Supporting Information

for the

Communication

Entitled

Fine-Tuning the Energy Barrier for Metal-Mediated Dinitrogen N≡N Bond Cleavage

Authored by

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Experimental details for all new compounds and description of kinetic studies and X-ray crystallographic information, including tables of bond lengths, angles, and anisotropic displacement parameters for complexes **1b**, **1c**, **2b**, **cis-3b, trans-3b**, **cis-3c, trans-3c**, **cis-4a, trans-4b**, **5**, **8**, **9a-c**, and **10** (254 Pages)

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Experimental Procedures

General Considerations

All manipulations with air and moisture sensitive compounds were carried out under N_2 or Ar atmospheres with standard Schlenk or glovebox techniques. All solvents were dried (Na for toluene and Na/benzophenone for pentane, Et_2O, and THF) and distilled under N_2 prior to use. Benzene-d_6, toluene-d_8 and methylcyclohexane were dried over Na/K alloy and isolated by vacuum transfer prior to use. Celite was oven dried (150 °C for several days) prior to use. Cooling was performed in the internal freezer of a glovebox maintained at -30 °C. N,N'-diisopropylcarbodiimide, PhLi (1.8M in n-butylether), $LiNMe_2$, MeLi, nitrous oxide (99 %), and methylcyclohexane (spectrophotometric grade) were purchased from Sigma-Aldrich, Cp^*TaCl_4 and $NbCl_5$ were purchased from Strem Chemicals, and $^{15}N_2$ (98%, ^{15}N enriched) was purchased from Cambridge Isotope Laboratories. All purchased chemicals were used as received unless otherwise noted. Compounds **6a**,[S1] **6c**,[S2] **1a**,[S3] **1a-$^{15}N_2$**,[S3] Cp^*NbCl_4[S4] and $[Cp^*V(\mu\text{-}Cl)_2]_3$[S5] were prepared according to previously reported procedures in similar yield and purity. ^1H NMR spectra were recorded at 400.132 MHz and referenced to $SiMe_4$ using residual ^1H chemical shifts of d_6-benzene and d_8-toluene. ^{15}N NMR spectra were recorded at 50.68 MHz and externally referenced to $NH_{3(l)}$ using neat $MeNO_2$ (380.2 ppm) as a standard. Mass spectrometry measurements were performed on a JEOL AccuTOF-CS mass spectrometer using electrospray ionization. Elemental analyses were carried out by Midwest Microlab, LLC.

{Cp*Ta[N(^{i}Pr)C(Ph)N(^{i}Pr)]}$_2$(μ-η^1:η^1-N$_2$) (1b). $Cp^*Ta[N(^iPr)C(Ph)N(^iPr)]Cl_3$ (105 mg, 0.17 mmol) and KC_8 (92 mg, 0.68 mmol) were placed in a storage tube with a Teflon valved stopper under an argon atmosphere. The storage tube was evacuated and cooled to -196 °C with 10 mL of THF added to the storage tube by vacuum transfer. The tube was charged with dinitrogen (~1 atm) at –196 °C, sealed, and warmed to –78 °C. After stirring at -78 °C for 6 h, the dark suspension was allowed to warm to 0 °C and stirred for 13 h. Volatiles were removed *in vacuo* at 0° C to give a black solid. The solid residue was extracted with –30 °C pentane and immediately filtered through a dry pad of Celite on a glass frit. Volatiles were removed *in vacuo* to give a black solid. The crude product was dissolved in minimal pentane and cooled to –30 °C to give black crystals of **1b** (51 mg, 57% yield). Anal. calc'd for $C_{46}H_{68}N_6Ta_2$: C, 51.76; H, 6.43; N, 7.88; Found: C, 51.70; H, 6.40; N, 7.69.

{Cp*Ta[N(^{i}Pr)C(NMe$_2$)N(^{i}Pr)]}$_2$(μ-η^1:η^1-N$_2$) (1c). $Cp^*Ta[N(^iPr)C(NMe_2)N(^iPr)]Cl_3$ (110 mg, 0.19 mmol) and KC_8 (100 mg, 0.74 mmol) were placed in a storage tube with a Teflon valved stopper under an argon atmosphere. The storage tube was evacuated and cooled to -196 °C with 10 mL of THF added to the storage tube by vacuum transfer. The tube was charged with dinitrogen (~1

atm) at –196 °C, sealed, and warmed to –78 °C. After stirring at -78 °C for 6 h, the reaction was allowed to warm to 0 °C and stirred for 12 h. Volatiles were removed *in vacuo* at 0° C to give a black solid. The solid residue was extracted with –30 °C pentane and immediately filtered through a dry pad of Celite on a glass frit. Volatiles were removed *in vacuo* to give a black solid. The crude product was dissolved in minimal pentane and cooled to –30 °C to give black crystals of **1c** (64 mg, 68% yield). Anal. calc'd for $C_{38}H_{70}N_8Ta_2$: C, 45.58; H, 7.05; N, 11.20; Found: C, 45.53; H, 7.01; N, 11.28.

{Cp*Ta[N(^{i}Pr)C(NMe$_2$)N(^{i}Pr)]}$_2$(μ-η^1:η^1-^{15}N$_2$) (1c-^{15}N$_2$). The ^{15}N-labeled version of **1c** was prepared in a similar yield and purity using labeled $^{15}N_2$ gas (98%, ^{15}N) in place of unlabeled N_2 gas.

{Cp*Nb[N(^{i}Pr)C(Ph)N(^{i}Pr)]}$_2$(μ-η^1:η^1-N$_2$) (2b). Compound **7b** (148 mg, 0.28 mmol) and KC_8 (151 mg, 1.11 mmol) were placed in a storage tube with a Teflon valved stopper under an argon atmosphere. The storage tube was evacuated and cooled to -196 °C with 10 mL of THF added to the storage tube by vacuum transfer. The tube was charged with dinitrogen (~1 atm) at –196 °C, sealed, and warmed to –78 °C. After stirring at -78 °C for 12 h, the reaction was allowed to warm to 0 °C and stirred for 1 h. Volatiles were removed *in vacuo* at 0° C to give a black solid. The solid residue was extracted with –30 °C pentane and immediately filtered through a dry pad of Celite on a glass frit. The filtrate was concentrated and cooled to –30 °C to give black crystals of **2b** (71 mg, 58% yield). Anal. calc'd for $C_{46}H_{68}N_6Nb_2$: C, 62.02; H, 7.69; N, 9.43; Found: C, 62.25; H, 7.62; N, 9.31.

{Cp*Ta[N(^{i}Pr)C(Ph)N(^{i}Pr)](μ-N)}$_2$ (3b). A solution of **1b** (38 mg, 0.04 mmol) in 0.5 mL of toluene was transferred into a J. Young tube with a teflon stopper. The contents of the J. Young tube were heated at 105 °C for 2 h to give a yellow solution. Solvents were removed *in vacuo* to give a yellow solid. The solid was dissolved in minimal pentane and cooled to -30 °C to give yellow crystals composed of a mixture of *cis* and *trans* isomers of **3b** (22 mg, 58% yield). Anal. calc'd for $C_{46}H_{68}N_6Ta_2$: C, 51.76; H, 6.43; N, 7.88; Found: C, 52.21; H, 6.32; N, 7.72. ^{1}H NMR (benzene-d_6): (*cis*-**3b**) δ 1.28 (24H, d, CH(CH_3)$_2$), 2.28 (30H, s, C$_5$(CH_3)$_5$), 3.62 (4H, sept, CH(CH$_3$)$_2$), 7.0-7.5 (10H, m, C(C$_6H_5$)). (*trans*-**3b**) δ 1.15 (12H, d, CH(CH_3)$_2$), 1.16 (12H, d, CH(CH_3)$_2$), 2.40 (30H, s, C$_5$(CH_3)$_5$), 3.70 (4H, sept, CH(CH$_3$)$_2$), 7.0-7.5 (10H, m, C(C$_6H_5$)).

{Cp*Ta[N(^{i}Pr)C(NMe$_2$)N(^{i}Pr)](μ-N)}$_2$ (3c). A solution of **1c** (41 mg, 0.04 mmol) was dissolved in 1 mL benzene and the solution was left at room temperature for one week to give yellow brown crystals composed of a mixture of *cis* and *trans* isomers of **3c** (24 mg, 59% yield).[S6]

{Cp*Nb[N(^{i}Pr)C(Me)N(^{i}Pr)](μ-N)}$_2$ (4a). Compound **7a** (100 mg, 0.21 mmol) and KC_8 (114 mg, 0.84 mmol) were placed in a storage tube with a Teflon valved stopper under an argon atmosphere. The storage tube was evacuated and cooled to -196 °C with 10 mL of THF added to the storage tube by vacuum transfer. The tube was charged with dinitrogen (~1 atm) at –196 °C, sealed, and warmed to –78 °C. After stirring at -78 °C for 10 h, the reaction was allowed to warm to 0 °C and stirred for 1 h. Volatiles were removed *in vacuo* to give a black solid. The solid residue was extracted with –30 °C pentane and immediately filtered through a dry pad of Celite on a glass frit. Volatiles were removed *in vacuo*, and crude NMR revealed a mixture of *cis*/*trans*-**4a** had formed. Crystallization of the mixture with minimal pentane at -30 °C led to the isolation of orange crystals of *cis*-**4a**, along with *trans*-**4a** (52.4 mg, 66% yield). ^{1}H NMR (benzene-d_6): (*cis*-**4a**) δ 1.17 (6H, d, *J* = 7.0 Hz, CH(CH_3)$_2$), 1.34 (6H, d, *J* = 6.8 Hz, CH(CH_3)$_2$), 1.66 (3H, s, N(^{i}Pr)C(CH_3)N(^{i}Pr), 2.09 (15H, s, C_5(CH_3)$_5$), 3.45 (1H, sept, *J* = 6.8 Hz, C*H*(CH$_3$)$_2$). (*trans*-**4a**) δ 1.18 (6H, d, *J* = 6.4 Hz, CH(CH_3)$_2$), 1.44 (6H, d, *J* = 6.4 Hz, CH(CH_3)$_2$), 1.65 (3H, s, N(^{i}Pr)C(CH_3)N(^{i}Pr), 2.10 (15H, s, C_5(CH_3)$_5$), 3.50 (1H, sept, *J* = 6.4 Hz, C*H*(CH$_3$)$_2$).

{Cp*Nb[N(^{i}Pr)C(Ph)N(^{i}Pr)](μ-N)}$_2$ (4b). A solution of **2b** (49 mg, 0.05 mmol) in 1 mL of benzene was transferred into a J Young tube with a teflon stopper. The contents of the J. Young tube were heated at 60 °C for 14 h to give an orange solution. Solvents were removed *in vacuo* to give an orange solid. The solid was dissolved in minimal pentane and cooled to -30 °C to give orange crystals of **4b** (30 mg, 61% yield). Anal. calc'd for $C_{46}H_{68}N_6Nb_2$: C, 62.02; H, 7.69; N, 9.43; Found: C, 62.07; H, 7.57; N, 9.39. ^{1}H NMR (benzene-d_6): δ 1.12 (12H, d, CH(CH_3)$_2$), 1.30 (12H, d, CH(CH_3)$_2$), 2.31 (30H, s, C_5(CH_3)$_5$), 3.64 (4H, sept, C*H*(CH$_3$)$_2$), 7.07-7.22 (6H, m, C(C_6H_5)), 7.24-7.30 (2H, m, C(C_6H_5)), 7.33-7.39 (2H, m, C(C_6H_5)).

{Cp*V[N(^{i}Pr)C(Me)N(^{i}Pr)]}$_2$(μ-η^1:η^1-N$_2$) (5). In an N_2 glovebox, compound **8** (504 mg, 1.39 mmol) was dissolved in 20 mL of THF and cooled to -30 °C. To the stirred solution, 0.5% w/w sodium amalgam (7.03 g, 1.53 mmol of Na) was added and the solution was allowed to warm to room temperature and stirred for 14 h. Solvents were removed *in vacuo* to give a green solid, which was subsequently dissolved in pentane and filtered through Celite on a glass frit. The filtrate was concentrated to saturation and stored at -30 °C to give green crystals of **8** (432 mg, 91% yield). Anal. calc'd for $C_{36}H_{64}N_6V_2$: C, 63.32; H, 9.45; N, 12.31; Found: C, 63.09; H, 9.19; N, 12.25.

Cp*Ta[N(^{i}Pr)C(Ph)N(^{i}Pr)]Cl$_3$ (6b). A 1.73 M solution of phenyl lithium in di-*n*-butylether (4.66 mL, 8.06 mmol) was added dropwise to a -30 °C solution of *N,N*-diisopropylcarbodiimide (1.017g, 8.06 mmol) in 50 mL of Et_2O over a period of 5 min. The solution was allowed to warm to room temperature and stirred for 14 h to give an opaque solution. Volatiles were removed *in vacuo* to give an oil, which was recrystallized in pentane to provide Li[N(^{i}Pr)C(Ph)N(^{i}Pr)]•(n-

Bu_2O), as a white solid. A -30 °C solution of the lithium etherate salt (252 mg, 0.75 mmol) in 10 mL of Et_2O was added dropwise to a -30 °C suspension of Cp^*TaCl_4 (320 mg, 0.70 mmol) in 50 mL of Et_2O. The suspension was allowed to warm to room temperature and stirred for 7 h to give a red colored suspension. Volatiles were removed *in vacuo* to give a red solid. The crude product was dissolved in toluene and filtered through a pad of Celite on a glass frit. The resulting red filtrate was concentrated and cooled to -30 °C to give red crystals of **6b** (372 mg , 85% yield). Anal. calc'd for $C_{23}H_{34}N_2Cl_3Ta_1$: C, 44.12; H, 5.48; N, 4.48; Found: C, 43.91; H 5.41; N, 4.35. ^{1}H NMR (benzene-d_6): δ 0.90 (6H, d, J = 7.0 Hz, CH(CH_3)$_2$), 1.72 (6H, d, J = 6.7 Hz, CH(CH_3)$_2$), 2.27 (15H, s, C_5(CH_3)$_5$), 4.35 (1H, sept, J = 7.0 Hz, CH(CH$_3$)$_2$), 4.47 (1H, sept, J = 6.7 Hz, CH(CH$_3$)$_2$), 6.85-7.0 (3H, m, C_6H_5), 7.18-7.27 (2H, m, C_6H_5).

Cp*Nb[N(^{i}Pr)C(Me)N(^{i}Pr)]Cl$_3$ (7a). A -30 °C solution of Li[N(^{i}Pr)C(Me)N(^{i}Pr)] (418 mg, 2.84 mmol) in 20 mL of Et_2O was added dropwise to a -30 °C suspension of Cp^*NbCl_4 (1.00 g, 2.71 mmol) in 40 mL of Et_2O. The suspension was allowed to warm to room temperature and stirred for 14 h to give a purple solution. Volatiles were removed *in vacuo*, and the crude product was dissolved in toluene and filtered through a pad of Celite on a glass frit. The resulting purple filtrate was concentrated and cooled to -30 °C to give dark purple crystals of **7a** (562 mg , 44% yield). Anal. calc'd for $C_{18}H_{32}N_2Cl_3Nb_1$: C, 45.45; H, 6.78; N, 5.89; Found: C, 45.23; H 6.87; N, 5.64. ^{1}H NMR (benzene-d_6): δ 1.00 (6H, d, J = 7.0 Hz, CH(CH_3)$_2$), 1.52 (3H, s, N(^{i}Pr)C(CH_3)N(^{i}Pr) 1.75 (6H, d, J = 7.0 Hz, CH(CH_3)$_2$), 2.00 (15H, s, C_5(CH_3)$_5$), 4.41 (1H, sept, J = 7.0 Hz, CH(CH$_3$)$_2$), 4.95 (1H, br, CH(CH$_3$)$_2$).

Cp*Nb[N(^{i}Pr)C(Ph)N(^{i}Pr)]Cl$_3$ (7b). A -30 °C solution of Li[N(^{i}Pr)C(Ph)N(^{i}Pr)]•n-Bu_2O (451 mg, 1.34 mmol) in 20 mL of Et_2O was added dropwise to a -30 °C suspension of Cp^*NbCl_4 (473 mg, 1.28 mmol) in 40 mL of Et_2O. The suspension was allowed to warm to room temperature and stirred for 14 h to give a purple solution. Volatiles were removed *in vacuo*, and the crude product was dissolved in toluene and filtered through a pad of Celite on a glass frit. The resulting purple filtrate was concentrated and cooled to -30 °C to give dark purple crystals of **7b** (411 mg , 61% yield). Anal. calc'd for $C_{23}H_{34}N_2Cl_3Nb_1$: C, 51.37; H, 6.37; N, 5.21; Found: C, 51.76; H 6.36; N, 5.06. ^{1}H NMR (benzene-d_6): δ 1.00 (6H, d, J = 7.0 Hz, CH(CH_3)$_2$), 1.52 (3H, s, N(^{i}Pr)C(CH_3)N(^{i}Pr), 1.75 (6H, d, J = 7.0 Hz, CH(CH_3)$_2$), 2.01 (15H, s, C_5(CH_3)$_5$), 4.41 (1H, sept, J = 7.0 Hz, CH(CH$_3$)$_2$), 4.95 (1H, br, J = 7.04 Hz, CH(CH$_3$)$_2$).

Cp*V[N(^{i}Pr)C(Me)N(^{i}Pr)]Cl (8). A -30 °C solution of Li[N(^{i}Pr)C(Me)N(^{i}Pr)] (178 mg, 1.21 mmol) in 10 mL of Et_2O was added dropwise to a -30 °C suspension of [Cp*V(μ-Cl)$_2$]$_3$ (306 mg, 0.40 mmol) in 20 mL of Et_2O. The reaction was allowed to warm to room temperature and stir for 14 h to give a maroon solution. Solvents were removed *in vacuo* to give a maroon solid, which was subsequently dissolved in pentane and filtered through Celite on a glass frit. The filtrate was

concentrated to saturation and stored at -30 °C to give maroon crystals of **8** (354 mg, 82% yield). Anal. calc'd for $C_{18}H_{32}N_2Cl_1V_1$: C, 59.58; H, 8.89; N, 7.72; Found: C, 59.69; H, 8.72; N, 7.86.

{Cp*Ta[N(ⁱPr)C(Me)N(ⁱPr)]}$_2$(μ-η^2:η^2-N$_2$)(μ-O) (9a). A solution of **1a** (42 mg, 0.05 mmol) in 8 mL of -30 °C toluene was transferred into a storage tube with a teflon valved stopper. The headspace of the storage tube was evacuated and the storage tube was placed in a 0 °C ice bath. The storage tube was charged with nitrous oxide (5 psi) and stirred at 0 °C for 20 h to yield a dark purple solution. Volatiles were removed *in vacuo*, and the dark purple crude product was dissolved in minimal pentane and stored at -30 °C to give dark purple crystals of **9a** (37 mg, 87% yield). Anal. calc'd for $C_{36}H_{64}N_6Ta_2O_1$: C, 45.36; H, 6.14; N, 8.82; Found: C, 44.93; H, 6.69; N, 8.64. ^{1}H NMR (toluene-*d*$_8$): δ 1.16 (6H, d, *J* = 6.4 Hz, CH(C*H*$_3$)$_2$), 1.17 (6H, d, *J* = 6.4 Hz, CH(C*H*$_3$)$_2$), 1.29 (6H, d, *J* = 6.6 Hz, CH(C*H*$_3$)$_2$), 1.36 (6H, d, *J* = 6.6 Hz, CH(C*H*$_3$)$_2$), 1.54 (6H, s, [N(ⁱPr)C(C*H*$_3$)N(ⁱPr)]), 2.12 (30H, s, C$_5$(C*H*$_3$)$_5$), 3.44 (2H, sept, *J* = 6.4 Hz, C*H*(CH$_3$)$_2$), 3.67 (2H, sept, *J* = 6.6 Hz, C*H*(CH$_3$)$_2$).

{Cp*Ta[N(ⁱPr)C(Ph)N(ⁱPr)]}$_2$(μ-η^2:η^2-N$_2$) (μ-O) (9b). A -30 °C solution of **1b** (44 mg, 0.04 mmol) in 5 mL of toluene was transferred into a storage tube with a Teflon valved stopper. The headspace of the storage tube was evacuated and the storage tube was placed in a 0 °C ice bath. The storage tube was charged with nitrous oxide (5 psi) and stirred at 0 °C for 4 h to give a dark purple solution. Volatiles were removed *in vacuo* to give a dark purple solid. The crude product was dissolved in minimal pentane and cooled to -30 °C to give dark purple crystals of **9b** (29 mg, 64% yield). Anal. calc'd for $C_{46}H_{68}N_6Ta_2O_1$:C, 51.00; H, 6.33; N, 7.76; Found: C, 50.82; H, 6.21; N, 7.38. ^{1}H NMR (benzene-*d*$_6$, 25 °C): δ 0.79 (6H, d, *J* = 6.5 Hz, CH(C*H*$_3$)$_2$), 1.20 (6H, d, *J* = 6.7 Hz, CH(C*H*$_3$)$_2$), 1.27 (12H, d, *J* = 6.7 Hz, CH(C*H*$_3$)$_2$), 2.34 (30H, s, C$_5$(C*H*$_3$)$_5$), 3.69 (2H, sept, *J* = 6.5 Hz, C*H*(CH$_3$)$_2$), 3.81 (2H, sept, *J* = 6.7 Hz, C*H*(CH$_3$)$_2$), 7.00-7.30 (8H, m, C$_6$*H*$_5$), 7.45 - 7.60 (2H, m, C$_6$*H*$_5$).

{Cp*Ta[N(ⁱPr)C(NMe$_2$)N(ⁱPr)]}$_2$(μ-η^2:η^2-N$_2$)(μ-O) (9c). Complex **1c** (63 mg, 0.06 mmol) was dissolved in 8 mL of -30 °C toluene and transferred to a storage tube with a teflon valve. The headspace of the storage tube was evacuated and the storage tube was placed in a 0 °C ice bath. The storage tube was charged with nitrous oxide (5 psi) and stirred at 0 °C for 18 h to yield a dark purple solution. Volatiles were removed *in vacuo* and the dark purple crude product was dissolved in benzene for crystallization at room temperature to give dark purple crystals of **9c** (59 mg, 92% yield). Anal. calc'd for $C_{38}H_{70}N_8Ta_2O_1$: C, 44.86; H, 6.94; N, 11.02; Found: C, 44.76; H, 6.75; N, 11.06. ^{1}H NMR (toluene-*d*$_8$): δ 1.10 (6H, d, *J* = 6.4 Hz, CH(C*H*$_3$)$_2$), 1.24 (6H, d, *J* = 6.6 Hz, CH(C*H*$_3$)$_2$), 1.34 (6H, d, CH(C*H*$_3$)$_2$, *J* = 6.6 Hz), 1.38 (6H, d, *J* = 6.6 Hz, CH(C*H*$_3$)$_2$), 2.18 (30H, s, C$_5$(C*H*$_3$)$_5$), 2.37 (12H, s, N(C*H*$_3$)$_2$), 3.46 (2H, sept, *J* = 6.6 Hz, C*H*(CH$_3$)$_2$), 3.75 (2H, sept, *J* = 6.6 Hz, C*H*(CH$_3$)$_2$).

{Cp*Ta[N(^{i}Pr)C(NMe$_2$)N(^{i}Pr)]}$_2$(μ-η^2:η^2-^{15}N$_2$)(μ-O) (9c-^{15}N$_2$). The ^{15}N-labeled version of **9c** was prepared in a similar yield and purity through the reaction of **1c-^{15}N** with unlabeled N_2O. ^{15}N NMR (toluene-d_8): δ 423.03 (2N, s, μ-η^2:η^2-N_2).

Cp*V[N(^{i}Pr)C(Me)N(^{i}Pr)][CN(2,6-Me$_2$C$_6$H$_3$)]$_2$ (10). Compound 5 (102 mg, 0.15 mmol) in 5 mL of pentane was added to a suspension of 2,6-xylylisocyanide (79 mg, 0.60 mmol) in 5 mL of pentane and stirred at room temperature. After reacting for 14 h to give a red solution, the solution was filtered through Celite supported by Kimwipe in a glass pipette. The filtrate was concentrated and stored at -30 °C to give dark red crystals of **10** (157 mg, 89% yield). Anal. calc'd for $C_{36}H_{50}N_4V_1$: C, 73.32; H, 8.55; N, 9.50; Found: C, 73.86; H, 8.54; N, 9.67. IR (KBr) ν_{CN} = 1902.47 cm^{-1} (s), 1991.77 cm^{-1} (s).

Kinetic Studies. Solutions of pre-cleaved N_2 complexes for Eyring analysis were prepared in an argon filled glovebox by dissolving 0.03 mmol – 0.08 mmol of **1a-c** or **2b** in 40.4 g of methylcyclohexane[S6] that was pre-cooled to -30 °C to give solutions with concentrations between 0.55 mM and 1.53 mM. These solutions were subsequently analyzed at 5 different temperatures within the range of 40 °C to 95 °C in triplicate. Stock solutions for concentration dependence analysis were prepared by dissolving **1a-c** (0.04 mmol – 0.05 mmol) in 23 g of methylcyclohexane that was pre-cooled to -30 °C.[S6] Dilutions of the stock solution were performed by mass to give solutions that were 0.75, 0.50, and 0.25 times the concentration of the stock solution. Solutions were stored and maintained at -30 °C and used immediately after preparation, with aliquots analyzed consecutively until the data set was complete.

For sample analysis, a teflon sealed quartz cuvette was charged with a magnetic stir bar and 3 mL of a sample solution. The cuvette was pumped out of the glovebox and then inserted into an Agilent Cary 60 Spectrophotometer equipped with a Quantum Northwest temperature controlled cuvette holder that was pre-equilibrated at the desired temperature, with data collection starting simultaneously. The cuvette solution was stirred while scans from 800 – 350 nm were collected at a rate to give 30 to 164 data points per run.

First-order rate constants for all kinetic runs were determined by a least-squares fit of absorbance data, monitored at 625 nm, to the equation ln(A) = -*k*t + A_0 using the LINEST function in Excel. The first 3 min of data acquisition were excluded to account for temperature equilibration of the cuvette solution, and the number of data points included was determined by a standard of linearity (R^2 > 0.999) for each kinetic run. Using this standard, up to 4.2 half-lives of first-order linear data were observed for the compounds examined. Initial rates from absorbance vs. time plots were determined by a least-squares linear fit of the first 5 data points

after the temperature equilibration period using the LINEST function in Excel. All rate constants and initial rates were analyzed in triplicate.

Temperature dependent rate constants collected for each compound were least-squares fitted to the Eyring equation, $k = (k_B T/h) \exp(\Delta S^{\ddagger}/R) \exp(-\Delta H^{\ddagger}/RT)$, using OriginPro 8 software. All rate constant, initial rate, and activation parameter errors are reported at the 95% confidence interval.[S7]

Crossover Experiment. Compounds **1a** (9.5 mg, 0.01 mmol) and **1c** (14.9 mg, 0.01 mmol) were dissolved in 0.25 mL of THF in a Teflon sealed NMR tube and heated to 70 °C for 3.5 hours to produce a yellow solution. The solution was diluted with THF to give a total volume of 2 mL, which was then analyzed by ESI-MS (positive ion mode). Only peaks corresponding to **3a** ($[M + H]^+$ = 943.21 m/z) and **3c** ($[M + H]^+$ = 1001.26 m/z) were present and no crossover product, {Cp*Ta[N(iPr)C(Me)N(iPr)]}(μ-η^1:η^1:N_2){Cp*Ta[N(iPr)C(Me)N(iPr)]} ($[M + H]^+$ m/z = 972.45), was observed.

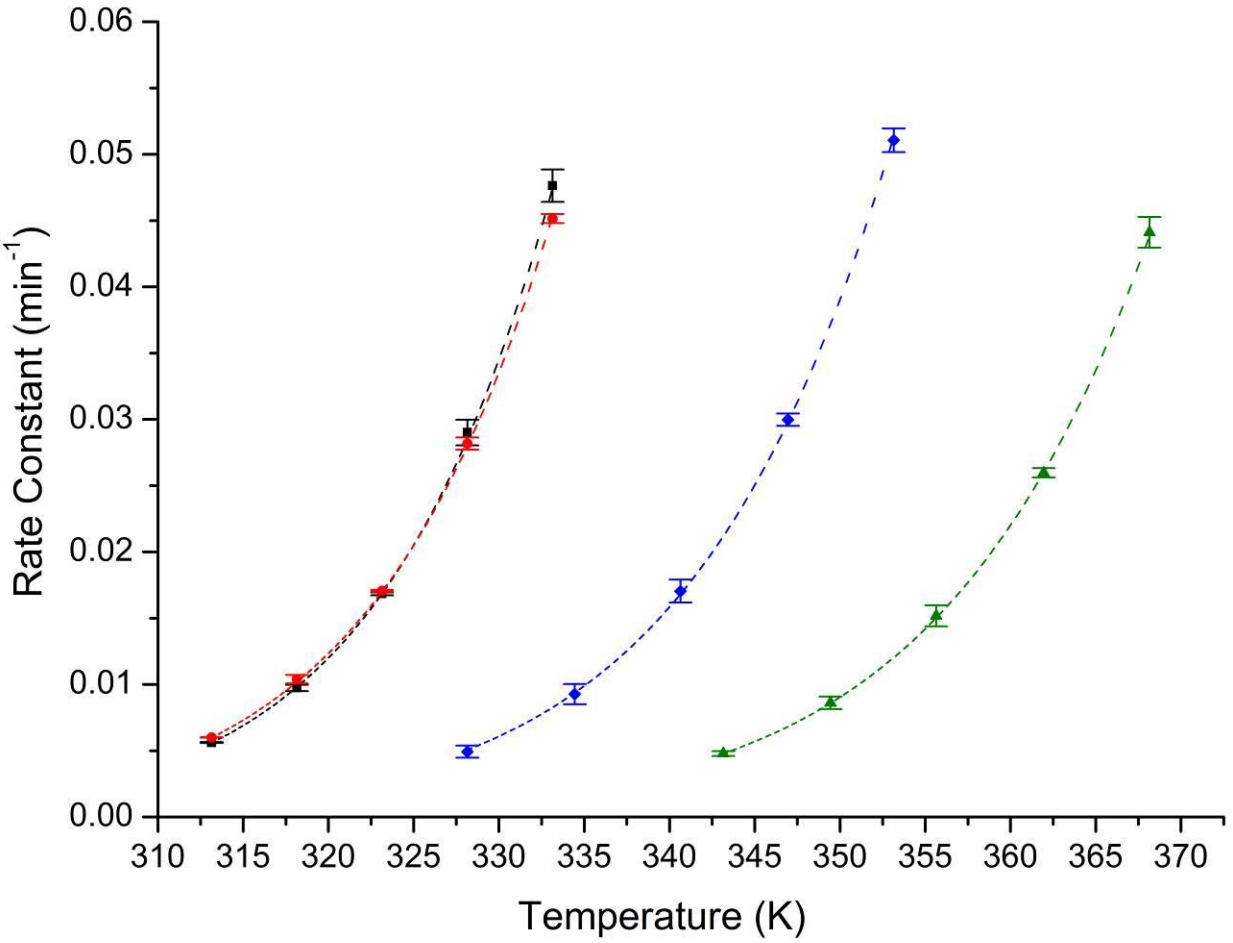


Figure S1. Temperature-dependent first-order rate constants with least-squares fit to the Eyring equation, $k = (k_B T/h) \exp(\Delta S^{\ddagger}/R) \exp(-\Delta H^{\ddagger}/RT)$, for the conversion of **1a** to **3a** (black/square), **1c** to **3c** (blue/diamond), **1b** to **3b** (green/triangle) and **2b** to **4b** (red/circle).

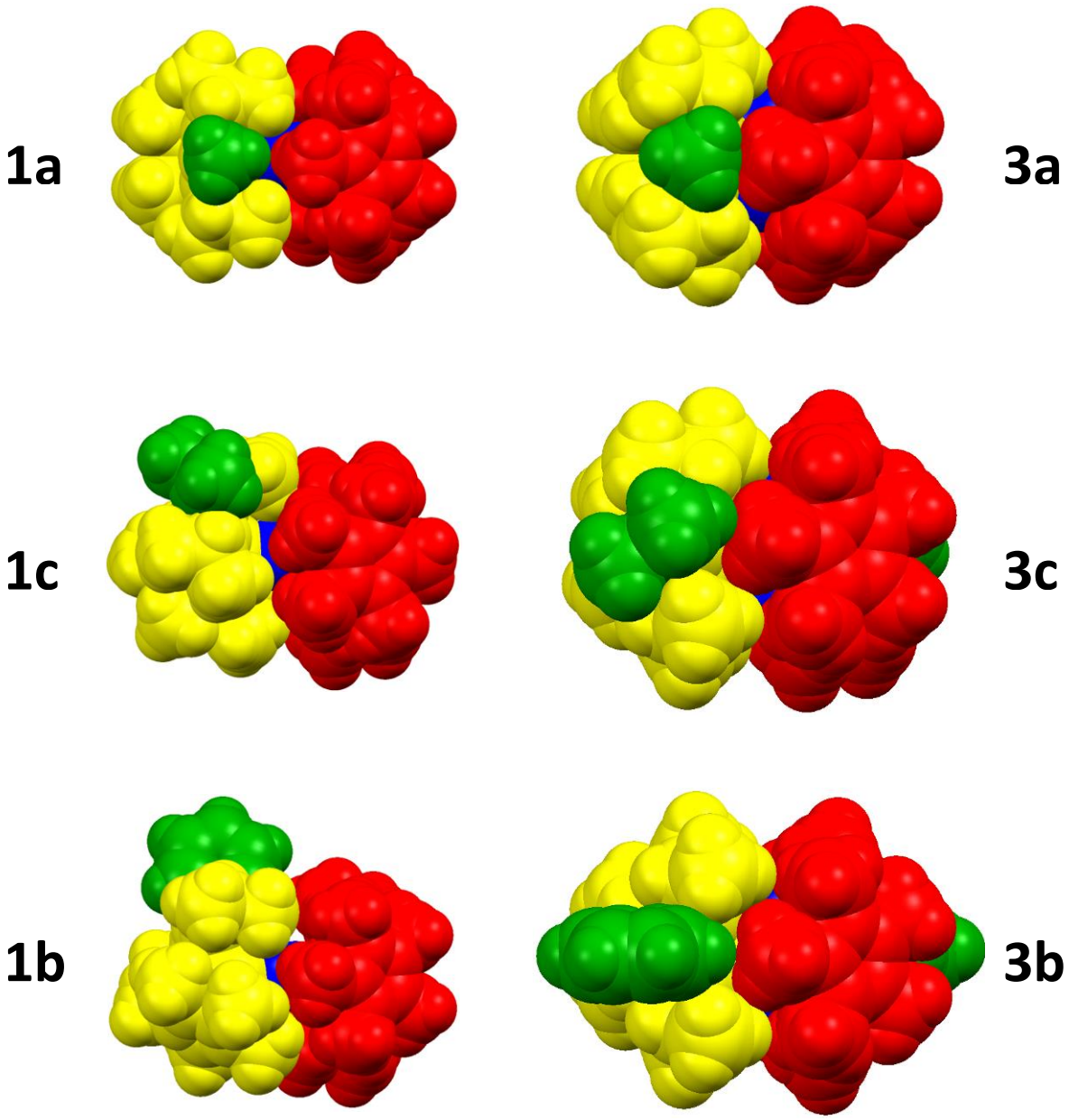


Figure S2. Space-fill models with view of red Cp* remaining constant. Rotation away from C_{2h} symmetry of **1a** going down the column to **1c** and **1b** (left column). Cleaved *trans* **3a-c** compounds locked in C_{2h} symmetry showing distal R group on yellow amidinate directly impinging with proximal red Cp*, leading to deflection of R group away from red Cp* (right column).

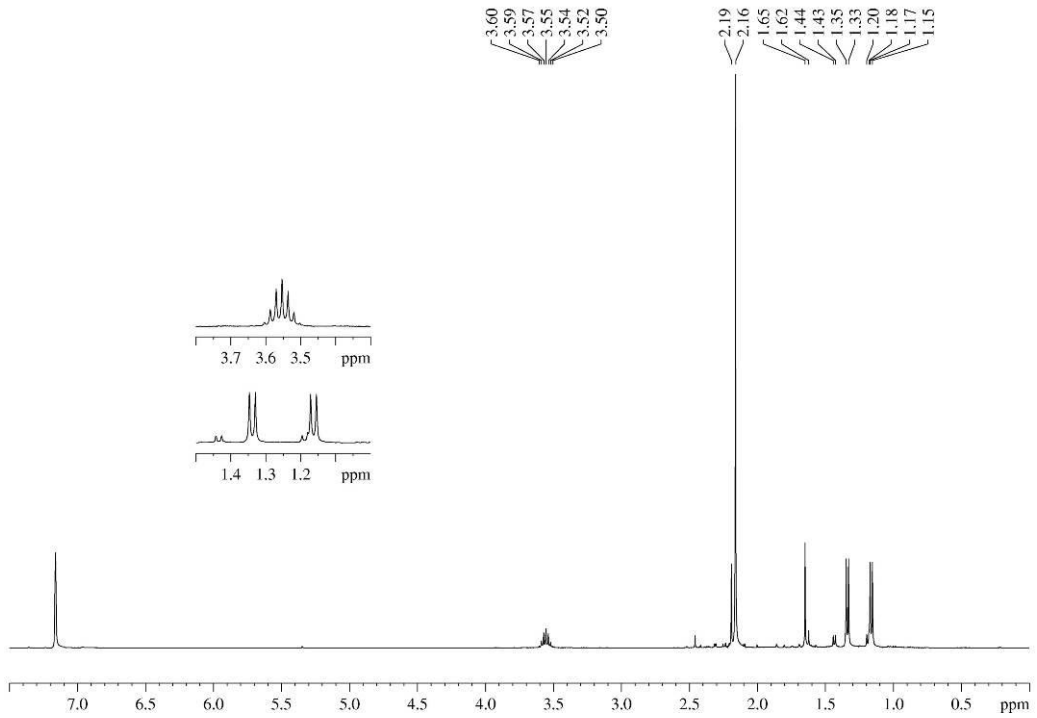


Figure S3. NMR experiment showing crude products (*cis*/*trans*-**3a**) obtained from thermolysis of **1a** at 70 °C for 2 h (400.132 MHz, C_6D_6, rt).

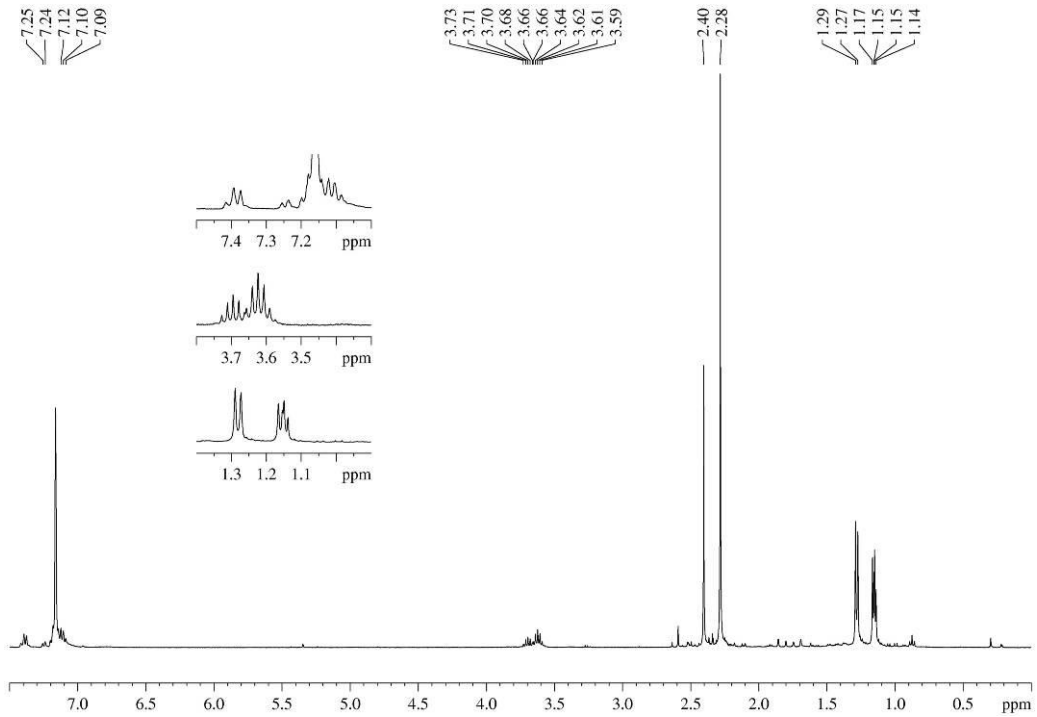


Figure S4. NMR experiment showing crude products (*cis*/*trans*-**3b**) obtained from thermolysis of **1b** at 85 °C for 2.5 h (400.132 MHz, C_6D_6, rt).

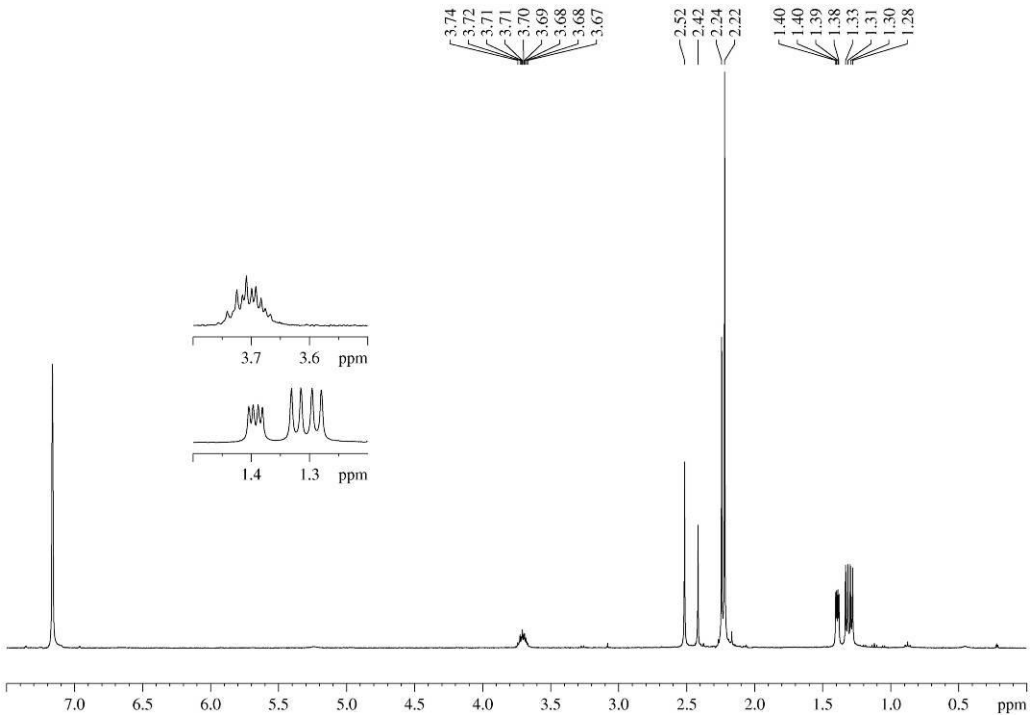


Figure S5. NMR experiment showing crude products (*cis*/*trans*-**3c**) obtained from thermolysis of **1c** at 70 °C for 2 h (400.132 MHz, C_6D_6, rt).

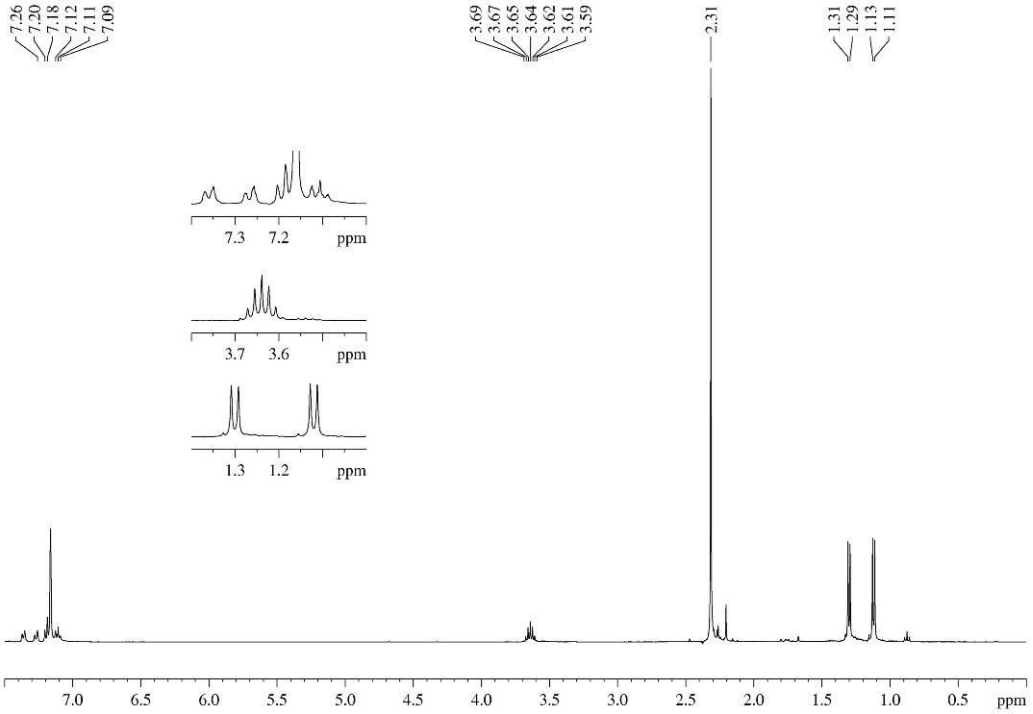


Figure S6. NMR experiment showing crude product (*trans*-**4b**) obtained from thermolysis of **2b** at 70 °C for 2 h (400.132 MHz, C_6D_6, rt).

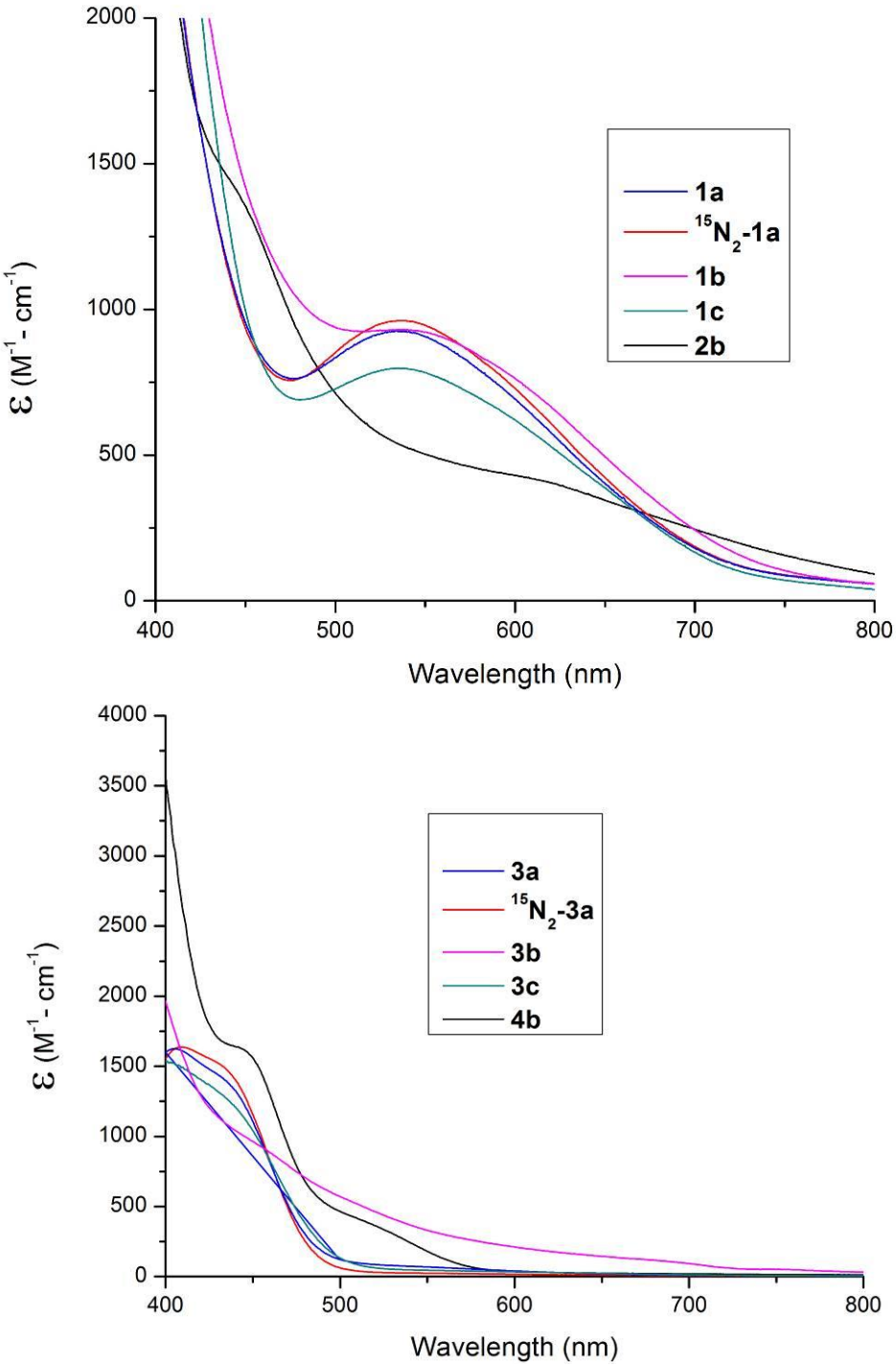


Figure S7. UV/Vis spectra of (top) **1a-c** and **2b**, and (right) **3a-c** and **4b**.

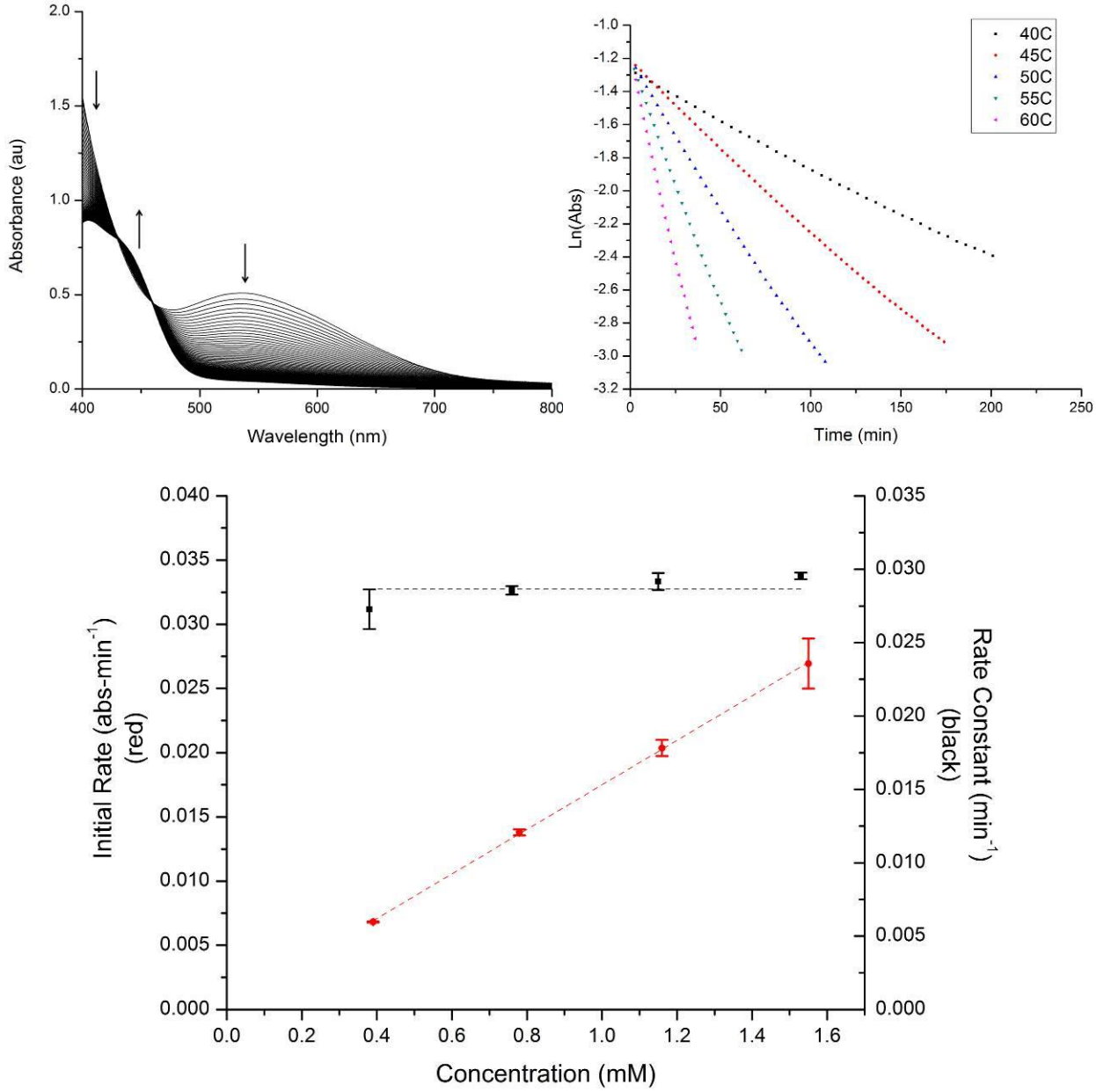


Figure S8. (top left) UV/Vis scanning kinetics at 323.15 K, Δt = 3 min, (top right) temperature dependent first order ln(A) = -*k*t + A_0 plots, and (bottom) rate constant and initial rate concentration dependence for the conversion of **1a** to **3a**.

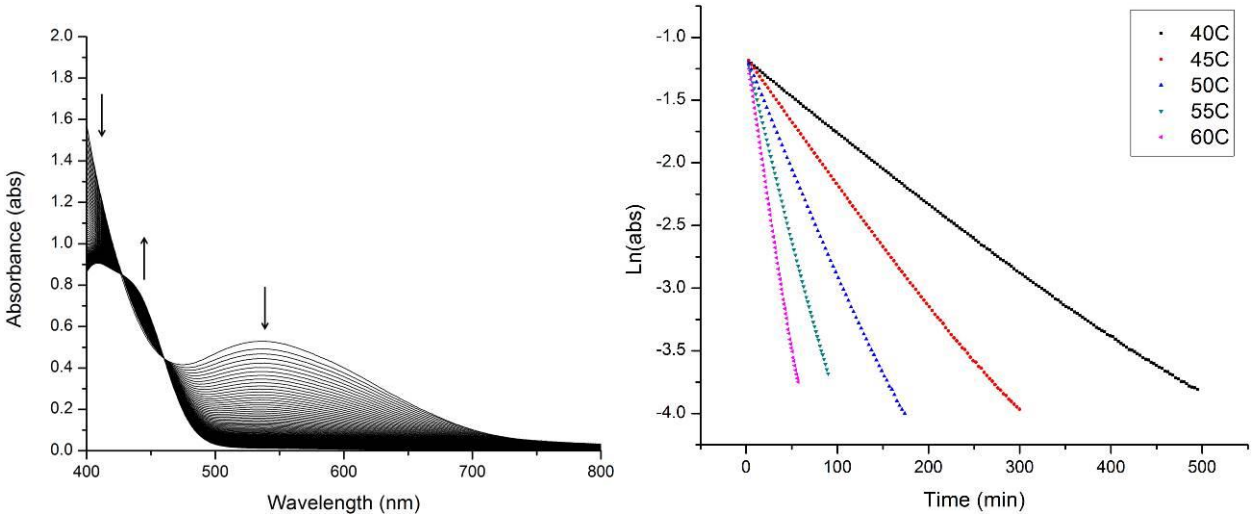


Figure S9. (left) UV/Vis scanning kinetics at 318.15 K, Δt = 2.8 min and (right) temperature dependent first order ln(A) = -*k*t + A_0 plots for the conversion of ($^{15}N_2$, 98%)-**1a** to ($^{15}N_2$, 98%)-**3a**.

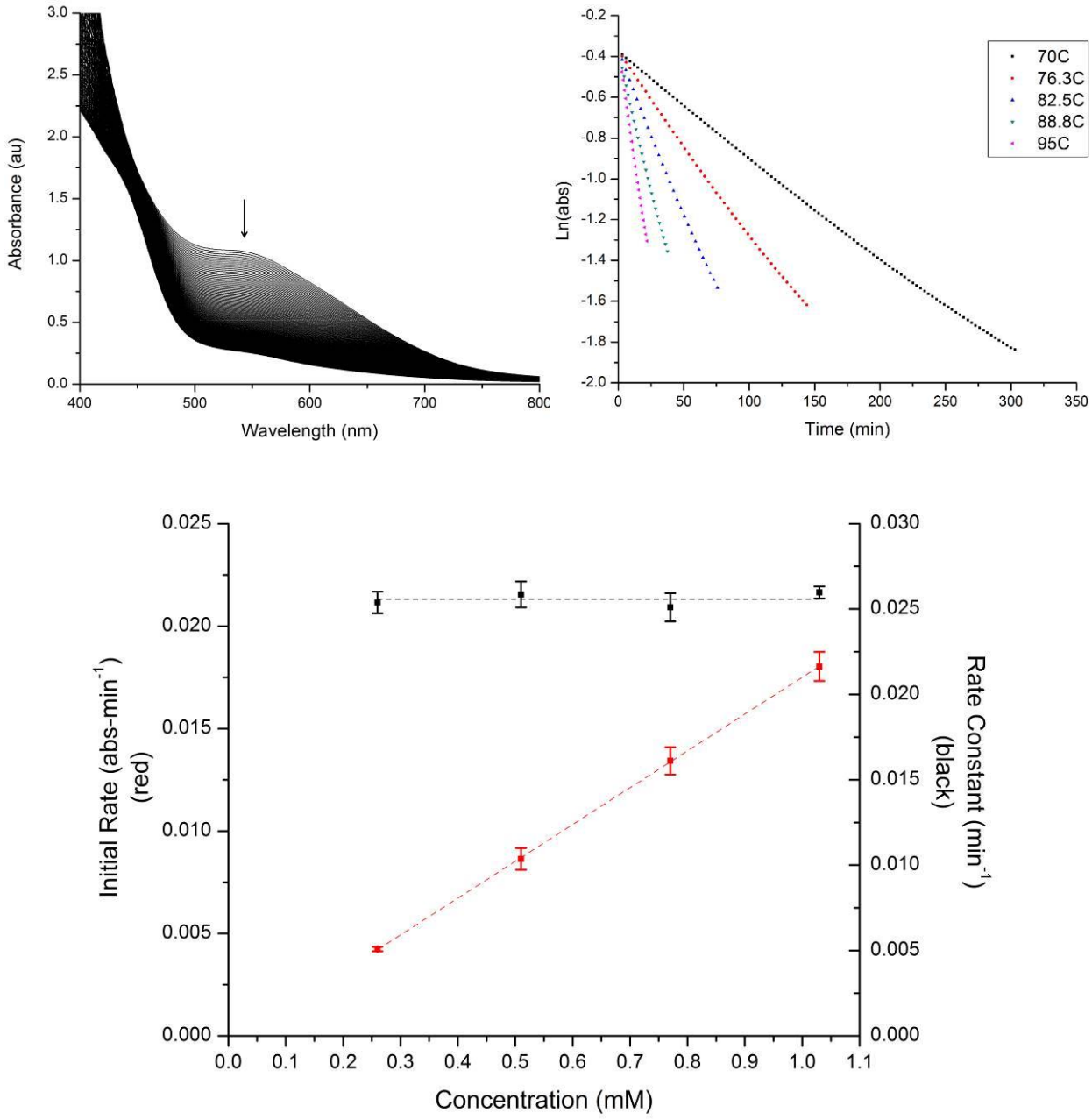


Figure S10. (top left) UV/Vis scanning kinetics at 343.15 K, Δt = 3 min, (top right) temperature dependent first order ln(A) = -*k*t + A_0 plots, and (bottom) rate constant and initial rate concentration dependence for the conversion of **1b** to **3b**.

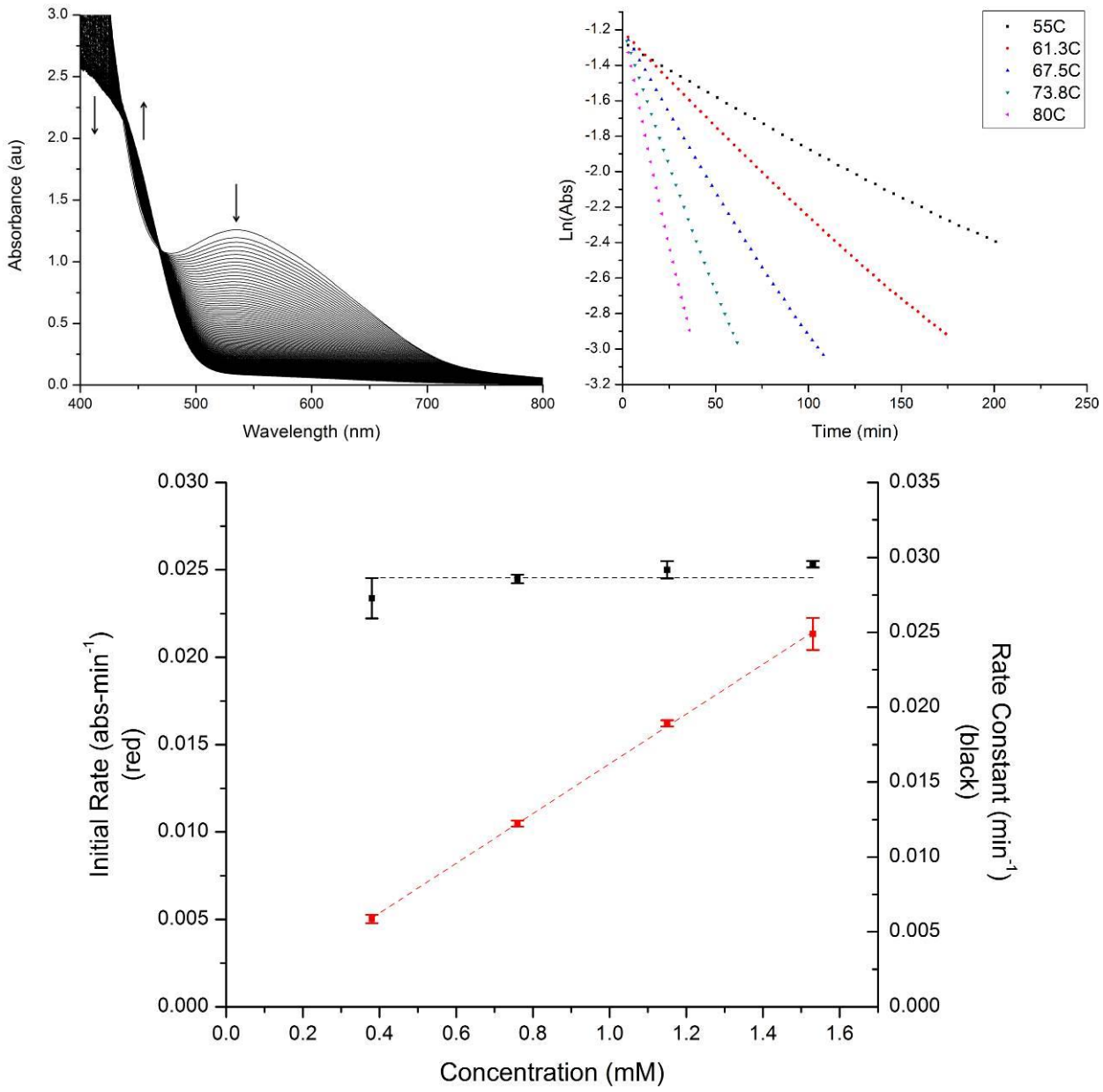


Figure S11. (top left) UV/Vis scanning kinetics at 334.45 K, Δt = 3 min, (top right) temperature dependent first order ln(A) = -*k*t + A_0 plots, and (bottom) rate constant and initial rate concentration dependence for the conversion of **1c** to **3c**.

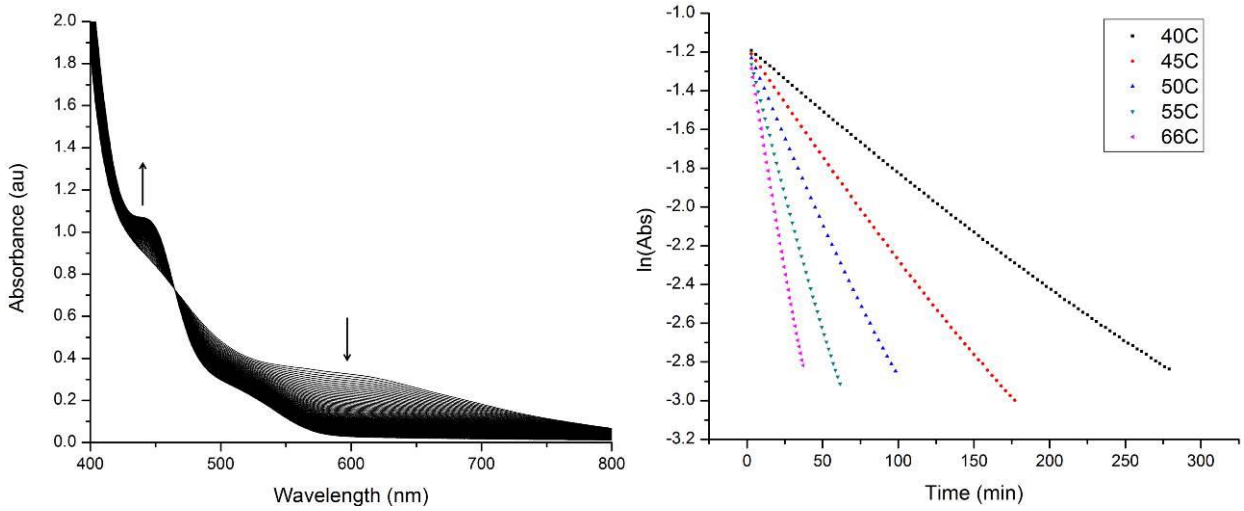


Figure S12. (left) UV/Vis scanning kinetics (338.15K, Δt = 3 min) and (right) temperature dependent first order ln(A) = -*k*t +A_0 plots for the conversion of **2b** to **4b**.

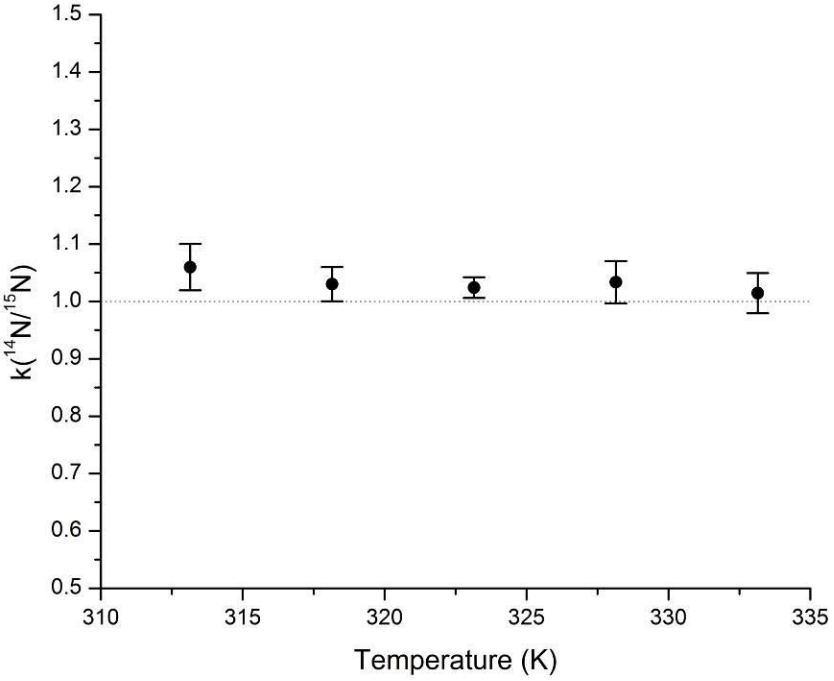


Figure S13. Kinetic isotope effect *k*(^{14}N)/*k*(^{15}N) for the conversion of **1a** to **3a**. Raw values and errors can be found in Table S9.

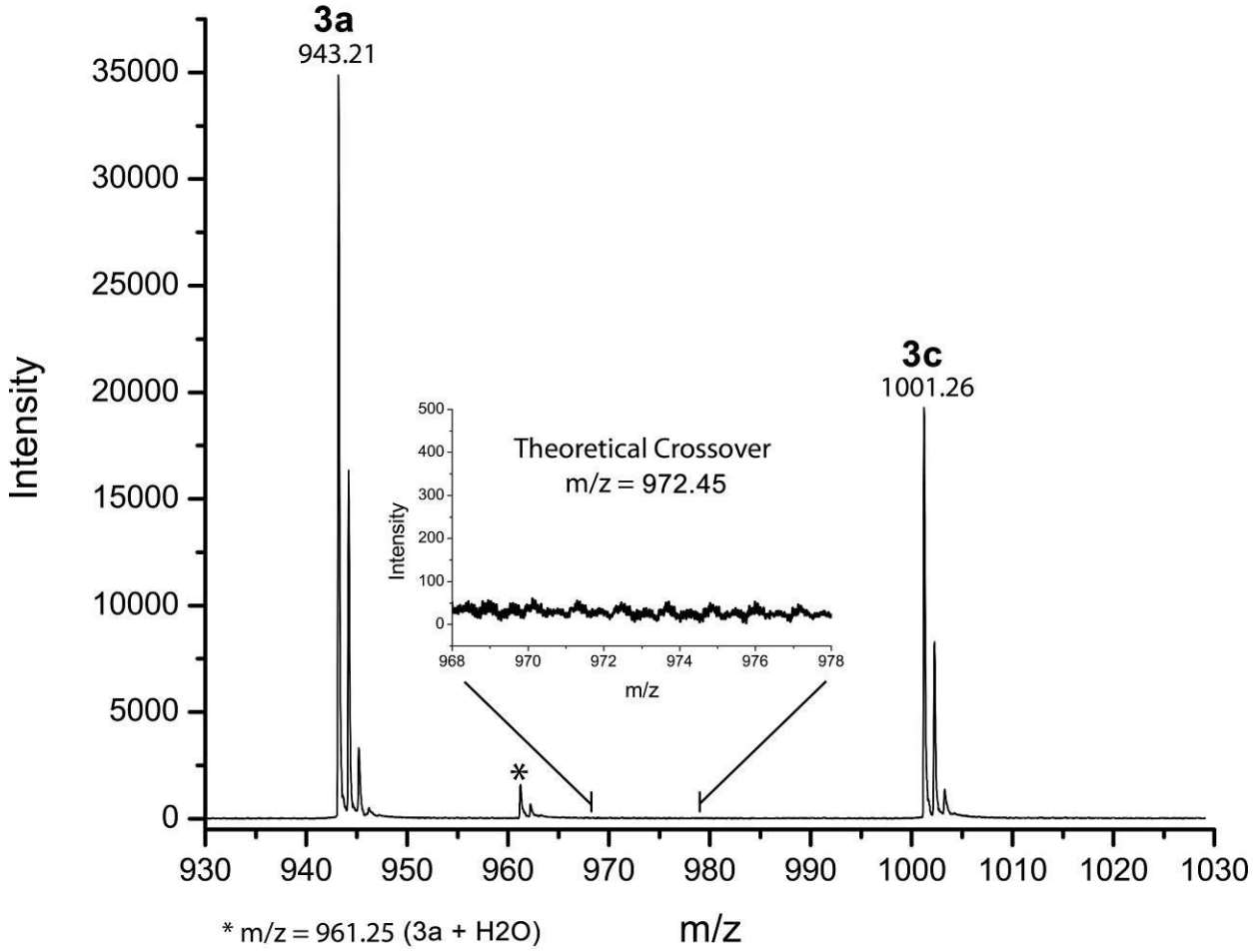


Figure S14. Crossover study: ESI-MS+ of products from heating a mixture of **1a** and **1c** in THF for 3.5 h.

Table S1. Temperature dependent rate constants for the conversion of 0.55 mM **1a** to **3a**.

Temp (K)	k (min^{-1})
313.15	0.00560(4)
318.15	0.0097(2)
323.15	0.0168(1)
328.15	0.029(1)
333.15	0.048(1)

Table S2. Temperature dependent rate constants for the conversion of 0.55 mM ($^{15}N_2$, 98%)-**1a** to ($^{15}N_2$, 98%)-**3a**.

Temp (K)	*k* (min^{-1})
313.15	0.0053(2)
318.15	0.0095(1)
323.15	0.0164(3)
328.15	0.0281(4)
333.15	0.047(1)

Table S3. Temperature dependent rate constants for the conversion of 1.03 mM **1b** to **3b**.

Temp (K)	*k* (min^{-1})
343.15	0.0048(2)
349.45	0.0086(5)
355.65	0.0152(8)
361.95	0.0260(4)
368.15	0.044(1)

Table S4. Temperature dependent rate constants for the conversion of 1.53 mM **1c** to **3c**.

Temp (K)	*k* (min^{-1})
328.15	0.0049(5)
334.45	0.0093(8)
340.65	0.0170(9)
346.95	0.0300(5)
353.15	0.0511(9)

Table S5. Temperature dependent rate constants for the conversion of 0.68 mM **2b** to **4b**.

Temp (K)	*k* (min^{-1})
313.15	0.00600(1)
318.15	0.0104(3)
323.15	0.0171(8)
328.15	0.0282(5)
333.15	0.0451(3)

Table S6. Concentration dependent rate constants and initial rates at 55 °C for the conversion of **1a** to **3a**.

Concentration	k (min^{-1})	Initial Rate (abs/min)
1.55 mM	0.0306(4)	0.027(2)
1.16 mM	0.0303(3)	0.0204(6)
0.78 mM	0.0300(3)	0.0138(2)
0.39 mM	0.0290(3)	0.00682(4)

Table S7. Concentration dependent rate constants and initial rates at 88.8 °C for the conversion of **1b** to **3b**.

Concentration	k (min^{-1})	Initial Rate (abs/min)
1.03 mM	0.0260(4)	0.0180(7)
0.77 mM	0.0251(8)	0.0134(3)
0.51 mM	0.0259(8)	0.0086(6)
0.26 mM	0.0254(6)	0.0042(1)

Table S8. Concentration dependent rate constants and initial rates at 73.8 °C for the conversion of **1c** to **3c**.

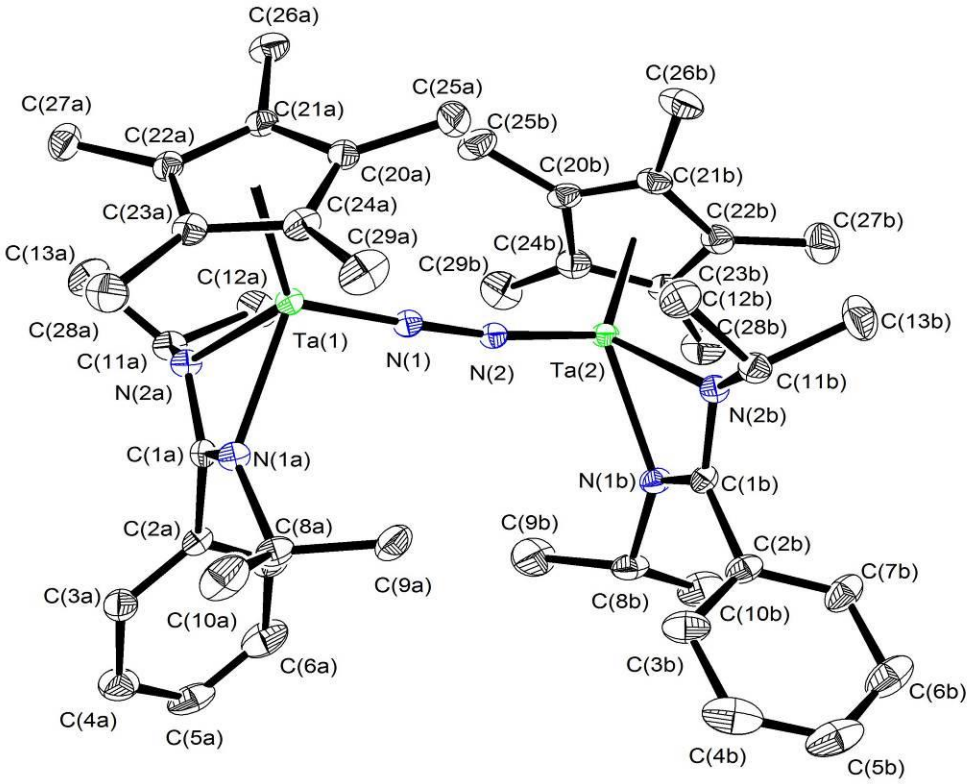
Concentration	k (min^{-1})	Initial Rate (abs/min)
1.53 mM	0.0296(2)	0.0213(9)
1.15 mM	0.0292(6)	0.0162(2)
0.76 mM	0.0286(3)	0.0105(2)
0.38 mM	0.027(1)	0.0050(2)

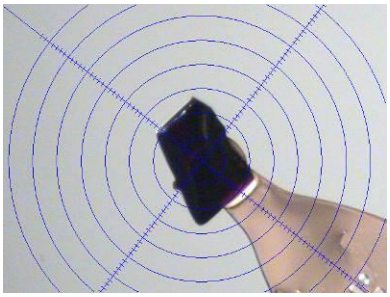
Table S9. Kinetic isotope effect ($k^{14}N/^{15}N$) for **1a** to **3a**.

Temp (K)	KIE
313.15	1.06(4)
318.15	1.03(3)
323.15	1.02(2)
328.15	1.03(4)
333.15	1.01(3)

X-Ray Crystallographic Information

{Cp*Ta[N(iPr)C(Ph)N(iPr]}$_2$(μ-η^1:η^1-N$_2$) (1b)





A dark-purple/black plate-like specimen of $C_{46}H_{68}N_6Ta_2$, approximate dimensions 0.07 mm x 0.30 mm x 0.47 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker Smart Apex2, CCD system equipped with a graphite monochromator and a MoK_α fine focus sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 6.73 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 68758 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 13539 were independent (average redundancy 5.079, completeness = 99.9%, R_{int} = 2.36%, R_{sig} = 1.78%) and 11810 (87.23%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.6870(8) Å, b = 16.2027(11) Å, c = 25.0686(17) Å, β = 101.8262(10)°, volume = 4646.3(5) Å^3, are based upon the refinement of the XYZ-centroids of 9966 reflections above 20 σ(I) with 5.018° < 2θ < 64.38°. Data were corrected for absorption effects using the integration method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.2116 and 0.7480.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/c$, with Z = 4 for the formula unit, $C_{46}H_{68}N_6Ta_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 516 variables converged at R1 = 2.06%, for the observed data and wR2 = 4.20% for all data. The goodness-of-fit was 1.002. The largest peak in the final difference electron density synthesis was 1.345 e$^-$/Å^3 and the largest hole

was -0.623 $e^-/Å^3$ with an RMS deviation of 0.081 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.525 g/cm^3 and F(000), 2128 e^-.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2008/4 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 1b.

Identification code	**1b**	
Chemical formula	$C_{46}H_{68}N_6Ta_2$	
Formula weight	1066.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.07 x 0.30 x 0.47 mm	
Crystal habit	dark-purple/black plate	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 11.6870(8) Å	α = 90°
	b = 16.2027(11) Å	β = 101.8262(10)°
	c = 25.0686(17) Å	γ = 90°
Volume	4646.3(5) $Å^3$	
Z	4	
Density (calculated)	1.525 Mg/cm^3	
Absorption coefficient	4.743 mm^{-1}	
F(000)	2128	

Table 2. Data collection and structure refinement for 1b.

Diffractometer	Bruker Smart Apex2, CCD
Radiation source	fine focus sealed tube, MoK_α
Theta range for data collection	2.08 to 30.00°
Index ranges	-16<=h<=16, -22<=k<=22, -35<=l<=35
Reflections collected	68758
Independent reflections	13539 [R(int) = 0.0236]
Coverage of independent reflections	99.9%
Absorption correction	integration
Max. and min. transmission	0.7480 and 0.2116
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	13539 / 45 / 516

Goodness-of-fit on F^2	1.002
Δ/σ_{max}	0.004
Final R indices	11810 data; I>2σ(I) R1 = 0.0206, wR2 = 0.0405
	all data R1 = 0.0267, wR2 = 0.0420
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.01P)^2+6.39P]$,$P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	1.345 and -0.623 eÅ^{-3}
R.M.S. deviation from mean	0.081 eÅ^{-3}

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$ $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$

GOOF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$ $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 1b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ta1	0.334681(7)	0.574222(5)	0.667751(3)	0.02139(2)
Ta2	0.210575(8)	0.565667(5)	0.843688(4)	0.02448(2)
N1	0.28162(15)	0.57680(10)	0.73073(7)	0.0241(3)
N2	0.25100(15)	0.57908(10)	0.77807(7)	0.0243(3)
C1A	0.15416(18)	0.63984(12)	0.60716(8)	0.0229(4)
C2A	0.03448(18)	0.67752(13)	0.59490(9)	0.0262(4)
C3A	0.9950(2)	0.71972(16)	0.54681(11)	0.0388(6)
C4A	0.8852(3)	0.75685(19)	0.53640(13)	0.0515(7)
C5A	0.8160(2)	0.75254(17)	0.57414(15)	0.0523(8)
C6A	0.8546(3)	0.7115(2)	0.62194(15)	0.0575(8)
C7A	0.9637(2)	0.67348(17)	0.63289(12)	0.0450(6)
N1A	0.25100(15)	0.68383(10)	0.62516(8)	0.0251(4)
C8A	0.2443(2)	0.77164(13)	0.63935(10)	0.0308(5)
C9A	0.2755(6)	0.7824(3)	0.7022(2)	0.0445(12)
C10A	0.3240(6)	0.8225(3)	0.6127(3)	0.0566(17)
C14A	0.2443(2)	0.77164(13)	0.63935(10)	0.0308(5)
C15A	0.3108(19)	0.7893(12)	0.6914(8)	0.0445(12)
C16A	0.286(2)	0.8221(12)	0.5894(10)	0.0566(17)
N2A	0.17574(15)	0.55904(10)	0.60491(8)	0.0253(4)
C11A	0.08082(19)	0.49793(13)	0.59490(10)	0.0299(5)
C12A	0.0674(2)	0.45736(16)	0.64793(12)	0.0424(6)
C13A	0.1044(2)	0.43335(16)	0.55444(13)	0.0462(7)
C20A	0.52110(18)	0.52260(14)	0.70791(9)	0.0284(4)
C21A	0.47203(19)	0.46307(13)	0.66794(9)	0.0279(4)
C22A	0.46497(18)	0.49961(14)	0.61550(9)	0.0269(4)
C23A	0.50552(18)	0.58156(14)	0.62288(10)	0.0290(4)
C24A	0.53900(18)	0.59704(14)	0.68020(10)	0.0304(5)
C25A	0.5556(2)	0.50848(19)	0.76831(10)	0.0446(6)
C26A	0.4494(2)	0.37381(14)	0.67854(12)	0.0398(6)
C27A	0.4307(2)	0.45479(17)	0.56224(10)	0.0384(6)

	x/a	y/b	z/c	U(eq)
C28A	0.5136(2)	0.64155(16)	0.57783(11)	0.0418(6)
C29A	0.5999(2)	0.67290(17)	0.70672(13)	0.0489(7)
C1B	0.21181(19)	0.71563(13)	0.88181(9)	0.0274(4)
C2B	0.22031(19)	0.80665(14)	0.89188(11)	0.0330(5)
C3B	0.2338(2)	0.86147(16)	0.85158(13)	0.0449(6)
C4B	0.2454(2)	0.94719(19)	0.86502(17)	0.0595(8)
C5B	0.2413(2)	0.97186(19)	0.91739(17)	0.0610(9)
C6B	0.2288(2)	0.91771(19)	0.95691(16)	0.0577(8)
C7B	0.2191(2)	0.83513(17)	0.94449(12)	0.0435(6)
N1B	0.11393(16)	0.67571(11)	0.86019(8)	0.0299(4)
C8B	0.0031(2)	0.71808(15)	0.84057(11)	0.0378(6)
C9B	0.9383(6)	0.6778(5)	0.7874(3)	0.078(2)
C10B	0.9302(4)	0.7184(4)	0.8843(3)	0.0578(13)
C14B	0.0031(2)	0.71808(15)	0.84057(11)	0.0378(6)
C15B	0.9796(15)	0.7073(12)	0.7819(9)	0.078(2)
C16B	0.9053(12)	0.6844(9)	0.8654(7)	0.0578(13)
N2B	0.30440(16)	0.66604(11)	0.89287(8)	0.0285(4)
C11B	0.4236(2)	0.69864(15)	0.90841(10)	0.0323(5)
C12B	0.4984(2)	0.66305(17)	0.87112(12)	0.0421(6)
C13B	0.4758(3)	0.6786(2)	0.96796(11)	0.0512(7)
C20B	0.2194(2)	0.42099(13)	0.83775(11)	0.0342(5)
C21B	0.2924(2)	0.44454(14)	0.88809(11)	0.0351(5)
C22B	0.2176(2)	0.47328(15)	0.92318(10)	0.0360(5)
C23B	0.1020(2)	0.46951(15)	0.89387(11)	0.0372(6)
C24B	0.1014(2)	0.43850(14)	0.84079(11)	0.0370(5)
C25B	0.2590(3)	0.38164(15)	0.79038(12)	0.0469(7)
C26B	0.4215(2)	0.42890(18)	0.90415(13)	0.0499(7)
C27B	0.2562(3)	0.5003(2)	0.98139(12)	0.0543(8)
C28B	0.9949(3)	0.4880(2)	0.91650(14)	0.0574(8)
C29B	0.9961(3)	0.41577(18)	0.79795(14)	0.0547(8)

Table 4. Bond lengths (Å) for 1b.

Ta1-N1	1.8111(18)	Ta1-N2A	2.1894(18)
Ta1-N1A	2.1959(18)	Ta1-C20A	2.358(2)
Ta1-C24A	2.373(2)	Ta1-C21A	2.412(2)
Ta1-C23A	2.487(2)	Ta1-C22A	2.513(2)
Ta2-N2	1.8152(18)	Ta2-N2B	2.1940(19)
Ta2-N1B	2.1950(18)	Ta2-C20B	2.352(2)
Ta2-C21B	2.360(2)	Ta2-C24B	2.417(2)
Ta2-C22B	2.480(2)	Ta2-C23B	2.505(2)
N1-N2	1.308(2)	C1A-N1A	1.335(3)
C1A-N2A	1.337(3)	C1A-C2A	1.499(3)

C2A-C3A	1.381(3)	C2A-C7A	1.385(3)
C3A-C4A	1.392(4)	C3A-H3A	0.95
C4A-C5A	1.367(4)	C4A-H4A	0.95
C5A-C6A	1.364(5)	C5A-H5A	0.95
C6A-C7A	1.392(4)	C6A-H6A	0.95
C7A-H7A	0.95	N1A-C8A	1.473(3)
C8A-C10A	1.500(5)	C8A-C9A	1.554(6)
C8A-H8A	1.0	C9A-H9A1	0.98
C9A-H9A2	0.98	C9A-H9A3	0.98
C10A-H10A	0.98	C10A-H10B	0.98
C10A-H10C	0.98	C15A-H15A	0.98
C15A-H15B	0.98	C15A-H15C	0.98
C16A-H16A	0.98	C16A-H16B	0.98
C16A-H16C	0.98	N2A-C11A	1.470(3)
C11A-C12A	1.520(3)	C11A-C13A	1.521(3)
C11A-H11A	1.0	C12A-H12A	0.98
C12A-H12B	0.98	C12A-H12C	0.98
C13A-H13A	0.98	C13A-H13B	0.98
C13A-H13C	0.98	C20A-C21A	1.424(3)
C20A-C24A	1.429(3)	C20A-C25A	1.503(3)
C21A-C22A	1.429(3)	C21A-C26A	1.504(3)
C22A-C23A	1.409(3)	C22A-C27A	1.500(3)
C23A-C24A	1.432(3)	C23A-C28A	1.507(3)
C24A-C29A	1.505(3)	C25A-H25A	0.98
C25A-H25B	0.98	C25A-H25C	0.98
C26A-H26A	0.98	C26A-H26B	0.98
C26A-H26C	0.98	C27A-H27A	0.98
C27A-H27B	0.98	C27A-H27C	0.98
C28A-H28A	0.98	C28A-H28B	0.98
C28A-H28C	0.98	C29A-H29A	0.98
C29A-H29B	0.98	C29A-H29C	0.98
C1B-N1B	1.329(3)	C1B-N2B	1.331(3)
C1B-C2B	1.496(3)	C2B-C3B	1.379(4)
C2B-C7B	1.400(4)	C3B-C4B	1.429(4)
C3B-H3B	0.95	C4B-C5B	1.383(5)
C4B-H4B	0.95	C5B-C6B	1.353(5)
C5B-H5B	0.95	C6B-C7B	1.373(4)
C6B-H6B	0.95	C7B-H7B	0.95
N1B-C8B	1.459(3)	C8B-C10B	1.521(6)
C8B-C9B	1.538(7)	C8B-H8B	1.0
C9B-H9B1	0.98	C9B-H9B2	0.98
C9B-H9B3	0.98	C10B-H10D	0.98
C10B-H10E	0.98	C10B-H10F	0.98
C15B-H15D	0.98	C15B-H15E	0.98

C15B-H15F	0.98	C16B-H16D	0.98
C16B-H16E	0.98	C16B-H16F	0.98
N2B-C11B	1.466(3)	C11B-C12B	1.519(3)
C11B-C13B	1.528(4)	C11B-H11B	1.0
C12B-H12D	0.98	C12B-H12E	0.98
C12B-H12F	0.98	C13B-H13D	0.98
C13B-H13E	0.98	C13B-H13F	0.98
C20B-C21B	1.423(4)	C20B-C24B	1.425(4)
C20B-C25B	1.502(4)	C21B-C22B	1.439(3)
C21B-C26B	1.501(4)	C22B-C23B	1.401(4)
C22B-C27B	1.501(4)	C23B-C24B	1.421(4)
C23B-C28B	1.506(4)	C24B-C29B	1.504(4)
C25B-H25D	0.98	C25B-H25E	0.98
C25B-H25F	0.98	C26B-H26D	0.98
C26B-H26E	0.98	C26B-H26F	0.98
C27B-H27D	0.98	C27B-H27E	0.98
C27B-H27F	0.98	C28B-H28D	0.98
C28B-H28E	0.98	C28B-H28F	0.98
C29B-H29D	0.98	C29B-H29E	0.98
C29B-H29F	0.98		

Table 5. Bond angles (°) for 1b.

N1-Ta1-N2A	103.78(7)	N1-Ta1-N1A	101.96(7)
N2A-Ta1-N1A	60.88(6)	N1-Ta1-C20A	95.02(8)
N2A-Ta1-C20A	147.22(7)	N1A-Ta1-C20A	140.79(7)
N1-Ta1-C24A	113.39(8)	N2A-Ta1-C24A	142.62(8)
N1A-Ta1-C24A	105.89(7)	C20A-Ta1-C24A	35.15(8)
N1-Ta1-C21A	111.23(8)	N2A-Ta1-C21A	112.57(7)
N1A-Ta1-C21A	146.59(7)	C20A-Ta1-C21A	34.71(8)
C24A-Ta1-C21A	57.63(8)	N1-Ta1-C23A	147.47(8)
N2A-Ta1-C23A	108.74(7)	N1A-Ta1-C23A	93.45(7)
C20A-Ta1-C23A	56.84(8)	C24A-Ta1-C23A	34.16(8)
C21A-Ta1-C23A	56.01(7)	N1-Ta1-C22A	144.88(7)
N2A-Ta1-C22A	94.95(7)	N1A-Ta1-C22A	113.12(7)
C20A-Ta1-C22A	56.38(7)	C24A-Ta1-C22A	56.11(7)
C21A-Ta1-C22A	33.65(7)	C23A-Ta1-C22A	32.74(7)
N2-Ta2-N2B	103.15(7)	N2-Ta2-N1B	108.25(7)
N2B-Ta2-N1B	60.60(7)	N2-Ta2-C20B	92.24(8)
N2B-Ta2-C20B	138.67(8)	N1B-Ta2-C20B	148.47(8)
N2-Ta2-C21B	111.81(8)	N2B-Ta2-C21B	104.12(8)
N1B-Ta2-C21B	139.56(8)	C20B-Ta2-C21B	35.15(9)
N2-Ta2-C24B	107.98(8)	N2B-Ta2-C24B	148.09(8)
N1B-Ta2-C24B	114.16(8)	C20B-Ta2-C24B	34.75(8)
C21B-Ta2-C24B	57.70(9)	N2-Ta2-C22B	145.94(8)

N2B-Ta2-C22B	93.75(8)	N1B-Ta2-C22B	105.81(8)
C20B-Ta2-C22B	56.96(9)	C21B-Ta2-C22B	34.47(8)
C24B-Ta2-C22B	55.95(9)	N2-Ta2-C23B	141.47(8)
N2B-Ta2-C23B	115.16(8)	N1B-Ta2-C23B	94.44(8)
C20B-Ta2-C23B	56.31(8)	C21B-Ta2-C23B	56.21(8)
C24B-Ta2-C23B	33.50(9)	C22B-Ta2-C23B	32.64(9)
N2-N1-Ta1	175.93(15)	N1-N2-Ta2	171.47(14)
N1A-C1A-N2A	112.51(18)	N1A-C1A-C2A	122.86(18)
N2A-C1A-C2A	124.50(18)	C3A-C2A-C7A	119.0(2)
C3A-C2A-C1A	120.8(2)	C7A-C2A-C1A	120.2(2)
C2A-C3A-C4A	120.5(3)	C2A-C3A-H3A	119.8
C4A-C3A-H3A	119.8	C5A-C4A-C3A	120.1(3)
C5A-C4A-H4A	119.9	C3A-C4A-H4A	119.9
C6A-C5A-C4A	119.8(3)	C6A-C5A-H5A	120.1
C4A-C5A-H5A	120.1	C5A-C6A-C7A	120.9(3)
C5A-C6A-H6A	119.5	C7A-C6A-H6A	119.5
C2A-C7A-C6A	119.7(3)	C2A-C7A-H7A	120.2
C6A-C7A-H7A	120.2	C1A-N1A-C8A	120.93(18)
C1A-N1A-Ta1	89.71(12)	C8A-N1A-Ta1	134.78(15)
N1A-C8A-C10A	110.8(3)	N1A-C8A-C9A	109.9(2)
C10A-C8A-C9A	110.7(3)	N1A-C8A-H8A	108.5
C10A-C8A-H8A	108.5	C9A-C8A-H8A	108.5
C8A-C9A-H9A1	109.5	C8A-C9A-H9A2	109.5
H9A1-C9A-H9A2	109.5	C8A-C9A-H9A3	109.5
H9A1-C9A-H9A3	109.5	H9A2-C9A-H9A3	109.5
C8A-C10A-H10A	109.5	C8A-C10A-H10B	109.5
H10A-C10A-H10B	109.5	C8A-C10A-H10C	109.5
H10A-C10A-H10C	109.5	H10B-C10A-H10C	109.5
H15A-C15A-H15B	109.5	H15A-C15A-H15C	109.5
H15B-C15A-H15C	109.5	H16A-C16A-H16B	109.5
H16A-C16A-H16C	109.5	H16B-C16A-H16C	109.5
C1A-N2A-C11A	121.65(18)	C1A-N2A-Ta1	89.95(12)
C11A-N2A-Ta1	134.26(14)	N2A-C11A-C12A	110.58(19)
N2A-C11A-C13A	110.11(19)	C12A-C11A-C13A	110.5(2)
N2A-C11A-H11A	108.5	C12A-C11A-H11A	108.5
C13A-C11A-H11A	108.5	C11A-C12A-H12A	109.5
C11A-C12A-H12B	109.5	H12A-C12A-H12B	109.5
C11A-C12A-H12C	109.5	H12A-C12A-H12C	109.5
H12B-C12A-H12C	109.5	C11A-C13A-H13A	109.5
C11A-C13A-H13B	109.5	H13A-C13A-H13B	109.5
C11A-C13A-H13C	109.5	H13A-C13A-H13C	109.5
H13B-C13A-H13C	109.5	C21A-C20A-C24A	107.9(2)
C21A-C20A-C25A	126.3(2)	C24A-C20A-C25A	125.6(2)
C21A-C20A-Ta1	74.71(12)	C24A-C20A-Ta1	72.99(12)

C25A-C20A-Ta1	121.20(16)	C20A-C21A-C22A	107.8(2)
C20A-C21A-C26A	126.0(2)	C22A-C21A-C26A	125.6(2)
C20A-C21A-Ta1	70.58(12)	C22A-C21A-Ta1	77.05(12)
C26A-C21A-Ta1	125.27(15)	C23A-C22A-C21A	108.4(2)
C23A-C22A-C27A	126.5(2)	C21A-C22A-C27A	124.9(2)
C23A-C22A-Ta1	72.64(12)	C21A-C22A-Ta1	69.30(12)
C27A-C22A-Ta1	128.08(15)	C22A-C23A-C24A	108.2(2)
C22A-C23A-C28A	125.5(2)	C24A-C23A-C28A	126.3(2)
C22A-C23A-Ta1	74.63(12)	C24A-C23A-Ta1	68.54(12)
C28A-C23A-Ta1	123.29(15)	C20A-C24A-C23A	107.64(19)
C20A-C24A-C29A	125.3(2)	C23A-C24A-C29A	126.4(2)
C20A-C24A-Ta1	71.86(12)	C23A-C24A-Ta1	77.29(12)
C29A-C24A-Ta1	123.88(16)	C20A-C25A-H25A	109.5
C20A-C25A-H25B	109.5	H25A-C25A-H25B	109.5
C20A-C25A-H25C	109.5	H25A-C25A-H25C	109.5
H25B-C25A-H25C	109.5	C21A-C26A-H26A	109.5
C21A-C26A-H26B	109.5	H26A-C26A-H26B	109.5
C21A-C26A-H26C	109.5	H26A-C26A-H26C	109.5
H26B-C26A-H26C	109.5	C22A-C27A-H27A	109.5
C22A-C27A-H27B	109.5	H27A-C27A-H27B	109.5
C22A-C27A-H27C	109.5	H27A-C27A-H27C	109.5
H27B-C27A-H27C	109.5	C23A-C28A-H28A	109.5
C23A-C28A-H28B	109.5	H28A-C28A-H28B	109.5
C23A-C28A-H28C	109.5	H28A-C28A-H28C	109.5
H28B-C28A-H28C	109.5	C24A-C29A-H29A	109.5
C24A-C29A-H29B	109.5	H29A-C29A-H29B	109.5
C24A-C29A-H29C	109.5	H29A-C29A-H29C	109.5
H29B-C29A-H29C	109.5	N1B-C1B-N2B	112.73(19)
N1B-C1B-C2B	124.8(2)	N2B-C1B-C2B	122.5(2)
C3B-C2B-C7B	120.2(2)	C3B-C2B-C1B	121.7(2)
C7B-C2B-C1B	118.1(2)	C2B-C3B-C4B	118.2(3)
C2B-C3B-H3B	120.9	C4B-C3B-H3B	120.9
C5B-C4B-C3B	119.0(3)	C5B-C4B-H4B	120.5
C3B-C4B-H4B	120.5	C6B-C5B-C4B	122.5(3)
C6B-C5B-H5B	118.7	C4B-C5B-H5B	118.7
C5B-C6B-C7B	118.8(3)	C5B-C6B-H6B	120.6
C7B-C6B-H6B	120.6	C6B-C7B-C2B	121.2(3)
C6B-C7B-H7B	119.4	C2B-C7B-H7B	119.4
C1B-N1B-C8B	122.60(19)	C1B-N1B-Ta2	92.24(13)
C8B-N1B-Ta2	140.72(16)	N1B-C8B-C10B	110.4(3)
N1B-C8B-C9B	109.8(3)	C10B-C8B-C9B	112.2(4)
N1B-C8B-H8B	108.1	C10B-C8B-H8B	108.1
C9B-C8B-H8B	108.1	C8B-C9B-H9B1	109.5
C8B-C9B-H9B2	109.5	H9B1-C9B-H9B2	109.5

C8B-C9B-H9B3	109.5	H9B1-C9B-H9B3	109.5
H9B2-C9B-H9B3	109.5	H15D-C15B-H15E	109.5
H15D-C15B-H15F	109.5	H15E-C15B-H15F	109.5
H16D-C16B-H16E	109.5	H16D-C16B-H16F	109.5
H16E-C16B-H16F	109.5	C1B-N2B-C11B	121.72(19)
C1B-N2B-Ta2	92.24(14)	C11B-N2B-Ta2	139.00(14)
N2B-C11B-C12B	109.6(2)	N2B-C11B-C13B	110.5(2)
C12B-C11B-C13B	110.8(2)	N2B-C11B-H11B	108.6
C12B-C11B-H11B	108.6	C13B-C11B-H11B	108.6
C11B-C12B-H12D	109.5	C11B-C12B-H12E	109.5
H12D-C12B-H12E	109.5	C11B-C12B-H12F	109.5
H12D-C12B-H12F	109.5	H12E-C12B-H12F	109.5
C11B-C13B-H13D	109.5	C11B-C13B-H13E	109.5
H13D-C13B-H13E	109.5	C11B-C13B-H13F	109.5
H13D-C13B-H13F	109.5	H13E-C13B-H13F	109.5
C21B-C20B-C24B	108.1(2)	C21B-C20B-C25B	126.1(2)
C24B-C20B-C25B	125.8(3)	C21B-C20B-Ta2	72.71(13)
C24B-C20B-Ta2	75.10(13)	C25B-C20B-Ta2	119.85(16)
C20B-C21B-C22B	107.5(2)	C20B-C21B-C26B	125.4(2)
C22B-C21B-C26B	126.4(3)	C20B-C21B-Ta2	72.13(12)
C22B-C21B-Ta2	77.35(13)	C26B-C21B-Ta2	123.69(17)
C23B-C22B-C21B	107.9(2)	C23B-C22B-C27B	126.0(2)
C21B-C22B-C27B	126.2(3)	C23B-C22B-Ta2	74.64(14)
C21B-C22B-Ta2	68.19(12)	C27B-C22B-Ta2	123.97(18)
C22B-C23B-C24B	109.0(2)	C22B-C23B-C28B	125.5(3)
C24B-C23B-C28B	125.3(3)	C22B-C23B-Ta2	72.72(13)
C24B-C23B-Ta2	69.86(13)	C28B-C23B-Ta2	127.66(18)
C23B-C24B-C20B	107.5(2)	C23B-C24B-C29B	127.0(3)
C20B-C24B-C29B	124.9(3)	C23B-C24B-Ta2	76.64(14)
C20B-C24B-Ta2	70.15(13)	C29B-C24B-Ta2	125.46(18)
C20B-C25B-H25D	109.5	C20B-C25B-H25E	109.5
H25D-C25B-H25E	109.5	C20B-C25B-H25F	109.5
H25D-C25B-H25F	109.5	H25E-C25B-H25F	109.5
C21B-C26B-H26D	109.5	C21B-C26B-H26E	109.5
H26D-C26B-H26E	109.5	C21B-C26B-H26F	109.5
H26D-C26B-H26F	109.5	H26E-C26B-H26F	109.5
C22B-C27B-H27D	109.5	C22B-C27B-H27E	109.5
H27D-C27B-H27E	109.5	C22B-C27B-H27F	109.5
H27D-C27B-H27F	109.5	H27E-C27B-H27F	109.5
C23B-C28B-H28D	109.5	C23B-C28B-H28E	109.5
H28D-C28B-H28E	109.5	C23B-C28B-H28F	109.5
H28D-C28B-H28F	109.5	H28E-C28B-H28F	109.5
C24B-C29B-H29D	109.5	C24B-C29B-H29E	109.5
H29D-C29B-H29E	109.5	C24B-C29B-H29F	109.5

H29D-C29B-H29F	109.5	H29E-C29B-H29F	109.5

Table 6. Torsion angles (°) for 1b.

N1A-C1A-C2A-C3A	78.9(3)	N2A-C1A-C2A-C3A	-105.6(3)
N1A-C1A-C2A-C7A	-98.2(3)	N2A-C1A-C2A-C7A	77.2(3)
C7A-C2A-C3A-C4A	-0.7(4)	C1A-C2A-C3A-C4A	-177.9(2)
C2A-C3A-C4A-C5A	0.7(4)	C3A-C4A-C5A-C6A	-0.2(5)
C4A-C5A-C6A-C7A	-0.3(5)	C3A-C2A-C7A-C6A	0.2(4)
C1A-C2A-C7A-C6A	177.4(2)	C5A-C6A-C7A-C2A	0.3(5)
N2A-C1A-N1A-C8A	-169.69(19)	C2A-C1A-N1A-C8A	6.2(3)
N2A-C1A-N1A-Ta1	-24.79(18)	C2A-C1A-N1A-Ta1	151.14(18)
N1-Ta1-N1A-C1A	-83.54(13)	N2A-Ta1-N1A-C1A	15.71(12)
C20A-Ta1-N1A-C1A	162.81(12)	C24A-Ta1-N1A-C1A	157.63(12)
C21A-Ta1-N1A-C1A	103.03(16)	C23A-Ta1-N1A-C1A	125.27(13)
C22A-Ta1-N1A-C1A	98.21(13)	N1-Ta1-N1A-C8A	52.4(2)
N2A-Ta1-N1A-C8A	151.7(2)	C20A-Ta1-N1A-C8A	-61.2(2)
C24A-Ta1-N1A-C8A	-66.4(2)	C21A-Ta1-N1A-C8A	-121.0(2)
C23A-Ta1-N1A-C8A	-98.8(2)	C22A-Ta1-N1A-C8A	-125.81(19)
C1A-N1A-C8A-C10A	-130.5(4)	Ta1-N1A-C8A-C10A	103.6(4)
C1A-N1A-C8A-C9A	106.9(3)	Ta1-N1A-C8A-C9A	-19.0(4)
N1A-C1A-N2A-C11A	169.89(19)	C2A-C1A-N2A-C11A	-6.0(3)
N1A-C1A-N2A-Ta1	24.87(18)	C2A-C1A-N2A-Ta1	-150.98(19)
N1-Ta1-N2A-C1A	80.48(13)	N1A-Ta1-N2A-C1A	-15.69(12)
C20A-Ta1-N2A-C1A	-156.33(14)	C24A-Ta1-N2A-C1A	-93.41(16)
C21A-Ta1-N2A-C1A	-159.14(12)	C23A-Ta1-N2A-C1A	-99.02(13)
C22A-Ta1-N2A-C1A	-129.46(13)	N1-Ta1-N2A-C11A	-56.6(2)
N1A-Ta1-N2A-C11A	-152.7(2)	C20A-Ta1-N2A-C11A	66.6(3)
C24A-Ta1-N2A-C11A	129.5(2)	C21A-Ta1-N2A-C11A	63.8(2)
C23A-Ta1-N2A-C11A	123.93(19)	C22A-Ta1-N2A-C11A	93.5(2)
C1A-N2A-C11A-C12A	-100.7(2)	Ta1-N2A-C11A-C12A	26.1(3)
C1A-N2A-C11A-C13A	136.8(2)	Ta1-N2A-C11A-C13A	-96.3(2)
N1-Ta1-C20A-C21A	120.77(13)	N2A-Ta1-C20A-C21A	-4.5(2)
N1A-Ta1-C20A-C21A	-123.33(14)	C24A-Ta1-C20A-C21A	-114.66(19)
C23A-Ta1-C20A-C21A	-76.74(14)	C22A-Ta1-C20A-C21A	-37.29(12)
N1-Ta1-C20A-C24A	-124.57(14)	N2A-Ta1-C20A-C24A	110.12(16)
N1A-Ta1-C20A-C24A	-8.67(19)	C21A-Ta1-C20A-C24A	114.66(19)
C23A-Ta1-C20A-C24A	37.92(13)	C22A-Ta1-C20A-C24A	77.37(14)
N1-Ta1-C20A-C25A	-2.7(2)	N2A-Ta1-C20A-C25A	-128.1(2)
N1A-Ta1-C20A-C25A	113.1(2)	C24A-Ta1-C20A-C25A	121.8(3)
C21A-Ta1-C20A-C25A	-123.5(3)	C23A-Ta1-C20A-C25A	159.7(2)
C22A-Ta1-C20A-C25A	-160.8(2)	C24A-C20A-C21A-C22A	2.7(2)
C25A-C20A-C21A-C22A	-173.5(2)	Ta1-C20A-C21A-C22A	68.72(15)
C24A-C20A-C21A-C26A	174.0(2)	C25A-C20A-C21A-C26A	-2.3(4)
Ta1-C20A-C21A-C26A	-120.0(2)	C24A-C20A-C21A-Ta1	-65.98(15)

C25A-C20A-C21A-Ta1	117.7(2)	N1-Ta1-C21A-C20A	-66.67(14)
N2A-Ta1-C21A-C20A	177.34(13)	N1A-Ta1-C21A-C20A	106.43(16)
C24A-Ta1-C21A-C20A	38.27(13)	C23A-Ta1-C21A-C20A	79.32(14)
C22A-Ta1-C21A-C20A	114.44(19)	N1-Ta1-C21A-C22A	178.89(12)
N2A-Ta1-C21A-C22A	62.90(14)	N1A-Ta1-C21A-C22A	-8.0(2)
C20A-Ta1-C21A-C22A	-114.44(19)	C24A-Ta1-C21A-C22A	-76.17(14)
C23A-Ta1-C21A-C22A	-35.12(12)	N1-Ta1-C21A-C26A	54.2(2)
N2A-Ta1-C21A-C26A	-61.8(2)	N1A-Ta1-C21A-C26A	-132.69(19)
C20A-Ta1-C21A-C26A	120.9(3)	C24A-Ta1-C21A-C26A	159.2(2)
C23A-Ta1-C21A-C26A	-159.8(2)	C22A-Ta1-C21A-C26A	-124.7(3)
C20A-C21A-C22A-C23A	-1.9(2)	C26A-C21A-C22A-C23A	-173.2(2)
Ta1-C21A-C22A-C23A	62.51(15)	C20A-C21A-C22A-C27A	172.9(2)
C26A-C21A-C22A-C27A	1.6(3)	Ta1-C21A-C22A-C27A	-122.7(2)
C20A-C21A-C22A-Ta1	-64.39(14)	C26A-C21A-C22A-Ta1	124.3(2)
N1-Ta1-C22A-C23A	-119.91(16)	N2A-Ta1-C22A-C23A	117.49(13)
N1A-Ta1-C22A-C23A	57.11(14)	C20A-Ta1-C22A-C23A	-79.60(14)
C24A-Ta1-C22A-C23A	-37.02(13)	C21A-Ta1-C22A-C23A	-118.11(19)
N1-Ta1-C22A-C21A	-1.8(2)	N2A-Ta1-C22A-C21A	-124.40(13)
N1A-Ta1-C22A-C21A	175.21(12)	C20A-Ta1-C22A-C21A	38.50(13)
C24A-Ta1-C22A-C21A	81.09(14)	C23A-Ta1-C22A-C21A	118.11(19)
N1-Ta1-C22A-C27A	117.0(2)	N2A-Ta1-C22A-C27A	-5.6(2)
N1A-Ta1-C22A-C27A	-66.0(2)	C20A-Ta1-C22A-C27A	157.3(2)
C24A-Ta1-C22A-C27A	-160.1(2)	C21A-Ta1-C22A-C27A	118.8(3)
C23A-Ta1-C22A-C27A	-123.1(3)	C21A-C22A-C23A-C24A	0.3(2)
C27A-C22A-C23A-C24A	-174.4(2)	Ta1-C22A-C23A-C24A	60.68(14)
C21A-C22A-C23A-C28A	179.4(2)	C27A-C22A-C23A-C28A	4.7(4)
Ta1-C22A-C23A-C28A	-120.2(2)	C21A-C22A-C23A-Ta1	-60.39(15)
C27A-C22A-C23A-Ta1	124.9(2)	N1-Ta1-C23A-C22A	111.95(17)
N2A-Ta1-C23A-C22A	-68.94(14)	N1A-Ta1-C23A-C22A	-129.32(13)
C20A-Ta1-C23A-C22A	78.07(14)	C24A-Ta1-C23A-C22A	117.13(19)
C21A-Ta1-C23A-C22A	36.12(13)	N1-Ta1-C23A-C24A	-5.2(2)
N2A-Ta1-C23A-C24A	173.93(12)	N1A-Ta1-C23A-C24A	113.55(13)
C20A-Ta1-C23A-C24A	-39.06(13)	C21A-Ta1-C23A-C24A	-81.00(14)
C22A-Ta1-C23A-C24A	-117.13(19)	N1-Ta1-C23A-C28A	-125.4(2)
N2A-Ta1-C23A-C28A	53.7(2)	N1A-Ta1-C23A-C28A	-6.7(2)
C20A-Ta1-C23A-C28A	-159.3(2)	C24A-Ta1-C23A-C28A	-120.2(3)
C21A-Ta1-C23A-C28A	158.7(2)	C22A-Ta1-C23A-C28A	122.6(3)
C21A-C20A-C24A-C23A	-2.6(2)	C25A-C20A-C24A-C23A	173.7(2)
Ta1-C20A-C24A-C23A	-69.69(15)	C21A-C20A-C24A-C29A	-173.7(2)
C25A-C20A-C24A-C29A	2.6(4)	Ta1-C20A-C24A-C29A	119.1(2)
C21A-C20A-C24A-Ta1	67.12(15)	C25A-C20A-C24A-Ta1	-116.6(2)
C22A-C23A-C24A-C20A	1.4(2)	C28A-C23A-C24A-C20A	-177.7(2)
Ta1-C23A-C24A-C20A	66.01(14)	C22A-C23A-C24A-C29A	172.5(2)
C28A-C23A-C24A-C29A	-6.7(4)	Ta1-C23A-C24A-C29A	-122.9(2)

C22A-C23A-C24A-Ta1	-64.59(15)	C28A-C23A-C24A-Ta1	116.3(2)
N1-Ta1-C24A-C20A	63.35(15)	N2A-Ta1-C24A-C20A	-123.12(14)
N1A-Ta1-C24A-C20A	174.32(13)	C21A-Ta1-C24A-C20A	-37.78(13)
C23A-Ta1-C24A-C20A	-113.62(19)	C22A-Ta1-C24A-C20A	-78.19(14)
N1-Ta1-C24A-C23A	176.97(12)	N2A-Ta1-C24A-C23A	-9.50(19)
N1A-Ta1-C24A-C23A	-72.06(14)	C20A-Ta1-C24A-C23A	113.62(19)
C21A-Ta1-C24A-C23A	75.84(14)	C22A-Ta1-C24A-C23A	35.43(12)
N1-Ta1-C24A-C29A	-57.5(2)	N2A-Ta1-C24A-C29A	116.1(2)
N1A-Ta1-C24A-C29A	53.5(2)	C20A-Ta1-C24A-C29A	-120.8(3)
C21A-Ta1-C24A-C29A	-158.6(3)	C23A-Ta1-C24A-C29A	125.6(3)
C22A-Ta1-C24A-C29A	161.0(3)	N1B-C1B-C2B-C3B	-84.6(3)
N2B-C1B-C2B-C3B	93.9(3)	N1B-C1B-C2B-C7B	98.1(3)
N2B-C1B-C2B-C7B	-83.4(3)	C7B-C2B-C3B-C4B	-0.5(4)
C1B-C2B-C3B-C4B	-177.8(2)	C2B-C3B-C4B-C5B	-0.7(4)
C3B-C4B-C5B-C6B	1.2(4)	C4B-C5B-C6B-C7B	-0.4(4)
C5B-C6B-C7B-C2B	-0.9(4)	C3B-C2B-C7B-C6B	1.3(4)
C1B-C2B-C7B-C6B	178.7(2)	N2B-C1B-N1B-C8B	-174.8(2)
C2B-C1B-N1B-C8B	3.8(4)	N2B-C1B-N1B-Ta2	-14.00(19)
C2B-C1B-N1B-Ta2	164.6(2)	N2-Ta2-N1B-C1B	-86.18(14)
N2B-Ta2-N1B-C1B	8.94(13)	C20B-Ta2-N1B-C1B	145.80(16)
C21B-Ta2-N1B-C1B	85.66(18)	C24B-Ta2-N1B-C1B	153.54(14)
C22B-Ta2-N1B-C1B	94.26(15)	C23B-Ta2-N1B-C1B	125.41(14)
N2-Ta2-N1B-C8B	67.9(3)	N2B-Ta2-N1B-C8B	163.0(3)
C20B-Ta2-N1B-C8B	-60.1(3)	C21B-Ta2-N1B-C8B	-120.3(3)
C24B-Ta2-N1B-C8B	-52.4(3)	C22B-Ta2-N1B-C8B	-111.7(3)
C23B-Ta2-N1B-C8B	-80.5(3)	C1B-N1B-C8B-C10B	-95.8(4)
Ta2-N1B-C8B-C10B	115.5(4)	C1B-N1B-C8B-C9B	140.1(4)
Ta2-N1B-C8B-C9B	-8.7(5)	N1B-C1B-N2B-C11B	169.8(2)
C2B-C1B-N2B-C11B	-8.9(3)	N1B-C1B-N2B-Ta2	14.01(19)
C2B-C1B-N2B-Ta2	-164.7(2)	N2-Ta2-N2B-C1B	94.80(14)
N1B-Ta2-N2B-C1B	-8.93(13)	C20B-Ta2-N2B-C1B	-156.14(13)
C21B-Ta2-N2B-C1B	-148.32(13)	C24B-Ta2-N2B-C1B	-98.00(18)
C22B-Ta2-N2B-C1B	-114.98(14)	C23B-Ta2-N2B-C1B	-89.34(14)
N2-Ta2-N2B-C11B	-53.1(2)	N1B-Ta2-N2B-C11B	-156.8(3)
C20B-Ta2-N2B-C11B	56.0(3)	C21B-Ta2-N2B-C11B	63.8(2)
C24B-Ta2-N2B-C11B	114.1(2)	C22B-Ta2-N2B-C11B	97.1(2)
C23B-Ta2-N2B-C11B	122.8(2)	C1B-N2B-C11B-C12B	-126.0(2)
Ta2-N2B-C11B-C12B	15.4(3)	C1B-N2B-C11B-C13B	111.6(3)
Ta2-N2B-C11B-C13B	-107.1(3)	N2-Ta2-C20B-C21B	126.17(14)
N2B-Ta2-C20B-C21B	13.3(2)	N1B-Ta2-C20B-C21B	-102.32(19)
C24B-Ta2-C20B-C21B	-114.8(2)	C22B-Ta2-C20B-C21B	-38.32(14)
C23B-Ta2-C20B-C21B	-77.64(15)	N2-Ta2-C20B-C24B	-119.07(16)
N2B-Ta2-C20B-C24B	128.03(16)	N1B-Ta2-C20B-C24B	12.4(2)
C21B-Ta2-C20B-C24B	114.8(2)	C22B-Ta2-C20B-C24B	76.45(16)

C23B-Ta2-C20B-C24B	37.13(15)	N2-Ta2-C20B-C25B	4.0(2)
N2B-Ta2-C20B-C25B	-108.9(2)	N1B-Ta2-C20B-C25B	135.5(2)
C21B-Ta2-C20B-C25B	-122.2(3)	C24B-Ta2-C20B-C25B	123.0(3)
C22B-Ta2-C20B-C25B	-160.5(3)	C23B-Ta2-C20B-C25B	160.2(3)
C24B-C20B-C21B-C22B	2.6(2)	C25B-C20B-C21B-C22B	-175.3(2)
Ta2-C20B-C21B-C22B	69.96(16)	C24B-C20B-C21B-C26B	173.6(2)
C25B-C20B-C21B-C26B	-4.4(4)	Ta2-C20B-C21B-C26B	-119.1(2)
C24B-C20B-C21B-Ta2	-67.37(15)	C25B-C20B-C21B-Ta2	114.7(2)
N2-Ta2-C21B-C20B	-60.32(16)	N2B-Ta2-C21B-C20B	-171.01(14)
N1B-Ta2-C21B-C20B	128.02(15)	C24B-Ta2-C21B-C20B	37.75(14)
C22B-Ta2-C21B-C20B	113.3(2)	C23B-Ta2-C21B-C20B	77.93(16)
N2-Ta2-C21B-C22B	-173.62(15)	N2B-Ta2-C21B-C22B	75.69(16)
N1B-Ta2-C21B-C22B	14.7(2)	C20B-Ta2-C21B-C22B	-113.3(2)
C24B-Ta2-C21B-C22B	-75.54(16)	C23B-Ta2-C21B-C22B	-35.36(15)
N2-Ta2-C21B-C26B	60.8(2)	N2B-Ta2-C21B-C26B	-49.9(2)
N1B-Ta2-C21B-C26B	-110.8(2)	C20B-Ta2-C21B-C26B	121.1(3)
C24B-Ta2-C21B-C26B	158.9(3)	C22B-Ta2-C21B-C26B	-125.6(3)
C23B-Ta2-C21B-C26B	-160.9(3)	C20B-C21B-C22B-C23B	-1.8(3)
C26B-C21B-C22B-C23B	-172.6(2)	Ta2-C21B-C22B-C23B	64.62(17)
C20B-C21B-C22B-C27B	176.7(2)	C26B-C21B-C22B-C27B	5.8(4)
Ta2-C21B-C22B-C27B	-116.9(2)	C20B-C21B-C22B-Ta2	-66.41(15)
C26B-C21B-C22B-Ta2	122.7(3)	N2-Ta2-C22B-C23B	-106.29(18)
N2B-Ta2-C22B-C23B	133.44(15)	N1B-Ta2-C22B-C23B	72.96(16)
C20B-Ta2-C22B-C23B	-77.79(16)	C21B-Ta2-C22B-C23B	-116.9(2)
C24B-Ta2-C22B-C23B	-35.82(14)	N2-Ta2-C22B-C21B	10.6(2)
N2B-Ta2-C22B-C21B	-109.66(16)	N1B-Ta2-C22B-C21B	-170.13(15)
C20B-Ta2-C22B-C21B	39.11(15)	C24B-Ta2-C22B-C21B	81.08(17)
C23B-Ta2-C22B-C21B	116.9(2)	N2-Ta2-C22B-C27B	130.4(2)
N2B-Ta2-C22B-C27B	10.1(2)	N1B-Ta2-C22B-C27B	-50.4(2)
C20B-Ta2-C22B-C27B	158.9(3)	C21B-Ta2-C22B-C27B	119.8(3)
C24B-Ta2-C22B-C27B	-159.1(3)	C23B-Ta2-C22B-C27B	-123.3(3)
C21B-C22B-C23B-C24B	0.3(3)	C27B-C22B-C23B-C24B	-178.2(2)
Ta2-C22B-C23B-C24B	60.74(16)	C21B-C22B-C23B-C28B	175.2(2)
C27B-C22B-C23B-C28B	-3.2(4)	Ta2-C22B-C23B-C28B	-124.3(3)
C21B-C22B-C23B-Ta2	-60.44(16)	C27B-C22B-C23B-Ta2	121.1(3)
N2-Ta2-C23B-C22B	120.33(17)	N2B-Ta2-C23B-C22B	-53.17(16)
N1B-Ta2-C23B-C22B	-112.67(15)	C20B-Ta2-C23B-C22B	79.98(16)
C21B-Ta2-C23B-C22B	37.39(15)	C24B-Ta2-C23B-C22B	118.5(2)
N2-Ta2-C23B-C24B	1.8(2)	N2B-Ta2-C23B-C24B	-171.71(14)
N1B-Ta2-C23B-C24B	128.79(15)	C20B-Ta2-C23B-C24B	-38.56(15)
C21B-Ta2-C23B-C24B	-81.15(16)	C22B-Ta2-C23B-C24B	-118.5(2)
N2-Ta2-C23B-C28B	-117.8(3)	N2B-Ta2-C23B-C28B	68.7(3)
N1B-Ta2-C23B-C28B	9.2(3)	C20B-Ta2-C23B-C28B	-158.2(3)
C21B-Ta2-C23B-C28B	159.2(3)	C24B-Ta2-C23B-C28B	-119.6(3)

C22B-Ta2-C23B-C28B	121.8(3)	C22B-C23B-C24B-C20B	1.3(3)
C28B-C23B-C24B-C20B	-173.6(2)	Ta2-C23B-C24B-C20B	63.84(15)
C22B-C23B-C24B-C29B	172.9(2)	C28B-C23B-C24B-C29B	-2.1(4)
Ta2-C23B-C24B-C29B	-124.6(3)	C22B-C23B-C24B-Ta2	-62.53(17)
C28B-C23B-C24B-Ta2	122.5(2)	C21B-C20B-C24B-C23B	-2.4(3)
C25B-C20B-C24B-C23B	175.5(2)	Ta2-C20B-C24B-C23B	-68.19(16)
C21B-C20B-C24B-C29B	-174.2(2)	C25B-C20B-C24B-C29B	3.7(4)
Ta2-C20B-C24B-C29B	120.0(2)	C21B-C20B-C24B-Ta2	65.78(15)
C25B-C20B-C24B-Ta2	-116.3(2)	N2-Ta2-C24B-C23B	-178.83(14)
N2B-Ta2-C24B-C23B	14.3(2)	N1B-Ta2-C24B-C23B	-58.40(16)
C20B-Ta2-C24B-C23B	114.5(2)	C21B-Ta2-C24B-C23B	76.29(16)
C22B-Ta2-C24B-C23B	34.88(14)	N2-Ta2-C24B-C20B	66.67(16)
N2B-Ta2-C24B-C20B	-100.21(19)	N1B-Ta2-C24B-C20B	-172.90(14)
C21B-Ta2-C24B-C20B	-38.21(15)	C22B-Ta2-C24B-C20B	-79.62(16)
C23B-Ta2-C24B-C20B	-114.5(2)	N2-Ta2-C24B-C29B	-52.7(3)
N2B-Ta2-C24B-C29B	140.5(2)	N1B-Ta2-C24B-C29B	67.8(3)
C20B-Ta2-C24B-C29B	-119.3(3)	C21B-Ta2-C24B-C29B	-157.5(3)
C22B-Ta2-C24B-C29B	161.1(3)	C23B-Ta2-C24B-C29B	126.2(3)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 1b.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.01708(4)	0.02239(4)	0.02554(4)	-0.00074(3)	0.00630(3)	-0.00149(3)
Ta2	0.02733(4)	0.02137(4)	0.02637(5)	0.00317(3)	0.00930(3)	0.00412(3)
N1	0.0213(8)	0.0237(8)	0.0283(9)	0.0002(7)	0.0071(7)	-0.0003(6)
N2	0.0248(8)	0.0214(8)	0.0273(9)	0.0009(7)	0.0070(7)	0.0014(6)
C1A	0.0220(9)	0.0244(9)	0.0228(10)	0.0001(8)	0.0057(8)	-0.0018(7)
C2A	0.0210(10)	0.0251(9)	0.0332(12)	-0.0072(8)	0.0072(8)	-0.0024(8)
C3A	0.0336(13)	0.0442(14)	0.0385(14)	-0.0013(11)	0.0066(10)	0.0094(11)
C4A	0.0407(15)	0.0517(16)	0.0554(18)	-0.0057(14)	-0.0056(13)	0.0174(13)
C5A	0.0286(13)	0.0412(14)	0.086(2)	-0.0201(15)	0.0088(14)	0.0076(11)
C6A	0.0419(16)	0.0557(18)	0.086(2)	-0.0103(17)	0.0381(17)	0.0036(14)
C7A	0.0423(15)	0.0472(15)	0.0524(17)	0.0022(13)	0.0259(13)	0.0059(12)
N1A	0.0219(8)	0.0214(8)	0.0323(10)	-0.0011(7)	0.0061(7)	-0.0032(6)
C8A	0.0272(11)	0.0206(9)	0.0455(14)	-0.0044(9)	0.0094(10)	-0.0039(8)
C9A	0.052(3)	0.0360(16)	0.045(2)	-0.0148(16)	0.0082(19)	0.0039(19)
C10A	0.078(4)	0.0276(13)	0.076(4)	-0.008(2)	0.042(3)	-0.019(2)
C14A	0.0272(11)	0.0206(9)	0.0455(14)	-0.0044(9)	0.0094(10)	-0.0039(8)
C15A	0.052(3)	0.0360(16)	0.045(2)	-0.0148(16)	0.0082(19)	0.0039(19)
C16A	0.078(4)	0.0276(13)	0.076(4)	-0.008(2)	0.042(3)	-0.019(2)
N2A	0.0214(8)	0.0222(8)	0.0316(10)	-0.0009(7)	0.0040(7)	-0.0030(6)
C11A	0.0223(10)	0.0249(10)	0.0414(13)	-0.0029(9)	0.0038(9)	-0.0058(8)
C12A	0.0329(13)	0.0381(13)	0.0554(17)	0.0084(12)	0.0076(12)	-0.0134(10)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C13A	0.0396(14)	0.0360(13)	0.0638(19)	-0.0186(13)	0.0126(13)	-0.0118(11)
C20A	0.0199(10)	0.0358(11)	0.0291(11)	-0.0015(9)	0.0041(8)	0.0051(8)
C21A	0.0236(10)	0.0277(10)	0.0336(12)	-0.0003(9)	0.0090(9)	0.0055(8)
C22A	0.0203(9)	0.0332(11)	0.0285(11)	-0.0023(9)	0.0082(8)	0.0030(8)
C23A	0.0194(9)	0.0341(11)	0.0361(12)	0.0023(9)	0.0118(8)	0.0009(8)
C24A	0.0177(9)	0.0322(11)	0.0417(13)	-0.0057(10)	0.0068(9)	-0.0024(8)
C25A	0.0409(14)	0.0584(17)	0.0327(14)	-0.0011(12)	0.0033(11)	0.0151(12)
C26A	0.0435(14)	0.0272(11)	0.0530(16)	0.0015(11)	0.0195(12)	0.0052(10)
C27A	0.0328(13)	0.0498(14)	0.0335(13)	-0.0081(11)	0.0089(10)	0.0023(11)
C28A	0.0377(14)	0.0434(14)	0.0496(16)	0.0109(12)	0.0214(12)	0.0015(11)
C29A	0.0302(13)	0.0457(15)	0.071(2)	-0.0180(14)	0.0106(13)	-0.0120(11)
C1B	0.0292(11)	0.0289(10)	0.0261(11)	-0.0027(8)	0.0104(9)	0.0047(8)
C2B	0.0223(10)	0.0296(10)	0.0480(14)	-0.0072(9)	0.0097(10)	0.0036(8)
C3B	0.0314(13)	0.0377(12)	0.0691(18)	0.0078(12)	0.0184(13)	0.0062(10)
C4B	0.0274(13)	0.0453(15)	0.106(2)	0.0194(16)	0.0141(16)	-0.0001(11)
C5B	0.0241(13)	0.0403(14)	0.116(3)	-0.0250(15)	0.0093(16)	-0.0002(11)
C6B	0.0320(14)	0.0518(16)	0.089(2)	-0.0341(15)	0.0119(15)	-0.0027(12)
C7B	0.0271(12)	0.0469(14)	0.0568(16)	-0.0223(12)	0.0092(11)	0.0002(10)
N1B	0.0260(9)	0.0272(9)	0.0361(11)	-0.0028(8)	0.0054(8)	0.0051(7)
C8B	0.0282(11)	0.0280(11)	0.0546(16)	-0.0037(10)	0.0024(11)	0.0060(9)
C9B	0.054(4)	0.079(5)	0.081(3)	-0.023(3)	-0.034(3)	0.023(3)
C10B	0.039(2)	0.056(3)	0.084(4)	-0.005(2)	0.025(2)	0.011(2)
C14B	0.0282(11)	0.0280(11)	0.0546(16)	-0.0037(10)	0.0024(11)	0.0060(9)
C15B	0.054(4)	0.079(5)	0.081(3)	-0.023(3)	-0.034(3)	0.023(3)
C16B	0.039(2)	0.056(3)	0.084(4)	-0.005(2)	0.025(2)	0.011(2)
N2B	0.0273(9)	0.0308(9)	0.0274(10)	-0.0003(7)	0.0056(8)	0.0055(7)
C11B	0.0266(11)	0.0342(11)	0.0351(13)	-0.0009(10)	0.0039(9)	0.0044(9)
C12B	0.0343(13)	0.0441(14)	0.0511(16)	-0.0026(12)	0.0163(12)	0.0009(11)
C13B	0.0385(15)	0.074(2)	0.0368(15)	-0.0003(14)	-0.0029(12)	0.0017(14)
C20B	0.0439(14)	0.0195(9)	0.0431(14)	0.0074(9)	0.0182(11)	0.0052(9)
C21B	0.0382(13)	0.0296(11)	0.0406(14)	0.0144(10)	0.0154(11)	0.0089(9)
C22B	0.0437(14)	0.0326(11)	0.0354(13)	0.0120(10)	0.0164(11)	0.0053(10)
C23B	0.0383(13)	0.0309(11)	0.0475(15)	0.0117(10)	0.0208(11)	0.0041(10)
C24B	0.0381(13)	0.0278(11)	0.0469(15)	0.0074(10)	0.0127(11)	-0.0024(9)
C25B	0.0655(19)	0.0251(11)	0.0562(18)	0.0000(11)	0.0265(15)	0.0052(11)
C26B	0.0434(15)	0.0521(16)	0.0566(18)	0.0255(14)	0.0159(13)	0.0174(13)
C27B	0.065(2)	0.0629(19)	0.0382(16)	0.0117(14)	0.0188(14)	0.0023(16)
C28B	0.0498(18)	0.0597(19)	0.074(2)	0.0155(16)	0.0386(17)	0.0065(14)
C29B	0.0493(17)	0.0444(15)	0.068(2)	0.0054(14)	0.0070(15)	-0.0141(13)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 1b.

	x/a	y/b	z/c	U(eq)
H3A	0.0431	0.7235	0.5206	0.047
H4A	-0.1416	0.7852	0.5030	0.062
H5A	-0.2588	0.7780	0.5671	0.063
H6A	-0.1936	0.7089	0.6481	0.069
H7A	-0.0105	0.6449	0.6663	0.054
H8A	0.1622	0.7910	0.6259	0.037
H9A1	0.2249	0.7469	0.7190	0.067
H9A2	0.2638	0.8402	0.7115	0.067
H9A3	0.3574	0.7671	0.7158	0.067
H10A	0.4042	0.8020	0.6237	0.085
H10B	0.3209	0.8803	0.6239	0.085
H10C	0.2989	0.8186	0.5730	0.085
H14A	0.1608	0.7857	0.6389	0.037
H15A	0.3204	0.7390	0.7135	0.067
H15B	0.2706	0.8313	0.7089	0.067
H15C	0.3878	0.8101	0.6880	0.067
H16A	0.3056	0.8791	0.6008	0.085
H16B	0.2225	0.8220	0.5572	0.085
H16C	0.3550	0.7951	0.5807	0.085
H11A	0.0062	0.5270	0.5789	0.036
H12A	0.1390	0.4270	0.6635	0.064
H12B	0.0011	0.4191	0.6408	0.064
H12C	0.0536	0.4999	0.6737	0.064
H13A	0.1767	0.4037	0.5699	0.069
H13B	0.1126	0.4605	0.5205	0.069
H13C	0.0391	0.3942	0.5469	0.069
H25A	0.6386	0.4938	0.7780	0.067
H25B	0.5087	0.4634	0.7788	0.067
H25C	0.5420	0.5590	0.7876	0.067
H26A	0.3863	0.3530	0.6498	0.06
H26B	0.4267	0.3686	0.7139	0.06
H26C	0.5206	0.3417	0.6789	0.06
H27A	0.4973	0.4226	0.5555	0.058
H27B	0.4071	0.4948	0.5327	0.058
H27C	0.3652	0.4176	0.5637	0.058
H28A	0.4401	0.6410	0.5507	0.05
H28B	0.5780	0.6254	0.5604	0.05
H28C	0.5279	0.6972	0.5931	0.05
H29A	0.5761	0.6830	0.7414	0.073
H29B	0.5786	0.7205	0.6826	0.073
H29C	0.6847	0.6646	0.7134	0.073
H3B	0.2354	0.8428	0.8158	0.054
H4B	0.2558	0.9866	0.8384	0.071

	x/a	y/b	z/c	U(eq)
H5B	0.2475	1.0290	0.9260	0.073
H6B	0.2268	0.9365	0.9926	0.069
H7B	0.2114	0.7966	0.9721	0.052
H8B	0.0206	0.7766	0.8325	0.045
H9B1	-0.0295	0.6226	0.7839	0.117
H9B2	-0.0519	0.7118	0.7563	0.117
H9B3	-0.1450	0.6732	0.7880	0.117
H10D	-0.1426	0.7487	0.8711	0.087
H10E	-0.0257	0.7452	0.9172	0.087
H10F	-0.0880	0.6614	0.8929	0.087
H14B	0.0133	0.7782	0.8493	0.045
H15D	0.0423	0.7329	0.7670	0.117
H15E	-0.0951	0.7335	0.7658	0.117
H15F	-0.0244	0.6483	0.7732	0.117
H16D	-0.1084	0.6264	0.8551	0.087
H16E	-0.1661	0.7163	0.8521	0.087
H16F	-0.0730	0.6889	0.9052	0.087
H11B	0.4206	0.7600	0.9039	0.039
H12D	0.5030	0.6030	0.8755	0.063
H12E	0.5772	0.6866	0.8806	0.063
H12F	0.4634	0.6766	0.8332	0.063
H13D	0.4276	0.7035	0.9914	0.077
H13E	0.5554	0.7007	0.9777	0.077
H13F	0.4778	0.6186	0.9731	0.077
H25D	0.2357	0.4164	0.7580	0.07
H25E	0.2228	0.3271	0.7834	0.07
H25F	0.3442	0.3758	0.7989	0.07
H26D	0.4576	0.4382	0.8727	0.075
H26E	0.4351	0.3717	0.9166	0.075
H26F	0.4561	0.4666	0.9337	0.075
H27D	0.3403	0.5115	0.9890	0.081
H27E	0.2394	0.4565	1.0056	0.081
H27F	0.2139	0.5505	0.9875	0.081
H28D	-0.0708	0.5005	0.8865	0.086
H28E	0.0103	0.5356	0.9410	0.086
H28F	-0.0243	0.4399	0.9367	0.086
H29D	-0.0261	0.3585	0.8034	0.082
H29E	0.0147	0.4215	0.7618	0.082
H29F	-0.0691	0.4525	0.8008	0.082

Table 9. Data collection details for 1b.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s
Omega	50.064	-31.50	-31.50	90.00	54.71	0.30	610	8.00
Omega	50.064	-31.50	-31.50	210.00	54.71	0.30	610	8.00
Omega	50.064	-31.50	-31.50	330.00	54.71	0.30	610	8.00
Phi	50.064	-31.50	-211.50	0.00	54.71	0.30	690	8.00

Table 10. Platon CheckCIF for 1b.

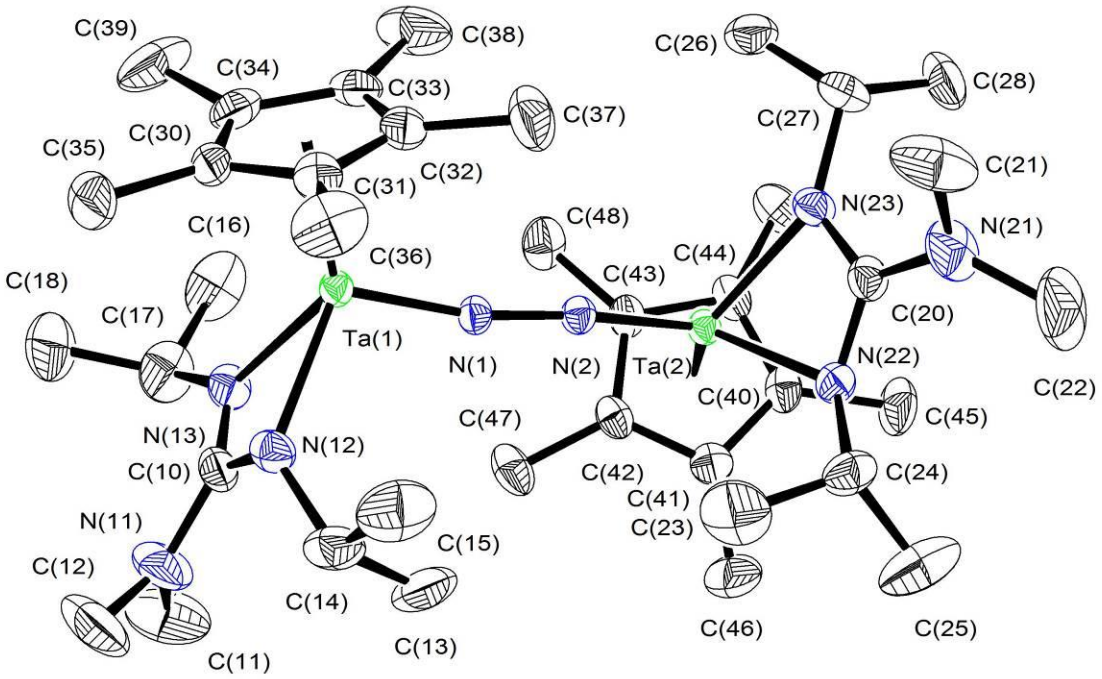
```
#===============================================================================
# PLATON/CHECK-(160910) versus check.def version of 160910  for entry: 2051
# Data From: 2051.cif - Data Type: CIF          Bond Precision   C-C = 0.0037 A
# Refl Data: 2051.fcf - Data Type: SHELXL                          Temp = 150 K
#
# UCL  11.6870(8) 16.2027(11) 25.0686(17)           90   101.826(1)          90
# WaveLength 0.71073    Volume Reported     4646.3(5)  Calculated     4646.3(5)
# SpaceGroup from Symmetry P 21/c        Hall: -P 2ybc
#                 Reported P21/c               -P 2ybc
# MoietyFormula C46 H68 N6 Ta2
#      Reported C46 H68 N6 Ta2
#    SumFormula C46 H68 N6 Ta2
#      Reported C46 H68 N6 Ta2
# Mr        =   1066.97[Calc],   1066.96[Rep]
# Dx,gcm-3  =     1.525[Calc],     1.525[Rep]
# Z         =         4[Calc],         4[Rep]
# Mu (mm-1) =     4.743[Calc],     4.743[Rep]
# F000      =    2128.0[Calc],    2128.0[Rep]  or F000' =   2123.10[Calc]
# Reported   T Limits: Tmin=0.149              Tmax=0.735  AbsCorr=INTEGRATION
# Calculated T Limits: Tmin=0.198 Tmin'=0.096  Tmax=0.735
# Reported   Hmax= 16, Kmax= 22, Lmax= 35, Nref= 13539        , Th(max)= 30.000
# Obs in FCF Hmax= 16, Kmax= 22, Lmax= 35, Nref= 13539        , Th(max)= 30.000
# Calculated Hmax= 16, Kmax= 22, Lmax= 35, Nref= 13548        , Ratio  =  0.999
# Reported   Rho(min) = -0.62, Rho(max) =  1.35 e/Ang**3 (From CIF)
# Calculated Rho(min) = -0.68, Rho(max) =  1.26 e/Ang**3 (From CIF+FCF data)
# w=1/[sigma**2(Fo**2)+(0.0100P)**2+  6.3900P], P=(Fo**2+2*Fc**2)/3
# R= 0.0206( 11810), wR2= 0.0419( 13539), S = 1.001      (From CIF+FCF data)
# R= 0.0206( 11810), wR2= 0.0419( 13539), S = 1.000      (From FCF data only)
# R= 0.0206( 11810), wR2= 0.0420( 13539), S = 1.002, Npar= 516
#===============================================================================

================================================================================
>>> The Following Model and Quality ALERTS were generated     - (Acta-Mode) <<<
================================================================================
094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.16
220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.41 Ratio
230_ALERT_2_C Hirshfeld Test Diff for    C3B    --  C4B     ..       6.33 su
230_ALERT_2_C Hirshfeld Test Diff for    C4B    --  C5B     ..       5.57 su
242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C8B
242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       C14B
910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) .....          3
#===============================================================================
083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       6.39
301_ALERT_3_G Note: Main Residue  Disorder ...................      10.00 Perc.
860_ALERT_3_G Note: Number of Least-Squares Restraints .......         45
#===============================================================================

================================================================================
>>> The Following Improvement and Query ALERTS were generated - (Acta-Mode) <<<
================================================================================
912_ALERT_4_C Missing # of FCF Reflections Above STh/L=  0.600          6
#===============================================================================
```

720_ALERT_4_G Number of Unusual/Non-Standard Labels 6
#==========

{Cp*Ta[N(iPr)C(NMe$_2$)N(iPr]}$_2$(μ-η^1:η^1-N$_2$) (1c)



A black prism of $C_{38}H_{70}N_8Ta_2$, approximate dimensions 0.105 × 0.13 × 0.20 mm^3, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 223(2) K on a three-circle diffractometer system equipped with Bruker Smart1000 CCD area detector using a graphite monochromator and a MoKα fine-focus sealed tube (λ= 0.71073 Å) operated at 50 kV and 30 mA. The detector was placed at a distance of 4.950 cm from the crystal.

A total of 2916 frames were collected with a scan width of 0.3° in ω and an exposure time of 38 sec/frame using SMART (Bruker, 1999). The total data collection time was 36.6 hours. The frames were integrated with SAINT software package using a narrow-frame integration algorithm. The integration of the data using a Monoclinic unit cell yielded a total of 34287 reflections to a maximum θ angle of 27.50°, of which 9992 were independent (completeness = 99.9%, R_{int} = 3.64%, R_{sig} = 3.21%) and 9375 were greater than 2σ(I). The final cell dimensions of *a* = 10.1527(12) Å, *b* = 16.0379(18) Å, *c* = 14.2362(16) Å, α= 90°, β= 110.774(2)°, γ= 90°, *V* = 2167.3(4) Å^3, are based upon the refinement of the XYZ-centroids of 6478 reflections with 2.1 < θ < 28.5° using SAINT. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.432 and 0.587.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick,

1997) software in the space group $P2_1$ with $Z = 2$ for the formula unit $C_{38}H_{70}N_8Ta_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 457 variables converged at $R_1 = 2.77$ % for the observed data and $wR_2 = 6.55$ % for all data. The goodness-of-fit was 1.000. The largest peak on the final difference map was 2.058 $\bar{e}/Å^3$ and the largest hole was -0.718 $\bar{e}/Å^3$. On the basis of the final model, the calculated density was 1.534 g/cm^3 and F(000), 1000 $\bar{e}$.

Overall structure quality considerations:

1. **Strong data set, no disorder, R_1 4% maximum. Publishable quality.**
2. Good data set, perhaps some minor disorder, R_1 6% maximum. Publishable quality.
3. Average data set and/or easily modeled disorder or twinning. Publishable with care.
4. Weak data and/or major disorder or twinning that is not easily modeled. Publishable in some cases.
5. Very weak data and/or unexplained features of data or model. Not of publishable quality.

A structure with a quality factor of 4 or 5 should not be used for a regulatory document without prior consultation.

Comments:

- Data quality: very good
- Twinning: none
- Disorder: none (not counting stacking fault disorder at the 1 e level)
- H-atoms: constrained geometry as riding on attached atom (A)
  Uiso(H)=1.5*U_{iso}(A) for CH_3 and 1.2*U_{iso}(A) for other groups
- Residual density: near heavy atoms & near disordered groups
- Structure quality: very good
  Publishable Yes

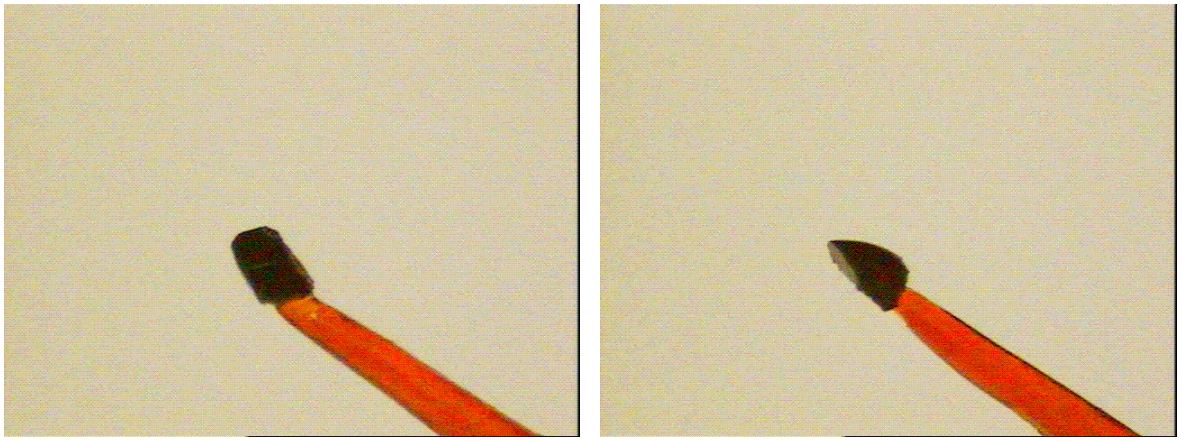


Table 1. Crystal data and structure refinement for **1c**.

X-ray lab book No.		**1c**
Crystal ID		**1c**
Empirical formula		C38 H70 N8 Ta2
Formula weight		1000.92
Temperature		223(2) K
Wavelength		0.71073 Å
Crystal size		0.20 × 0.13 × 0.105 mm^3
Crystal habit		black prism
Crystal system		Monoclinic
Space group		$P2_1$
Unit cell dimensions		a = 10.1527(12) Å α = 90°
		b = 16.0379(18) Å β = 110.774(2)°
		c = 14.2362(16) Å γ = 90°
Volume		2167.3(4) $Å^3$
Z		2
Density, ρ_{calc}		1.534 g/cm^3
Absorption coefficient, μ		5.079 mm^{-1}
F(000)		1000 $\bar{e}$
Diffractometer		Bruker Smart1000 CCD area detector
Radiation source		fine-focus sealed tube, MoKα
Generator power		50 kV, 30 mA
Detector distance		4.950 cm
Detector resolution		8.33 pixels/mm
Total frames		2916
Frame size		512 pixels
Frame width		0.3 °
Exposure per frame		38 sec
Total measurement time		36.6 hours
Data collection method		ω scans
θ range for data collection		2.15 to 27.50°
Index ranges		$-12 \le h \le 13$, $-20 \le k \le 20$, $-18 \le l \le 18$
Reflections collected		34287
Independent reflections		9992
Observed reflection, I>2σ(I)		9375
Coverage of independent reflections		99.9 %
Variation in check reflections		0 %
Absorption correction		Semi-empirical from equivalents
		SADABS (Sheldrick, 1996)
Max. and min. transmission		0.587 and 0.432
Structure solution technique		direct
Structure solution program		SHELXS-97 (Sheldrick, 1990)
Refinement technique		Full-matrix least-squares on F^2
Refinement program		SHELXL-97 (Sheldrick, 1997)
Function minimized		$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters		9992 / 1 / 457
Goodness-of-fit on F^2		1.000
Δ/σ_{max}		0.001
Final R indices:	R_1, I>2σ(I)	0.0277
	wR_2, all data	0.0655
	R_{int}	0.0364
	R_{sig}	0.0321
Weighting scheme		$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 5.965P]$,
		$P = [\max(F_o^2, 0) + 2F_o^2]/3$
Absolute structure parameter		0.017(11)
Largest diff. peak and hole		2.058 and -0.718 $\bar{e}/Å^3$

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table 2. Atomic coordinates and equivalent* isotropic atomic displacement parameters (Å^2) for **1c**.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Ta1	0.30228(2)	0.503405(14)	0.863637(14)	0.03280(5)
Ta2	0.28318(2)	0.598660(13)	0.532029(15)	0.03307(5)
N1	0.2829(5)	0.5434(3)	0.7404(3)	0.0355(10)
N2	0.2752(5)	0.5550(3)	0.6478(3)	0.0354(10)
N11	0.1015(10)	0.6602(4)	0.9871(7)	0.085(2)
N12	0.1105(6)	0.5408(3)	0.8901(4)	0.0481(13)
N13	0.3087(7)	0.6113(3)	0.9600(4)	0.0523(14)
C10	0.1740(8)	0.6059(5)	0.9483(5)	0.0536(16)
C11	0.1227(15)	0.7495(6)	0.9909(12)	0.132(5)
C12	-0.0075(14)	0.6295(7)	1.0234(10)	0.123(5)
C13	-0.0368(9)	0.6198(7)	0.7419(8)	0.093(3)
C14	-0.0330(8)	0.5518(6)	0.8178(7)	0.070(2)
C15	-0.0851(10)	0.4714(7)	0.7602(9)	0.103(4)
C16	0.5489(11)	0.6625(6)	1.0125(8)	0.099(4)
C17	0.4142(12)	0.6629(6)	1.0354(7)	0.086(3)
C18	0.4407(13)	0.6314(8)	1.1411(7)	0.116(4)
N21	0.1230(8)	0.4207(5)	0.3233(6)	0.079(2)
N22	0.1050(5)	0.5501(3)	0.4045(4)	0.0436(11)
N23	0.3149(6)	0.4909(3)	0.4475(4)	0.0448(12)
C20	0.1816(7)	0.4861(4)	0.3903(5)	0.0469(14)
C21	0.1452(11)	0.3355(6)	0.3541(10)	0.107(4)
C22	0.0316(13)	0.4375(9)	0.2216(8)	0.127(5)
C23	-0.0776(10)	0.5426(8)	0.4769(9)	0.105(4)
C24	-0.0472(7)	0.5396(5)	0.3823(6)	0.0599(18)
C25	-0.1313(10)	0.6016(9)	0.3065(9)	0.124(4)
C26	0.5583(8)	0.4469(5)	0.5296(6)	0.066(2)
C27	0.4276(8)	0.4393(5)	0.4362(6)	0.0579(18)
C28	0.4588(11)	0.4626(7)	0.3435(6)	0.091(3)
C30	0.3545(9)	0.3806(4)	0.9729(5)	0.0490(17)
C31	0.2771(9)	0.3554(4)	0.8736(5)	0.0522(17)
C32	0.3553(9)	0.3680(4)	0.8144(5)	0.0542(17)
C33	0.4837(8)	0.4032(4)	0.8720(6)	0.0559(18)
C34	0.4856(8)	0.4114(5)	0.9746(6)	0.0601(18)
C35	0.3092(12)	0.3722(6)	1.0614(7)	0.081(3)
C36	0.1354(10)	0.3084(6)	0.8432(8)	0.088(3)
C37	0.3125(14)	0.3459(6)	0.7030(6)	0.089(3)
C38	0.6039(11)	0.4256(7)	0.8377(10)	0.108(4)
C39	0.6113(11)	0.4322(7)	1.0655(8)	0.111(4)
C40	0.3178(9)	0.7242(4)	0.4477(5)	0.0494(16)
C41	0.2360(8)	0.7457(4)	0.5069(5)	0.0492(15)
C42	0.3235(7)	0.7349(4)	0.6086(5)	0.0447(14)
C43	0.4554(7)	0.7046(4)	0.6128(4)	0.0436(13)
C44	0.4546(8)	0.6982(4)	0.5123(5)	0.0477(15)
C45	0.2679(12)	0.7299(6)	0.3331(6)	0.078(3)
C46	0.0934(11)	0.7859(6)	0.4696(8)	0.087(3)
C47	0.2834(10)	0.7543(5)	0.6991(6)	0.064(2)
C48	0.5768(8)	0.6841(6)	0.7071(6)	0.069(2)
C49	0.5766(9)	0.6789(5)	0.4797(7)	0.068(2)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic atomic displacement parameters * ($Å^2$) for **1c**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.03862(11)	0.03024(10)	0.03019(10)	0.00144(8)	0.01301(8)	0.00176(9)
Ta2	0.03857(11)	0.03094(10)	0.03052(10)	0.00144(8)	0.01327(8)	0.00024(9)
N1	0.042(3)	0.034(2)	0.030(2)	-0.0015(18)	0.012(2)	-0.0004(19)
N2	0.039(3)	0.035(2)	0.033(2)	0.0019(19)	0.014(2)	-0.0011(19)
N11	0.112(6)	0.057(4)	0.107(6)	-0.006(4)	0.066(5)	0.028(4)
N12	0.050(3)	0.046(3)	0.057(3)	0.008(2)	0.030(3)	0.003(2)
N13	0.074(4)	0.032(3)	0.048(3)	-0.011(2)	0.019(3)	0.002(3)
C10	0.077(5)	0.047(4)	0.047(3)	0.007(3)	0.035(3)	0.014(4)
C11	0.149(12)	0.058(6)	0.206(15)	-0.019(7)	0.083(11)	0.030(7)
C12	0.160(11)	0.116(9)	0.154(11)	0.016(8)	0.130(10)	0.038(8)
C13	0.054(5)	0.119(9)	0.100(7)	0.043(6)	0.018(5)	0.035(5)
C14	0.043(4)	0.080(5)	0.092(6)	0.010(5)	0.029(4)	0.010(4)
C15	0.054(5)	0.107(8)	0.129(9)	-0.009(7)	0.010(6)	-0.010(5)
C16	0.092(7)	0.086(7)	0.092(7)	-0.005(5)	0.000(6)	-0.046(6)
C17	0.113(8)	0.055(5)	0.073(6)	-0.025(4)	0.014(6)	-0.014(5)
C18	0.121(9)	0.156(12)	0.050(5)	-0.036(6)	0.007(5)	0.003(8)
N21	0.078(5)	0.073(5)	0.077(5)	-0.040(4)	0.018(4)	-0.021(4)
N22	0.037(3)	0.050(3)	0.040(2)	-0.003(2)	0.010(2)	-0.001(2)
N23	0.047(3)	0.039(3)	0.049(3)	-0.007(2)	0.018(2)	0.003(2)
C20	0.054(4)	0.043(4)	0.042(3)	-0.006(2)	0.015(3)	-0.003(3)
C21	0.080(7)	0.057(5)	0.188(13)	-0.043(6)	0.053(8)	-0.014(5)
C22	0.111(9)	0.178(13)	0.076(7)	-0.069(8)	0.013(6)	-0.035(9)
C23	0.053(5)	0.146(10)	0.124(9)	-0.011(8)	0.041(6)	-0.023(6)
C24	0.038(4)	0.061(4)	0.069(5)	-0.002(3)	0.004(3)	-0.001(3)
C25	0.064(6)	0.122(9)	0.146(10)	0.030(9)	-0.012(6)	0.013(7)
C26	0.053(4)	0.075(5)	0.077(5)	0.015(4)	0.029(4)	0.020(4)
C27	0.051(4)	0.051(4)	0.079(5)	-0.016(3)	0.031(4)	0.004(3)
C28	0.092(7)	0.131(9)	0.060(5)	-0.026(5)	0.041(5)	0.012(6)
C30	0.074(5)	0.035(3)	0.043(3)	0.011(3)	0.028(3)	0.014(3)
C31	0.074(5)	0.027(3)	0.056(4)	0.002(3)	0.024(4)	0.001(3)
C32	0.076(5)	0.035(3)	0.053(4)	-0.001(3)	0.024(4)	0.013(3)
C33	0.056(4)	0.046(3)	0.078(5)	0.020(3)	0.040(4)	0.018(3)
C34	0.059(4)	0.047(4)	0.058(4)	0.005(3)	0.002(3)	0.015(3)
C35	0.129(9)	0.063(5)	0.072(5)	0.029(5)	0.062(6)	0.024(5)
C36	0.083(6)	0.054(5)	0.118(8)	0.004(5)	0.024(6)	-0.019(4)
C37	0.163(11)	0.055(5)	0.058(5)	-0.004(4)	0.052(6)	0.013(6)
C38	0.092(7)	0.100(8)	0.167(11)	0.037(8)	0.090(8)	0.029(6)
C39	0.094(7)	0.078(6)	0.102(8)	-0.003(6)	-0.037(6)	0.021(6)
C40	0.073(5)	0.037(3)	0.041(3)	0.004(2)	0.023(3)	-0.008(3)
C41	0.067(4)	0.027(3)	0.055(4)	0.005(3)	0.023(3)	0.003(3)
C42	0.060(4)	0.034(3)	0.047(3)	-0.007(2)	0.027(3)	-0.008(3)
C43	0.045(3)	0.045(3)	0.040(3)	-0.006(2)	0.014(3)	-0.012(3)
C44	0.061(4)	0.041(3)	0.051(3)	-0.005(3)	0.031(3)	-0.014(3)
C45	0.121(8)	0.068(5)	0.041(4)	0.016(4)	0.025(5)	0.004(5)
C46	0.088(7)	0.069(6)	0.093(7)	0.014(5)	0.020(5)	0.034(5)
C47	0.099(6)	0.045(4)	0.064(5)	-0.014(3)	0.046(5)	-0.005(4)
C48	0.052(4)	0.094(6)	0.057(4)	-0.010(4)	0.015(4)	-0.020(4)
C49	0.069(5)	0.069(5)	0.085(5)	-0.006(4)	0.051(5)	-0.014(4)

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table 4. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å^2) for **1c**.

Atom	*x/a*	*y/b*	*z/c*	U_{iso}
H11A	0.1786	0.7644	0.9506	0.198
H11B	0.1715	0.7666	1.0599	0.198
H11C	0.0321	0.7773	0.9647	0.198
H12A	0.0083	0.6521	1.0897	0.185
H12B	-0.0037	0.5691	1.0268	0.185
H12C	-0.0993	0.6470	0.9776	0.185
H13A	-0.0254	0.6739	0.7743	0.140
H13B	-0.1264	0.6179	0.6866	0.140
H13C	0.0390	0.6108	0.7165	0.140
H14	-0.0962	0.5674	0.8542	0.085
H15A	-0.1799	0.4795	0.7125	0.154
H15B	-0.0855	0.4274	0.8068	0.154
H15C	-0.0232	0.4560	0.7245	0.154
H16A	0.6194	0.6963	1.0618	0.148
H16B	0.5305	0.6852	0.9460	0.148
H16C	0.5830	0.6058	1.0152	0.148
H17	0.3786	0.7209	1.0300	0.103
H18A	0.4703	0.5736	1.1462	0.173
H18B	0.3547	0.6359	1.1558	0.173
H18C	0.5139	0.6647	1.1889	0.173
H21A	0.0582	0.3046	0.3239	0.160
H21B	0.1745	0.3323	0.4267	0.160
H21C	0.2178	0.3118	0.3328	0.160
H22A	0.0275	0.4971	0.2096	0.191
H22B	-0.0622	0.4167	0.2115	0.191
H22C	0.0680	0.4099	0.1752	0.191
H23A	-0.0585	0.5982	0.5054	0.157
H23B	-0.0183	0.5026	0.5244	0.157
H23C	-0.1758	0.5289	0.4628	0.157
H24	-0.0736	0.4834	0.3529	0.072
H25A	-0.1247	0.6558	0.3382	0.186
H25B	-0.2290	0.5841	0.2799	0.186
H25C	-0.0947	0.6052	0.2523	0.186
H26A	0.5883	0.5047	0.5391	0.099
H26B	0.6329	0.4129	0.5222	0.099
H26C	0.5373	0.4281	0.5875	0.099
H27	0.3963	0.3805	0.4295	0.069
H28A	0.3766	0.4515	0.2842	0.136
H28B	0.5377	0.4299	0.3408	0.136
H28C	0.4822	0.5214	0.3460	0.136
H35A	0.3802	0.3963	1.1201	0.121
H35B	0.2974	0.3136	1.0736	0.121
H35C	0.2205	0.4011	1.0480	0.121
H36A	0.1530	0.2495	0.8584	0.132
H36B	0.0845	0.3153	0.7718	0.132
H36C	0.0796	0.3306	0.8804	0.132
H37A	0.3662	0.2980	0.6955	0.133
H37B	0.3313	0.3930	0.6668	0.133
H37C	0.2128	0.3328	0.6760	0.133
H38A	0.5686	0.4590	0.7770	0.161
H38B	0.6463	0.3750	0.8240	0.161
H38C	0.6740	0.4572	0.8899	0.161

H39A	0.6617	0.3815	1.0938	0.166
H39B	0.5806	0.4594	1.1151	0.166
H39C	0.6731	0.4694	1.0466	0.166
H45A	0.1887	0.6927	0.3037	0.117
H45B	0.3442	0.7140	0.3107	0.117
H45C	0.2393	0.7867	0.3122	0.117
H46A	0.0388	0.7661	0.5089	0.130
H46B	0.0453	0.7716	0.3995	0.130
H46C	0.1039	0.8459	0.4763	0.130
H47A	0.3006	0.8129	0.7161	0.096
H47B	0.3396	0.7205	0.7556	0.096
H47C	0.1844	0.7420	0.6835	0.096
H48A	0.6457	0.6513	0.6902	0.103
H48B	0.5430	0.6523	0.7520	0.103
H48C	0.6202	0.7353	0.7399	0.103
H49A	0.6139	0.7304	0.4634	0.102
H49B	0.5453	0.6432	0.4210	0.102
H49C	0.6497	0.6508	0.5338	0.102

Table 5. Bond lengths (Å) and angles (°) for **1c**.

Ta1-N1	1.812(5)	Ta1-N12	2.194(6)	Ta1-N13	2.194(5)
Ta1-C31	2.396(6)	Ta1-C32	2.401(6)	Ta1-C33	2.415(6)
Ta1-C30	2.449(6)	Ta1-C34	2.460(7)	Ta2-N2	1.819(5)
Ta2-N23	2.194(5)	Ta2-N22	2.201(5)	Ta2-C41	2.408(6)
Ta2-C42	2.411(6)	Ta2-C43	2.416(6)	Ta2-C40	2.432(6)
Ta2-C44	2.450(6)	N1-N2	1.306(5)	N11-C10	1.376(9)
N11-C11	1.446(13)	N11-C12	1.462(13)	N12-C10	1.347(9)
N12-C14	1.466(10)	N13-C10	1.320(9)	N13-C17	1.474(10)
C13-C14	1.527(12)	C14-C15	1.518(13)	C17-C18	1.519(14)
N21-C20	1.401(8)	N21-C21	1.427(13)	N21-C22	1.442(13)
N22-C20	1.346(8)	N22-C24	1.473(8)	N23-C20	1.311(8)
N23-C27	1.466(8)	C23-C24	1.486(13)	C24-C25	1.492(12)
C26-C27	1.515(11)	C27-C28	1.508(11)	C30-C31	1.411(10)
C30-C34	1.412(11)	C30-C35	1.493(10)	C31-C32	1.362(11)
C31-C36	1.545(12)	C32-C33	1.391(11)	C32-C37	1.530(10)
C33-C34	1.459(11)	C33-C38	1.510(11)	C34-C39	1.498(11)
C40-C41	1.419(10)	C40-C44	1.428(11)	C40-C45	1.530(10)
C41-C42	1.416(10)	C41-C46	1.499(11)	C42-C43	1.405(9)
C42-C47	1.514(9)	C43-C44	1.432(8)	C43-C48	1.502(10)
C44-C49	1.502(10)				

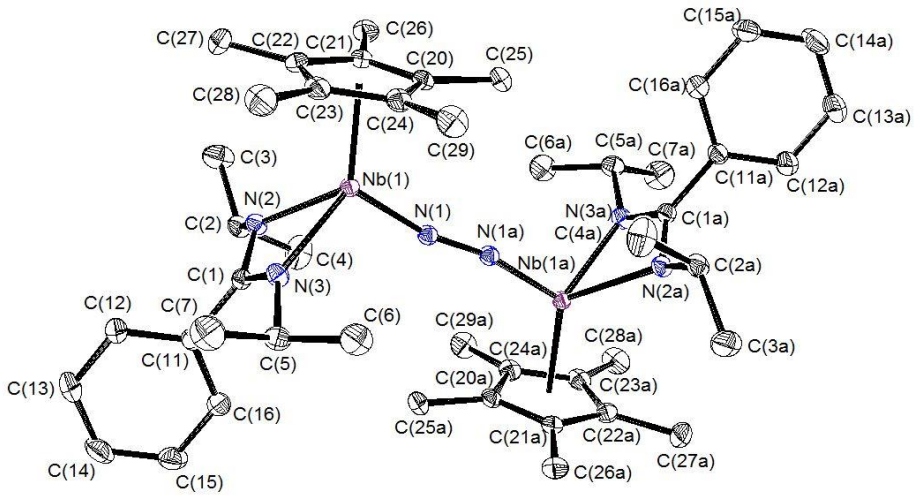
N1-Ta1-N12	105.8(2)	N1-Ta1-N13	107.2(2)	N12-Ta1-N13	60.6(2)
N2-Ta2-N23	104.8(2)	N2-Ta2-N22	108.9(2)	N23-Ta2-N22	60.4(2)
N2-N1-Ta1	167.2(4)	N1-N2-Ta2	164.5(4)	C10-N11-C11	123.2(9)
C10-N11-C12	120.5(8)	C11-N11-C12	116.2(9)	C10-N12-C14	118.6(6)
C10-N12-Ta1	93.3(4)	C14-N12-Ta1	129.3(5)	C10-N13-C17	125.5(7)
C10-N13-Ta1	94.0(4)	C17-N13-Ta1	138.7(6)	N13-C10-N12	112.1(6)
N13-C10-N11	125.9(8)	N12-C10-N11	122.0(7)	N12-C14-C15	110.3(7)
N12-C14-C13	110.6(7)	C15-C14-C13	107.9(8)	N13-C17-C16	108.7(8)
N13-C17-C18	111.2(8)	C16-C17-C18	110.8(9)	C20-N21-C21	121.7(8)
C20-N21-C22	120.7(8)	C21-N21-C22	117.6(9)	C20-N22-C24	119.9(6)
C20-N22-Ta2	92.5(4)	C24-N22-Ta2	135.3(4)	C20-N23-C27	124.9(6)
C20-N23-Ta2	93.8(4)	C27-N23-Ta2	141.0(5)	N23-C20-N22	112.7(5)
N23-C20-N21	124.2(6)	N22-C20-N21	123.1(6)	N22-C24-C23	110.0(6)
N22-C24-C25	111.5(7)	C23-C24-C25	112.6(9)	N23-C27-C28	111.8(7)
N23-C27-C26	109.4(6)	C28-C27-C26	111.0(7)	C31-C30-C34	107.7(6)
C31-C30-C35	126.2(8)	C34-C30-C35	126.0(8)	C32-C31-C30	109.8(7)
C32-C31-C36	126.0(7)	C30-C31-C36	123.6(8)	C31-C32-C33	108.9(6)

C31-C32-C37	126.4(8)	C33-C32-C37	124.6(8)	C32-C33-C34	107.7(6)
C32-C33-C38	127.0(8)	C34-C33-C38	125.3(9)	C30-C34-C33	105.9(6)
C30-C34-C39	127.0(9)	C33-C34-C39	126.1(9)	C41-C40-C44	109.2(6)
C41-C40-C45	125.2(8)	C44-C40-C45	125.6(7)	C42-C41-C40	106.9(6)
C42-C41-C46	126.3(7)	C40-C41-C46	126.1(7)	C43-C42-C41	109.2(6)
C43-C42-C47	125.0(6)	C41-C42-C47	125.8(7)	C42-C43-C44	108.3(6)
C42-C43-C48	125.6(6)	C44-C43-C48	126.1(6)	C40-C44-C43	106.4(6)
C40-C44-C49	125.6(6)	C43-C44-C49	127.6(7)		

Table 6. Torsion angles (°) for **1c**.

N12-Ta1-N1-N2	-127.6(19)	N13-Ta1-N1-N2	169.0(19)	C31-Ta1-N1-N2	-20(2)
C32-Ta1-N1-N2	1.0(19)	C33-Ta1-N1-N2	34.1(19)	C30-Ta1-N1-N2	1(2)
C34-Ta1-N1-N2	45(2)	Ta1-N1-N2-Ta2	-146.8(13)	N23-Ta2-N2-N1	151.4(15)
N22-Ta2-N2-N1	-145.3(15)	C41-Ta2-N2-N1	-34.3(16)	C42-Ta2-N2-N1	-11.9(15)
C43-Ta2-N2-N1	21.4(15)	C40-Ta2-N2-N1	-10.8(18)	C44-Ta2-N2-N1	33.1(16)
N1-Ta1-N12-C10	-100.2(4)	N13-Ta1-N12-C10	0.9(4)	C31-Ta1-N12-C10	140.4(4)
C32-Ta1-N12-C10	157.9(4)	C33-Ta1-N12-C10	121.2(6)	C30-Ta1-N12-C10	106.2(4)
C34-Ta1-N12-C10	86.4(4)	N1-Ta1-N12-C14	31.7(7)	N13-Ta1-N12-C14	132.8(7)
C31-Ta1-N12-C14	-87.8(6)	C32-Ta1-N12-C14	-70.3(7)	C33-Ta1-N12-C14	-106.9(8)
C30-Ta1-N12-C14	-121.9(6)	C34-Ta1-N12-C14	-141.7(6)	N1-Ta1-N13-C10	97.8(4)
N12-Ta1-N13-C10	-1.0(4)	C31-Ta1-N13-C10	-70.0(5)	C32-Ta1-N13-C10	-118.5(7)
C33-Ta1-N13-C10	-148.8(4)	C30-Ta1-N13-C10	-89.3(4)	C34-Ta1-N13-C10	-123.7(4)
N1-Ta1-N13-C17	-97.8(8)	N12-Ta1-N13-C17	163.5(9)	C31-Ta1-N13-C17	94.4(9)
C32-Ta1-N13-C17	46.0(12)	C33-Ta1-N13-C17	15.6(9)	C30-Ta1-N13-C17	75.1(9)
C34-Ta1-N13-C17	40.7(9)	C17-N13-C10-N12	-166.0(7)	Ta1-N13-C10-N12	1.5(6)
C17-N13-C10-N11	15.8(12)	Ta1-N13-C10-N11	-176.8(7)	C14-N12-C10-N13	-140.5(7)
Ta1-N12-C10-N13	-1.5(6)	C14-N12-C10-N11	37.8(10)	Ta1-N12-C10-N11	176.8(6)
C11-N11-C10-N13	39.4(15)	C12-N11-C10-N13	-143.3(10)	C11-N11-C10-N12	-138.6(11)
C12-N11-C10-N12	38.7(13)	C10-N12-C14-C15	-179.9(7)	Ta1-N12-C14-C15	58.0(10)
C10-N12-C14-C13	60.8(9)	Ta1-N12-C14-C13	-61.3(10)	C10-N13-C17-C16	-170.7(7)
Ta1-N13-C17-C16	28.5(12)	C10-N13-C17-C18	67.0(11)	Ta1-N13-C17-C18	-93.8(11)
N2-Ta2-N22-C20	-92.5(4)	N23-Ta2-N22-C20	4.2(4)	N2-Ta2-N22-C24	46.3(7)
N23-Ta2-N22-C24	143.1(7)	N2-Ta2-N23-C20	99.3(4)	N22-Ta2-N23-C20	-4.3(4)
N2-Ta2-N23-C27	-87.2(8)	N22-Ta2-N23-C27	169.2(8)	C27-N23-C20-N22	-168.4(6)
Ta2-N23-C20-N22	6.6(6)	C27-N23-C20-N21	13.3(11)	Ta2-N23-C20-N21	-171.7(7)
C24-N22-C20-N23	-154.3(6)	Ta2-N22-C20-N23	-6.6(6)	C24-N22-C20-N21	24.0(10)
Ta2-N22-C20-N21	171.7(6)	C21-N21-C20-N23	50.7(12)	C22-N21-C20-N23	-132.6(9)
C21-N21-C20-N22	-127.4(9)	C22-N21-C20-N22	49.3(12)	C20-N22-C24-C23	112.2(8)
Ta2-N22-C24-C23	-18.5(11)	C20-N22-C24-C25	-122.2(9)	Ta2-N22-C24-C25	107.1(9)
C20-N23-C27-C28	70.8(9)	Ta2-N23-C27-C28	-101.2(9)	C20-N23-C27-C26	-165.8(6)
Ta2-N23-C27-C26	22.1(11)	C34-C30-C31-C32	1.0(8)	C35-C30-C31-C32	-176.2(7)
C34-C30-C31-C36	172.3(7)	C35-C30-C31-C36	-4.9(11)	C30-C31-C32-C33	-1.4(8)
C36-C31-C32-C33	-172.3(7)	C30-C31-C32-C37	177.5(7)	C36-C31-C32-C37	6.5(12)
C31-C32-C33-C34	1.1(8)	C37-C32-C33-C34	-177.7(7)	C31-C32-C33-C38	178.5(8)
C37-C32-C33-C38	-0.4(12)	C31-C30-C34-C33	-0.3(7)	C35-C30-C34-C33	176.9(6)
C31-C30-C34-C39	-169.4(7)	C35-C30-C34-C39	7.8(12)	C32-C33-C34-C30	-0.5(7)
C38-C33-C34-C30	-177.9(7)	C32-C33-C34-C39	168.7(7)	C38-C33-C34-C39	-8.7(12)
C44-C40-C41-C42	1.3(7)	C45-C40-C41-C42	-177.4(7)	C44-C40-C41-C46	171.9(7)
C45-C40-C41-C46	-6.7(12)	C40-C41-C42-C43	-2.0(7)	C46-C41-C42-C43	-172.6(7)
C40-C41-C42-C47	177.0(6)	C46-C41-C42-C47	6.4(11)	C41-C42-C43-C44	1.9(7)
C47-C42-C43-C44	-177.1(6)	C41-C42-C43-C48	-179.2(6)	C47-C42-C43-C48	1.8(10)
C41-C40-C44-C43	-0.2(7)	C45-C40-C44-C43	178.5(7)	C41-C40-C44-C49	-173.3(6)
C45-C40-C44-C49	5.4(11)				

{Cp*Nb[N(iPr)C(Ph)N(iPr)]$_2$(μ-η^1:η^1-N$_2$) (2b)



A black prism-like specimen of $C_{46}H_{68}N_6Nb_2$, approximate dimensions 0.06 mm × 0.09 mm × 0.21 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 20.33 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 18628 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 6695 were independent (average redundancy 2.782, completeness = 98.6%, R_{int} = 2.72%) and 5436 (81.19%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.7368(5) Å, b = 20.4387(10) Å, c = 12.3870(6) Å, β = 109.4510(10)°, V = 2324.4(2) Å^3, are based upon the refinement of the XYZ-centroids of 6448 reflections above 20 σ(I) with 4.863° < 2θ < 62.20°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8680 and 0.9690.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 21/n, with Z = 2 for the formula unit, $C_{46}H_{68}N_6Nb_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 254 variables converged at R_1 = 3.11%, for the observed data and wR_2 = 6.20% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.795 e$^-$/Å^3 and the largest hole was -0.427 e$^-$/Å^3 with an RMS deviation of 0.064 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.273 g/cm^3 and F(000), 936 e$^-$.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 2b.

Identification code	**2b**	
Chemical formula	$C_{46}H_{68}N_6Nb_2$	
Formula weight	890.88	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.06 × 0.09 × 0.21 mm	
Crystal habit	black prism	
Crystal system	monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.7368(5) Å	α = 90°
	b = 20.4387(10) Å	β = 109.4510(10)°
	c = 12.3870(6) Å	γ = 90°
Volume	2324.4(2) $Å^3$	
Z	2	
Density (calculated)	1.273 Mg/cm^3	
Absorption coefficient	0.529 mm^{-1}	
F(000)	936	

Table 2. Data collection and structure refinement for 2b.

Diffractometer	Bruker APEX-II CCD
Radiation source	sealed tube, MoKα
Theta range for data collection	2.32 to 30.00°
Index ranges	$-12 \leq h \leq 13$, $-28 \leq k \leq 28$, $-17 \leq l \leq 17$
Reflections collected	18628
Independent reflections	6695 [R(int) = 0.0272]
Coverage of independent reflections	98.6%
Absorption correction	multi-scan
Max. and min. transmission	0.9690 and 0.8680
Structure solution technique	direct methods
Structure solution program	ShelXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	ShelXL-2012 (Sheldrick, 2012)

Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6695 / 0 / 254	
Goodness-of-fit on F^2	1.000	
Final R indices	5436 data; $I>2\sigma(I)$	$R_1 = 0.0311$, $wR_2 = 0.0580$
	all data	$R_1 = 0.0434$, $wR_2 = 0.0620$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0100P)^2+2.0470P]$, $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.795 and -0.427 eÅ^{-3}	
R.M.S. deviation from mean	0.064 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 2b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Nb1	0.85335(2)	0.06005(2)	0.82805(2)	0.02164(4)
N1	0.96992(16)	0.01939(7)	0.95701(12)	0.0242(3)
C1	0.00453(19)	0.16228(9)	0.80398(15)	0.0255(4)
N2	0.89909(16)	0.16623(7)	0.84986(13)	0.0270(3)
C2	0.8965(2)	0.21731(9)	0.93221(17)	0.0317(4)
C3	0.7409(2)	0.23762(12)	0.9134(2)	0.0519(6)
C4	0.9693(3)	0.19214(12)	0.05348(19)	0.0545(7)
N3	0.00541(17)	0.10509(8)	0.75243(13)	0.0274(3)
C5	0.1217(2)	0.08617(10)	0.70777(17)	0.0326(4)
C6	0.1411(3)	0.01238(11)	0.7174(2)	0.0487(6)
C7	0.0887(3)	0.10883(14)	0.5850(2)	0.0562(7)
C11	0.1122(2)	0.21595(9)	0.81083(16)	0.0281(4)
C12	0.0721(3)	0.26907(11)	0.7371(2)	0.0459(6)
C13	0.1724(3)	0.31806(13)	0.7409(2)	0.0587(7)

	x/a	y/b	z/c	U(eq)
C14	0.3119(3)	0.31469(12)	0.8175(2)	0.0514(6)
C15	0.3519(2)	0.26251(11)	0.8909(2)	0.0450(5)
C16	0.2530(2)	0.21321(10)	0.88800(18)	0.0356(4)
C20	0.66570(19)	0.98133(9)	0.80872(16)	0.0280(4)
C21	0.60001(19)	0.04390(9)	0.80493(16)	0.0289(4)
C22	0.5979(2)	0.07490(10)	0.70082(17)	0.0331(4)
C23	0.6647(2)	0.03232(10)	0.64322(16)	0.0337(4)
C24	0.7077(2)	0.97426(10)	0.71002(16)	0.0313(4)
C25	0.6818(2)	0.93008(10)	0.89951(18)	0.0364(5)
C26	0.5305(2)	0.06807(11)	0.88921(19)	0.0397(5)
C27	0.5330(2)	0.14048(11)	0.6570(2)	0.0460(6)
C28	0.6827(3)	0.04536(13)	0.52856(17)	0.0496(6)
C29	0.7687(3)	0.91285(11)	0.6765(2)	0.0449(5)

Table 4. Bond lengths (Å) for 2b.

Nb1-N1	1.8230(14)	Nb1-N3	2.2001(15)
Nb1-N2	2.2138(15)	Nb1-C20	2.3861(18)
Nb1-C21	2.4094(18)	Nb1-C24	2.4170(18)
Nb1-C23	2.4773(18)	Nb1-C22	2.4803(18)
N1-N1	1.300(3)	C1-N2	1.331(2)
C1-N3	1.333(2)	C1-C11	1.500(3)
N2-C2	1.466(2)	C2-C3	1.512(3)
C2-C4	1.521(3)	C2-H2	1.0
C3-H3A	0.98	C3-H3B	0.98
C3-H3C	0.98	C4-H4A	0.98
C4-H4B	0.98	C4-H4C	0.98
N3-C5	1.468(2)	C5-C7	1.518(3)
C5-C6	1.520(3)	C5-H5	1.0
C6-H6A	0.98	C6-H6B	0.98
C6-H6C	0.98	C7-H7A	0.98
C7-H7B	0.98	C7-H7C	0.98
C11-C16	1.387(3)	C11-C12	1.388(3)
C12-C13	1.389(3)	C12-H12	0.95
C13-C14	1.375(4)	C13-H13	0.95
C14-C15	1.371(3)	C14-H14	0.95
C15-C16	1.386(3)	C15-H15	0.95

C16-H16	0.95	C20-C24	1.420(3)
C20-C21	1.424(3)	C20-C25	1.506(3)
C21-C22	1.431(3)	C21-C26	1.504(3)
C22-C23	1.414(3)	C22-C27	1.504(3)
C23-C24	1.427(3)	C23-C28	1.512(3)
C24-C29	1.505(3)	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C25-H25D	0.98	C25-H25E	0.98
C25-H25F	0.98	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C28-H28A	0.98
C28-H28B	0.98	C28-H28C	0.98
C29-H29A	0.98	C29-H29B	0.98
C29-H29C	0.98		

Table 5. Bond angles (°) for 2b.

N1-Nb1-N3	104.65(6)	N1-Nb1-N2	107.38(6)
N3-Nb1-N2	60.35(6)	N1-Nb1-C20	90.74(6)
N3-Nb1-C20	147.23(6)	N2-Nb1-C20	142.14(6)
N1-Nb1-C21	110.84(7)	N3-Nb1-C21	144.51(6)
N2-Nb1-C21	107.77(6)	C20-Nb1-C21	34.54(6)
N1-Nb1-C24	105.54(7)	N3-Nb1-C24	112.86(6)
N2-Nb1-C24	147.00(6)	C20-Nb1-C24	34.38(7)
C21-Nb1-C24	57.15(7)	N1-Nb1-C23	139.40(7)
N3-Nb1-C23	95.70(6)	N2-Nb1-C23	113.22(6)
C20-Nb1-C23	56.33(6)	C21-Nb1-C23	56.22(7)
C24-Nb1-C23	33.89(7)	N1-Nb1-C22	144.35(7)
N3-Nb1-C22	110.67(6)	N2-Nb1-C22	94.36(6)
C20-Nb1-C22	56.39(6)	C21-Nb1-C22	33.99(6)
C24-Nb1-C22	56.10(7)	C23-Nb1-C22	33.13(7)
N1-N1-Nb1	167.17(17)	N2-C1-N3	112.74(16)
N2-C1-C11	123.72(17)	N3-C1-C11	123.53(17)
C1-N2-C2	122.33(16)	C1-N2-Nb1	92.33(11)
C2-N2-Nb1	137.21(12)	N2-C2-C3	109.69(17)
N2-C2-C4	109.63(16)	C3-C2-C4	111.0(2)
N2-C2-H2	108.8	C3-C2-H2	108.8

C4-C2-H2	108.8	C2-C3-H3A	109.5
C2-C3-H3B	109.5	H3A-C3-H3B	109.5
C2-C3-H3C	109.5	H3A-C3-H3C	109.5
H3B-C3-H3C	109.5	C2-C4-H4A	109.5
C2-C4-H4B	109.5	H4A-C4-H4B	109.5
C2-C4-H4C	109.5	H4A-C4-H4C	109.5
H4B-C4-H4C	109.5	C1-N3-C5	122.70(16)
C1-N3-Nb1	92.88(11)	C5-N3-Nb1	139.74(13)
N3-C5-C7	111.36(17)	N3-C5-C6	108.86(17)
C7-C5-C6	111.1(2)	N3-C5-H5	108.5
C7-C5-H5	108.5	C6-C5-H5	108.5
C5-C6-H6A	109.5	C5-C6-H6B	109.5
H6A-C6-H6B	109.5	C5-C6-H6C	109.5
H6A-C6-H6C	109.5	H6B-C6-H6C	109.5
C5-C7-H7A	109.5	C5-C7-H7B	109.5
H7A-C7-H7B	109.5	C5-C7-H7C	109.5
H7A-C7-H7C	109.5	H7B-C7-H7C	109.5
C16-C11-C12	118.79(19)	C16-C11-C1	121.42(17)
C12-C11-C1	119.77(17)	C11-C12-C13	120.1(2)
C11-C12-H12	120.0	C13-C12-H12	120.0
C14-C13-C12	120.6(2)	C14-C13-H13	119.7
C12-C13-H13	119.7	C15-C14-C13	119.6(2)
C15-C14-H14	120.2	C13-C14-H14	120.2
C14-C15-C16	120.5(2)	C14-C15-H15	119.8
C16-C15-H15	119.8	C15-C16-C11	120.5(2)
C15-C16-H16	119.8	C11-C16-H16	119.8
C24-C20-C21	108.54(17)	C24-C20-C25	125.73(18)
C21-C20-C25	125.67(18)	C24-C20-Nb1	74.00(11)
C21-C20-Nb1	73.63(10)	C25-C20-Nb1	120.55(12)
C20-C21-C22	107.40(17)	C20-C21-C26	124.97(18)
C22-C21-C26	127.26(18)	C20-C21-Nb1	71.84(10)
C22-C21-Nb1	75.72(11)	C26-C21-Nb1	123.49(13)
C23-C22-C21	108.14(17)	C23-C22-C27	125.12(19)
C21-C22-C27	126.7(2)	C23-C22-Nb1	73.31(10)
C21-C22-Nb1	70.29(10)	C27-C22-Nb1	123.38(13)
C22-C23-C24	108.35(17)	C22-C23-C28	125.6(2)
C24-C23-C28	126.0(2)	C22-C23-Nb1	73.55(10)
C24-C23-Nb1	70.74(10)	C28-C23-Nb1	123.07(14)

C20-C24-C23	107.55(18)	C20-C24-C29	125.15(19)
C23-C24-C29	126.87(19)	C20-C24-Nb1	71.62(10)
C23-C24-Nb1	75.37(11)	C29-C24-Nb1	124.46(14)
C20-C25-H25A	109.5	C20-C25-H25B	109.5
H25A-C25-H25B	109.5	C20-C25-H25C	109.5
H25A-C25-H25C	109.5	H25B-C25-H25C	109.5
C20-C25-H25D	109.5	H25A-C25-H25D	141.1
H25B-C25-H25D	56.3	H25C-C25-H25D	56.3
C20-C25-H25E	109.5	H25A-C25-H25E	56.3
H25B-C25-H25E	141.1	H25C-C25-H25E	56.3
H25D-C25-H25E	109.5	C20-C25-H25F	109.5
H25A-C25-H25F	56.3	H25B-C25-H25F	56.3
H25C-C25-H25F	141.1	H25D-C25-H25F	109.5
H25E-C25-H25F	109.5	C21-C26-H26A	109.5
C21-C26-H26B	109.5	H26A-C26-H26B	109.5
C21-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C22-C27-H27A	109.5
C22-C27-H27B	109.5	H27A-C27-H27B	109.5
C22-C27-H27C	109.5	H27A-C27-H27C	109.5
H27B-C27-H27C	109.5	C23-C28-H28A	109.5
C23-C28-H28B	109.5	H28A-C28-H28B	109.5
C23-C28-H28C	109.5	H28A-C28-H28C	109.5
H28B-C28-H28C	109.5	C24-C29-H29A	109.5
C24-C29-H29B	109.5	H29A-C29-H29B	109.5
C24-C29-H29C	109.5	H29A-C29-H29C	109.5
H29B-C29-H29C	109.5		

Table 6. Torsion angles (°) for 2b.

N3-Nb1-N1-N1	-144.0(8)	N2-Nb1-N1-N1	153.0(8)
C20-Nb1-N1-N1	6.8(8)	C21-Nb1-N1-N1	35.6(8)
C24-Nb1-N1-N1	-24.7(8)	C23-Nb1-N1-N1	-26.4(9)
C22-Nb1-N1-N1	28.1(9)	N3-C1-N2-C2	165.76(16)
C11-C1-N2-C2	-13.4(3)	N3-C1-N2-Nb1	12.26(15)
C11-C1-N2-Nb1	-166.94(15)	C1-N2-C2-C3	144.32(19)
Nb1-N2-C2-C3	-76.7(2)	C1-N2-C2-C4	-93.5(2)
Nb1-N2-C2-C4	45.5(3)	N2-C1-N3-C5	-172.44(16)
C11-C1-N3-C5	6.8(3)	N2-C1-N3-Nb1	-12.34(15)

C11-C1-N3-Nb1	166.86(15)	C1-N3-C5-C7	-88.7(2)
Nb1-N3-C5-C7	123.0(2)	C1-N3-C5-C6	148.41(18)
Nb1-N3-C5-C6	0.1(3)	N2-C1-C11-C16	101.8(2)
N3-C1-C11-C16	-77.3(2)	N2-C1-C11-C12	-79.6(3)
N3-C1-C11-C12	101.3(2)	C16-C11-C12-C13	0.4(4)
C1-C11-C12-C13	-178.3(2)	C11-C12-C13-C14	-0.2(4)
C12-C13-C14-C15	-0.2(4)	C13-C14-C15-C16	0.3(4)
C14-C15-C16-C11	-0.1(4)	C12-C11-C16-C15	-0.3(3)
C1-C11-C16-C15	178.4(2)	C24-C20-C21-C22	1.7(2)
C25-C20-C21-C22	-175.84(17)	Nb1-C20-C21-C22	67.99(12)
C24-C20-C21-C26	175.04(17)	C25-C20-C21-C26	-2.5(3)
Nb1-C20-C21-C26	-118.63(18)	C24-C20-C21-Nb1	-66.33(13)
C25-C20-C21-Nb1	116.18(18)	C20-C21-C22-C23	-1.4(2)
C26-C21-C22-C23	-174.54(18)	Nb1-C21-C22-C23	64.00(13)
C20-C21-C22-C27	177.12(18)	C26-C21-C22-C27	3.9(3)
Nb1-C21-C22-C27	-117.51(19)	C20-C21-C22-Nb1	-65.36(12)
C26-C21-C22-Nb1	121.45(19)	C21-C22-C23-C24	0.6(2)
C27-C22-C23-C24	-177.96(18)	Nb1-C22-C23-C24	62.60(13)
C21-C22-C23-C28	178.71(18)	C27-C22-C23-C28	0.2(3)
Nb1-C22-C23-C28	-119.24(19)	C21-C22-C23-Nb1	-62.05(12)
C27-C22-C23-Nb1	119.44(19)	C21-C20-C24-C23	-1.3(2)
C25-C20-C24-C23	176.17(17)	Nb1-C20-C24-C23	-67.40(13)
C21-C20-C24-C29	-174.23(18)	C25-C20-C24-C29	3.3(3)
Nb1-C20-C24-C29	119.69(19)	C21-C20-C24-Nb1	66.08(12)
C25-C20-C24-Nb1	-116.43(18)	C22-C23-C24-C20	0.5(2)
C28-C23-C24-C20	-177.68(18)	Nb1-C23-C24-C20	64.89(12)
C22-C23-C24-C29	173.22(19)	C28-C23-C24-C29	-4.9(3)
Nb1-C23-C24-C29	-122.4(2)	C22-C23-C24-Nb1	-64.42(13)
C28-C23-C24-Nb1	117.43(19)		

Table 7. Anisotropic atomic displacement parameters (Å^2) for 2b.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	0.02109(7)	0.02220(8)	0.01984(7)	0.00007(6)	0.00442(5)	-0.00216(7)
N1	0.0239(7)	0.0239(7)	0.0235(7)	-0.0009(6)	0.0061(6)	-0.0028(6)
C1	0.0256(9)	0.0252(9)	0.0241(8)	0.0031(7)	0.0061(7)	-0.0007(7)

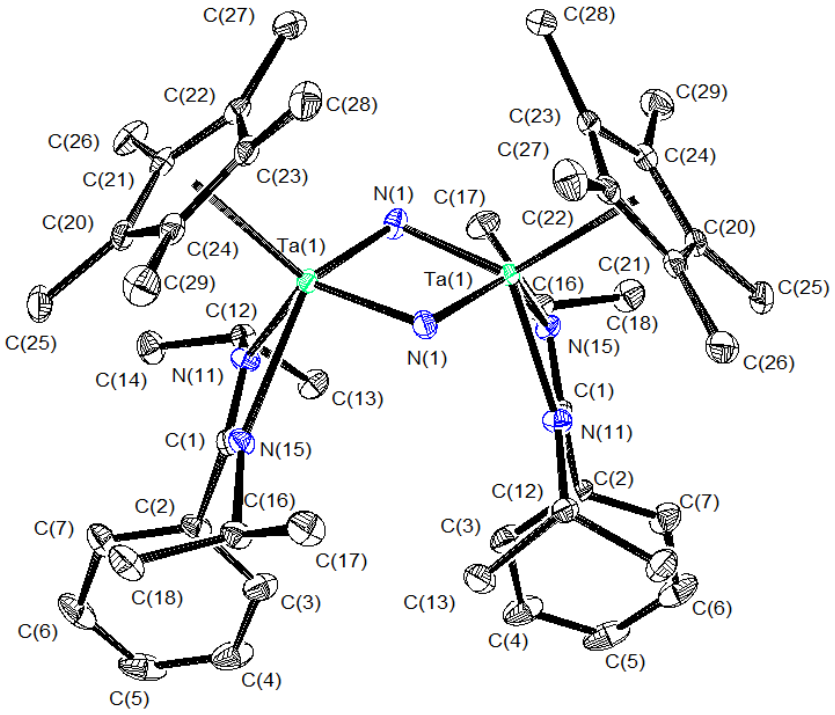
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	0.0277(8)	0.0236(8)	0.0318(8)	-0.0029(6)	0.0127(6)	-0.0015(6)
C2	0.0338(10)	0.0233(9)	0.0420(11)	-0.0054(8)	0.0179(9)	-0.0025(8)
C3	0.0407(13)	0.0378(13)	0.0825(19)	-0.0182(12)	0.0275(13)	0.0011(10)
C4	0.0804(19)	0.0416(13)	0.0386(12)	-0.0117(10)	0.0160(12)	0.0073(13)
N3	0.0313(8)	0.0273(8)	0.0271(8)	-0.0013(6)	0.0142(6)	-0.0023(6)
C5	0.0314(10)	0.0372(11)	0.0327(10)	-0.0035(8)	0.0153(8)	-0.0011(8)
C6	0.0515(14)	0.0402(13)	0.0625(15)	-0.0104(11)	0.0298(12)	0.0035(11)
C7	0.0615(16)	0.0760(19)	0.0425(13)	0.0038(13)	0.0327(12)	0.0043(14)
C11	0.0285(9)	0.0258(9)	0.0319(9)	0.0010(7)	0.0126(8)	-0.0018(7)
C12	0.0377(12)	0.0416(13)	0.0523(14)	0.0178(10)	0.0067(10)	-0.0045(10)
C13	0.0574(16)	0.0444(14)	0.0727(18)	0.0259(13)	0.0194(14)	-0.0089(12)
C14	0.0456(13)	0.0430(13)	0.0711(17)	0.0000(12)	0.0268(13)	-0.0176(11)
C15	0.0311(11)	0.0438(13)	0.0573(14)	-0.0064(11)	0.0109(10)	-0.0068(9)
C16	0.0327(10)	0.0309(10)	0.0411(11)	0.0009(9)	0.0095(9)	-0.0017(8)
C20	0.0241(9)	0.0270(9)	0.0304(9)	-0.0001(7)	0.0056(7)	-0.0073(7)
C21	0.0211(8)	0.0309(10)	0.0332(9)	0.0019(7)	0.0069(7)	-0.0033(7)
C22	0.0237(9)	0.0347(11)	0.0326(10)	0.0049(8)	-0.0018(7)	-0.0037(8)
C23	0.0310(10)	0.0406(11)	0.0233(9)	-0.0011(8)	0.0008(7)	-0.0112(8)
C24	0.0309(10)	0.0311(10)	0.0272(9)	-0.0057(8)	0.0036(8)	-0.0077(8)
C25	0.0363(10)	0.0294(11)	0.0431(11)	0.0059(8)	0.0130(9)	-0.0064(8)
C26	0.0303(10)	0.0425(12)	0.0499(12)	0.0018(10)	0.0181(9)	0.0014(9)
C27	0.0378(12)	0.0404(12)	0.0493(13)	0.0143(10)	0.0002(10)	0.0038(10)
C28	0.0520(14)	0.0650(16)	0.0248(10)	0.0007(10)	0.0033(9)	-0.0141(12)
C29	0.0528(14)	0.0388(12)	0.0424(12)	-0.0140(10)	0.0151(11)	-0.0057(10)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 2b.

	x/a	y/b	z/c	U(eq)
H2	0.9519	0.2561	0.9197	0.038
H3A	0.6971	0.2545	0.8354	0.078
H3B	0.7396	0.2719	0.9685	0.078
H3C	0.6852	0.1997	0.9242	0.078
H4A	0.9258	0.1502	1.0627	0.082
H4B	0.9553	0.2238	1.1082	0.082
H4C	1.0738	0.1862	1.0676	0.082
H5	1.2145	0.1072	0.7562	0.039

	x/a	y/b	z/c	U(eq)
H6A	1.1612	-0.0010	0.7972	0.073
H6B	1.2227	-0.0004	0.6924	0.073
H6C	1.0519	-0.0090	0.6688	0.073
H7A	0.9979	0.0885	0.5364	0.084
H7B	1.1686	0.0960	0.5580	0.084
H7C	1.0781	0.1565	0.5814	0.084
H12	0.9759	0.2719	0.6840	0.055
H13	1.1445	0.3542	0.6901	0.07
H14	1.3801	0.3483	0.8195	0.062
H15	1.4480	0.2602	0.9442	0.054
H16	1.2819	0.1773	0.9392	0.043
H25A	0.6633	-0.1133	0.8637	0.055
H25B	0.6117	-0.0614	0.9391	0.055
H25C	0.7809	-0.0685	0.9547	0.055
H25D	0.7073	-0.0488	0.9747	0.055
H25E	0.7589	-0.1007	0.8993	0.055
H25F	0.5897	-0.0936	0.8837	0.055
H26A	0.4395	0.0443	0.8780	0.06
H26B	0.5099	0.1149	0.8772	0.06
H26C	0.5970	0.0608	0.9673	0.06
H27A	0.5061	0.1631	0.7168	0.069
H27B	0.4461	0.1343	0.5895	0.069
H27C	0.6046	0.1668	0.6362	0.069
H28A	0.5950	0.0310	0.4671	0.074
H28B	0.7673	0.0212	0.5236	0.074
H28C	0.6974	0.0923	0.5206	0.074
H29A	0.8363	-0.1078	0.7451	0.067
H29B	0.8206	-0.0762	0.6234	0.067
H29C	0.6890	-0.1174	0.6393	0.067

cis-{Cp*Ta[N(iPr)C(Ph)N(iPr](μ-N)}$_2$ (*cis*-3b)



A yellow prism-like specimen of $C_{46}H_{68}N_6Ta_2$, approximate dimensions 0.05 mm × 0.13 mm × 0.17 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 16.83 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 32820 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 6446 were independent (average redundancy 5.092, completeness = 99.9%, R_{int} = 2.58%) and 5692 (88.30%) were greater than $2\sigma(F^2)$. The final cell constants of a = 13.3148(10) Å, b = 17.9841(13) Å, c = 18.9403(14) Å, β = 102.7560(10)°, V = 4423.4(6) $Å^3$, are based upon the refinement of the XYZ-centroids of 9990 reflections above 20 σ(I) with 4.784° < 2θ < 64.32°. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.4740 and 0.7800.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group C2/c, with Z = 4 for the formula unit, $C_{46}H_{68}N_6Ta_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 254 variables converged at R_1 = 1.91%, for the observed data and wR_2 = 3.83% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 1.095 $e^-/Å^3$ and the largest hole was -0.538 $e^-/Å^3$ with an RMS deviation of 0.086 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.602 g/cm^3 and F(000), 2128 e^-.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)

XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for *cis*-3b.

Identification code	***cis*-3b**	
Chemical formula	$C_{46}H_{68}N_6Ta_2$	
Formula weight	1066.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.05 × 0.13 × 0.17 mm	
Crystal habit	yellow prism	
Crystal system	monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 13.3148(10) Å	α = 90°
	b = 17.9841(13) Å	β = 102.7560(10)°
	c = 18.9403(14) Å	γ = 90°
Volume	4423.4(6) $Å^3$	
Z	4	
Density (calculated)	1.602 Mg/cm^3	
Absorption coefficient	4.982 mm^{-1}	
F(000)	2128	

Table 2. Data collection and structure refinement for *cis*-3b.

Diffractometer	Bruker APEX-II CCD
Radiation source	sealed tube, MoKα
Theta range for data collection	1.93 to 30.00°
Index ranges	$-18 \le h \le 18$, $-25 \le k \le 25$, $-26 \le l \le 26$
Reflections collected	32820
Independent reflections	6446 [R(int) = 0.0258]
Coverage of independent reflections	99.9%
Absorption correction	multi-scan
Max. and min. transmission	0.7800 and 0.4740
Structure solution technique	direct methods
Structure solution	ShelXS-97 (Sheldrick, 2008)

program		
Refinement method	Full-matrix least-squares on F^2	
Refinement program	ShelXL-2012 (Sheldrick, 2012)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6446 / 0 / 254	
Goodness-of-fit on F^2	1.000	
Δ/σ_{max}	0.006	
Final R indices	5692 data; $I>2\sigma(I)$	$R_1 = 0.0191$, $wR_2 = 0.0367$
	all data	$R_1 = 0.0239$, $wR_2 = 0.0383$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0065P)^2+14.9030P]$, $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.095 and -0.538 eÅ^{-3}	
R.M.S. deviation from mean	0.086 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for *cis*-3b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ta1	0.54274(2)	0.14135(2)	0.68833(2)	0.01744(3)
N1	0.40810(14)	0.13679(12)	0.70952(10)	0.0244(4)
C1	0.58839(17)	0.28180(12)	0.64875(11)	0.0209(4)
C2	0.60116(17)	0.36265(13)	0.63163(12)	0.0260(5)
C3	0.5880(2)	0.41807(15)	0.67961(14)	0.0360(6)
C4	0.5928(3)	0.49266(16)	0.66125(16)	0.0468(8)
C5	0.6130(2)	0.51262(17)	0.59595(19)	0.0514(9)
C6	0.6285(2)	0.45845(18)	0.54803(18)	0.0481(8)
C7	0.6226(2)	0.38354(16)	0.56545(15)	0.0369(6)
N11	0.49941(14)	0.24533(11)	0.62979(10)	0.0238(4)

	x/a	y/b	z/c	U(eq)
C12	0.39828(17)	0.27446(13)	0.59224(11)	0.0225(4)
C13	0.3540(2)	0.33063(15)	0.63716(14)	0.0322(5)
C14	0.3943(2)	0.30544(16)	0.51640(13)	0.0354(6)
N15	0.66233(14)	0.23835(11)	0.68494(10)	0.0220(4)
C16	0.76480(17)	0.26814(14)	0.71860(13)	0.0268(5)
C17	0.8143(2)	0.22084(16)	0.78432(14)	0.0358(6)
C18	0.8357(2)	0.27306(17)	0.66532(15)	0.0383(6)
C20	0.59720(19)	0.10620(13)	0.56879(12)	0.0257(5)
C21	0.49329(18)	0.08284(13)	0.55916(11)	0.0257(5)
C22	0.48811(18)	0.02850(13)	0.61188(12)	0.0251(5)
C23	0.58984(19)	0.01762(13)	0.65483(12)	0.0254(5)
C24	0.65722(18)	0.06493(13)	0.62702(12)	0.0253(5)
C25	0.6373(2)	0.16199(15)	0.52266(14)	0.0357(6)
C26	0.4036(2)	0.10531(16)	0.50031(13)	0.0377(6)
C27	0.3924(2)	0.98638(16)	0.61524(15)	0.0378(6)
C28	0.6255(2)	0.95424(14)	0.70617(14)	0.0361(6)
C29	0.7726(2)	0.06263(17)	0.64928(15)	0.0384(6)

Table 4. Bond lengths (Å) for *cis*-3b.

Ta1-N1	1.9024(18)	Ta1-N1	1.9232(19)
Ta1-N11	2.1856(19)	Ta1-N15	2.3723(19)
Ta1-C23	2.434(2)	Ta1-C22	2.506(2)
Ta1-C24	2.519(2)	Ta1-C20	2.603(2)
Ta1-C21	2.610(2)	Ta1-Ta1	2.8153(2)
N1-Ta1	1.9025(18)	C1-N15	1.324(3)
C1-N11	1.332(3)	C1-C2	1.507(3)
C2-C3	1.386(4)	C2-C7	1.397(3)
C3-C4	1.391(4)	C3-H3	0.95
C4-C5	1.370(5)	C4-H4	0.95
C5-C6	1.378(5)	C5-H5	0.95
C6-C7	1.393(4)	C6-H6	0.95
C7-H7	0.95	N11-C12	1.473(3)
C12-C13	1.521(3)	C12-C14	1.531(3)
C12-H12	1.0	C13-H13A	0.98
C13-H13B	0.98	C13-H13C	0.98
C14-H14A	0.98	C14-H14B	0.98

C14-H14C	0.98	N15-C16	1.473(3)
C16-C18	1.529(3)	C16-C17	1.531(3)
C16-H16	1.0	C17-H17A	0.98
C17-H17B	0.98	C17-H17C	0.98
C18-H18A	0.98	C18-H18B	0.98
C18-H18C	0.98	C20-C21	1.419(3)
C20-C24	1.420(3)	C20-C25	1.504(3)
C21-C22	1.410(3)	C21-C26	1.498(3)
C22-C23	1.431(3)	C22-C27	1.496(3)
C23-C24	1.420(3)	C23-C28	1.505(3)
C24-C29	1.501(3)	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C25-H25D	0.98	C25-H25E	0.98
C25-H25F	0.98	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C28-H28A	0.98
C28-H28B	0.98	C28-H28C	0.98
C29-H29A	0.98	C29-H29B	0.98
C29-H29C	0.98		

Table 5. Bond angles (°) for *cis*-3b.

N1-Ta1-N1	85.02(8)	N1-Ta1-N11	123.08(8)
N1-Ta1-N11	89.34(8)	N1-Ta1-N15	88.68(7)
N1-Ta1-N15	134.36(8)	N11-Ta1-N15	57.36(7)
N1-Ta1-C23	100.09(8)	N1-Ta1-C23	108.73(9)
N11-Ta1-C23	134.78(7)	N15-Ta1-C23	116.88(7)
N1-Ta1-C22	122.93(8)	N1-Ta1-C22	85.47(8)
N11-Ta1-C22	112.91(7)	N15-Ta1-C22	133.69(7)
C23-Ta1-C22	33.64(8)	N1-Ta1-C24	109.76(8)
N1-Ta1-C24	139.45(8)	N11-Ta1-C24	110.59(7)
N15-Ta1-C24	84.87(7)	C23-Ta1-C24	33.26(8)
C22-Ta1-C24	54.52(8)	N1-Ta1-C20	140.78(8)
N1-Ta1-C20	128.50(8)	N11-Ta1-C20	81.92(7)
N15-Ta1-C20	80.65(7)	C23-Ta1-C20	54.12(7)
C22-Ta1-C20	53.26(8)	C24-Ta1-C20	32.14(7)
N1-Ta1-C21	153.47(8)	N1-Ta1-C21	97.15(8)

N11-Ta1-C21	83.44(7)	N15-Ta1-C21	107.63(7)
C23-Ta1-C21	54.08(7)	C22-Ta1-C21	31.90(7)
C24-Ta1-C21	53.20(7)	C20-Ta1-C21	31.58(7)
N1-Ta1-Ta1	42.91(6)	N1-Ta1-Ta1	42.33(5)
N11-Ta1-Ta1	108.13(5)	N15-Ta1-Ta1	114.78(4)
C23-Ta1-Ta1	113.02(5)	C22-Ta1-Ta1	111.13(5)
C24-Ta1-Ta1	141.20(5)	C20-Ta1-Ta1	164.35(5)
C21-Ta1-Ta1	135.49(6)	Ta1-N1-Ta1	94.77(8)
N15-C1-N11	111.4(2)	N15-C1-C2	125.1(2)
N11-C1-C2	123.6(2)	C3-C2-C7	118.4(2)
C3-C2-C1	121.1(2)	C7-C2-C1	120.5(2)
C2-C3-C4	120.7(3)	C2-C3-H3	119.7
C4-C3-H3	119.7	C5-C4-C3	120.5(3)
C5-C4-H4	119.8	C3-C4-H4	119.8
C4-C5-C6	119.8(3)	C4-C5-H5	120.1
C6-C5-H5	120.1	C5-C6-C7	120.2(3)
C5-C6-H6	119.9	C7-C6-H6	119.9
C6-C7-C2	120.4(3)	C6-C7-H7	119.8
C2-C7-H7	119.8	C1-N11-C12	128.22(19)
C1-N11-Ta1	99.50(14)	C12-N11-Ta1	131.29(14)
N11-C12-C13	113.08(18)	N11-C12-C14	114.92(19)
C13-C12-C14	110.2(2)	N11-C12-H12	106.0
C13-C12-H12	106.0	C14-C12-H12	106.0
C12-C13-H13A	109.5	C12-C13-H13B	109.5
H13A-C13-H13B	109.5	C12-C13-H13C	109.5
H13A-C13-H13C	109.5	H13B-C13-H13C	109.5
C12-C14-H14A	109.5	C12-C14-H14B	109.5
H14A-C14-H14B	109.5	C12-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
C1-N15-C16	121.41(19)	C1-N15-Ta1	91.22(13)
C16-N15-Ta1	144.95(14)	N15-C16-C18	112.5(2)
N15-C16-C17	109.94(19)	C18-C16-C17	110.5(2)
N15-C16-H16	107.9	C18-C16-H16	107.9
C17-C16-H16	107.9	C16-C17-H17A	109.5
C16-C17-H17B	109.5	H17A-C17-H17B	109.5
C16-C17-H17C	109.5	H17A-C17-H17C	109.5
H17B-C17-H17C	109.5	C16-C18-H18A	109.5
C16-C18-H18B	109.5	H18A-C18-H18B	109.5

C16-C18-H18C	109.5	H18A-C18-H18C	109.5
H18B-C18-H18C	109.5	C21-C20-C24	108.1(2)
C21-C20-C25	125.8(2)	C24-C20-C25	126.1(2)
C21-C20-Ta1	74.50(12)	C24-C20-Ta1	70.64(12)
C25-C20-Ta1	123.11(16)	C22-C21-C20	108.2(2)
C22-C21-C26	124.0(2)	C20-C21-C26	127.6(2)
C22-C21-Ta1	69.96(12)	C20-C21-Ta1	73.93(12)
C26-C21-Ta1	125.69(16)	C21-C22-C23	108.0(2)
C21-C22-C27	123.8(2)	C23-C22-C27	127.9(2)
C21-C22-Ta1	78.14(13)	C23-C22-Ta1	70.41(12)
C27-C22-Ta1	121.79(16)	C24-C23-C22	107.7(2)
C24-C23-C28	124.0(2)	C22-C23-C28	126.5(2)
C24-C23-Ta1	76.65(13)	C22-C23-Ta1	75.95(13)
C28-C23-Ta1	125.91(15)	C23-C24-C20	107.9(2)
C23-C24-C29	124.8(2)	C20-C24-C29	126.7(2)
C23-C24-Ta1	70.09(12)	C20-C24-Ta1	77.22(13)
C29-C24-Ta1	124.86(16)	C20-C25-H25A	109.5
C20-C25-H25B	109.5	H25A-C25-H25B	109.5
C20-C25-H25C	109.5	H25A-C25-H25C	109.5
H25B-C25-H25C	109.5	C20-C25-H25D	109.5
H25A-C25-H25D	141.1	H25B-C25-H25D	56.3
H25C-C25-H25D	56.3	C20-C25-H25E	109.5
H25A-C25-H25E	56.3	H25B-C25-H25E	141.1
H25C-C25-H25E	56.3	H25D-C25-H25E	109.5
C20-C25-H25F	109.5	H25A-C25-H25F	56.3
H25B-C25-H25F	56.3	H25C-C25-H25F	141.1
H25D-C25-H25F	109.5	H25E-C25-H25F	109.5
C21-C26-H26A	109.5	C21-C26-H26B	109.5
H26A-C26-H26B	109.5	C21-C26-H26C	109.5
H26A-C26-H26C	109.5	H26B-C26-H26C	109.5
C22-C27-H27A	109.5	C22-C27-H27B	109.5
H27A-C27-H27B	109.5	C22-C27-H27C	109.5
H27A-C27-H27C	109.5	H27B-C27-H27C	109.5
C23-C28-H28A	109.5	C23-C28-H28B	109.5
H28A-C28-H28B	109.5	C23-C28-H28C	109.5
H28A-C28-H28C	109.5	H28B-C28-H28C	109.5
C24-C29-H29A	109.5	C24-C29-H29B	109.5
H29A-C29-H29B	109.5	C24-C29-H29C	109.5

H29A-C29-H29C	109.5	H29B-C29-H29C	109.5

Table 6. Torsion angles (°) for *cis*-3b.

N15-C1-C2-C3	-88.0(3)	N11-C1-C2-C3	90.9(3)
N15-C1-C2-C7	94.6(3)	N11-C1-C2-C7	-86.5(3)
C7-C2-C3-C4	1.9(4)	C1-C2-C3-C4	-175.5(2)
C2-C3-C4-C5	-1.4(5)	C3-C4-C5-C6	0.0(5)
C4-C5-C6-C7	0.8(5)	C5-C6-C7-C2	-0.2(4)
C3-C2-C7-C6	-1.2(4)	C1-C2-C7-C6	176.3(2)
N15-C1-N11-C12	176.9(2)	C2-C1-N11-C12	-2.2(4)
N15-C1-N11-Ta1	7.3(2)	C2-C1-N11-Ta1	-171.76(18)
C1-N11-C12-C13	-66.5(3)	Ta1-N11-C12-C13	99.8(2)
C1-N11-C12-C14	61.3(3)	Ta1-N11-C12-C14	-132.5(2)
N11-C1-N15-C16	-173.18(19)	C2-C1-N15-C16	5.9(3)
N11-C1-N15-Ta1	-6.67(18)	C2-C1-N15-Ta1	172.4(2)
C1-N15-C16-C18	-84.3(3)	Ta1-N15-C16-C18	119.7(2)
C1-N15-C16-C17	152.0(2)	Ta1-N15-C16-C17	-4.0(4)
C24-C20-C21-C22	1.2(3)	C25-C20-C21-C22	178.1(2)
Ta1-C20-C21-C22	-61.93(15)	C24-C20-C21-C26	-173.9(2)
C25-C20-C21-C26	3.1(4)	Ta1-C20-C21-C26	123.0(2)
C24-C20-C21-Ta1	63.09(15)	C25-C20-C21-Ta1	-119.9(2)
C20-C21-C22-C23	-0.1(2)	C26-C21-C22-C23	175.2(2)
Ta1-C21-C22-C23	-64.63(15)	C20-C21-C22-C27	-175.0(2)
C26-C21-C22-C27	0.3(4)	Ta1-C21-C22-C27	120.5(2)
C20-C21-C22-Ta1	64.50(16)	C26-C21-C22-Ta1	-120.2(2)
C21-C22-C23-C24	-0.9(2)	C27-C22-C23-C24	173.7(2)
Ta1-C22-C23-C24	-70.76(16)	C21-C22-C23-C28	-165.7(2)
C27-C22-C23-C28	9.0(4)	Ta1-C22-C23-C28	124.5(2)
C21-C22-C23-Ta1	69.81(16)	C27-C22-C23-Ta1	-115.6(2)
C22-C23-C24-C20	1.7(2)	C28-C23-C24-C20	166.8(2)
Ta1-C23-C24-C20	-68.62(16)	C22-C23-C24-C29	-170.5(2)
C28-C23-C24-C29	-5.3(4)	Ta1-C23-C24-C29	119.3(2)
C22-C23-C24-Ta1	70.27(15)	C28-C23-C24-Ta1	-124.5(2)
C21-C20-C24-C23	-1.7(3)	C25-C20-C24-C23	-178.7(2)
Ta1-C20-C24-C23	63.86(15)	C21-C20-C24-C29	170.2(2)
C25-C20-C24-C29	-6.8(4)	Ta1-C20-C24-C29	-124.2(2)
C21-C20-C24-Ta1	-65.61(16)	C25-C20-C24-Ta1	117.4(2)

Table 7. Anisotropic atomic displacement parameters (Å^2) for *cis*-3b.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

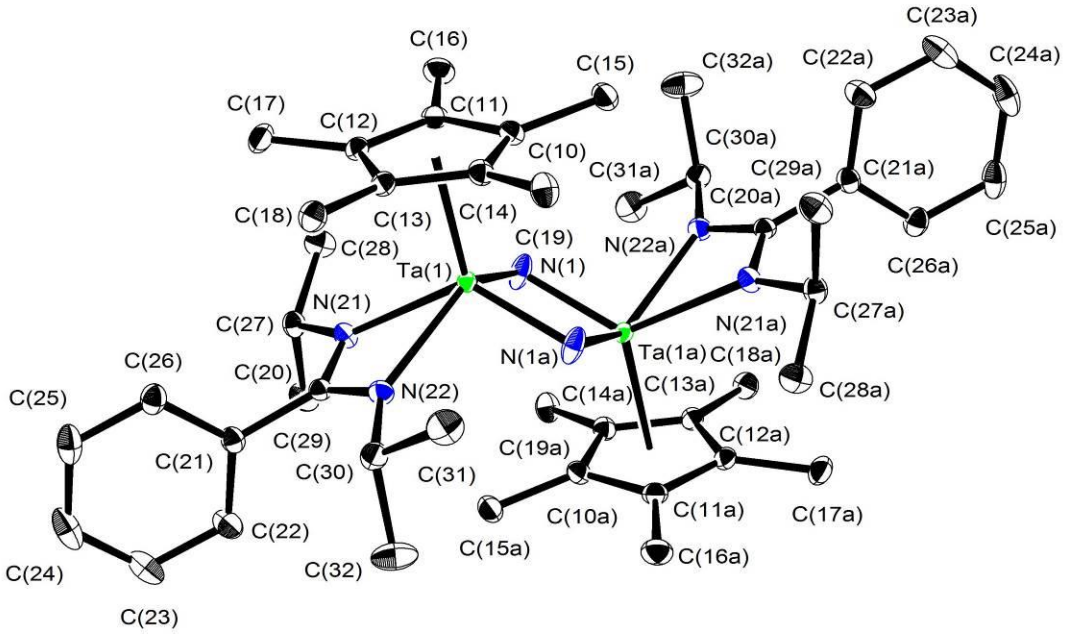
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.02261(4)	0.01523(4)	0.01481(4)	-0.00007(3)	0.00485(3)	0.00187(4)
N1	0.0225(8)	0.0319(11)	0.0189(8)	-0.0017(8)	0.0050(7)	0.0056(8)
C1	0.0250(10)	0.0216(11)	0.0176(9)	0.0022(8)	0.0076(8)	-0.0014(8)
C2	0.0241(10)	0.0223(11)	0.0295(11)	0.0081(9)	0.0011(9)	-0.0027(9)
C3	0.0474(15)	0.0249(13)	0.0300(12)	0.0028(10)	-0.0039(11)	-0.0026(11)
C4	0.064(2)	0.0228(13)	0.0436(16)	0.0024(12)	-0.0102(14)	-0.0034(13)
C5	0.0500(18)	0.0267(14)	0.066(2)	0.0204(14)	-0.0128(15)	-0.0116(13)
C6	0.0450(16)	0.0458(18)	0.0528(18)	0.0283(15)	0.0094(14)	-0.0091(14)
C7	0.0356(13)	0.0393(15)	0.0377(13)	0.0120(12)	0.0122(11)	-0.0029(12)
N11	0.0216(9)	0.0199(9)	0.0299(10)	0.0021(8)	0.0054(8)	0.0004(7)
C12	0.0229(10)	0.0217(11)	0.0217(10)	0.0013(8)	0.0026(8)	0.0013(8)
C13	0.0302(12)	0.0325(13)	0.0327(12)	-0.0049(10)	0.0043(10)	0.0061(10)
C14	0.0340(13)	0.0436(16)	0.0276(12)	0.0091(11)	0.0049(10)	0.0018(12)
N15	0.0227(9)	0.0218(9)	0.0216(8)	0.0039(7)	0.0052(7)	-0.0019(7)
C16	0.0224(10)	0.0275(12)	0.0292(11)	0.0033(9)	0.0029(9)	-0.0033(9)
C17	0.0285(12)	0.0386(15)	0.0361(13)	0.0083(11)	-0.0018(10)	-0.0012(11)
C18	0.0299(13)	0.0433(16)	0.0439(15)	0.0089(12)	0.0126(11)	-0.0064(12)
C20	0.0374(13)	0.0220(11)	0.0209(10)	-0.0014(8)	0.0132(9)	0.0030(10)
C21	0.0322(12)	0.0267(12)	0.0181(9)	-0.0065(9)	0.0055(9)	0.0059(10)
C22	0.0315(12)	0.0219(11)	0.0232(10)	-0.0075(9)	0.0088(9)	0.0008(9)
C23	0.0365(12)	0.0206(11)	0.0214(10)	-0.0028(8)	0.0112(9)	0.0048(9)
C24	0.0289(11)	0.0254(12)	0.0235(10)	-0.0028(9)	0.0099(9)	0.0051(9)
C25	0.0507(16)	0.0348(14)	0.0267(12)	0.0023(10)	0.0198(11)	0.0041(12)
C26	0.0452(15)	0.0366(15)	0.0260(12)	-0.0088(11)	-0.0032(11)	0.0103(12)
C27	0.0400(14)	0.0356(15)	0.0394(14)	-0.0121(12)	0.0124(12)	-0.0103(12)
C28	0.0531(17)	0.0257(13)	0.0322(13)	0.0032(10)	0.0152(12)	0.0131(12)
C29	0.0318(13)	0.0414(16)	0.0431(15)	-0.0013(12)	0.0107(11)	0.0080(12)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for *cis*-3b.

	x/a	y/b	z/c	U(eq)

	x/a	y/b	z/c	U(eq)
H3	0.5755	0.4050	0.7255	0.043
H4	0.5821	0.5300	0.6943	0.056
H5	0.6162	0.5637	0.5837	0.062
H6	0.6433	0.4722	0.5030	0.058
H7	0.6331	0.3465	0.5321	0.044
H12	0.3502	0.2310	0.5854	0.027
H13A	0.3615	0.3117	0.6866	0.048
H13B	0.2808	0.3385	0.6155	0.048
H13C	0.3910	0.3779	0.6384	0.048
H14A	0.4269	0.3546	0.5204	0.053
H14B	0.3223	0.3098	0.4901	0.053
H14C	0.4310	0.2718	0.4901	0.053
H16	0.7553	0.3196	0.7361	0.032
H17A	0.7653	0.2142	0.8155	0.054
H17B	0.8762	0.2459	0.8116	0.054
H17C	0.8332	0.1722	0.7679	0.054
H18A	0.9024	0.2934	0.6901	0.057
H18B	0.8045	0.3056	0.6249	0.057
H18C	0.8455	0.2233	0.6469	0.057
H25A	0.6360	0.2117	0.5436	0.054
H25B	0.5939	0.1614	0.4736	0.054
H25C	0.7082	0.1492	0.5207	0.054
H25D	0.6561	0.1365	0.4817	0.054
H25E	0.6982	0.1868	0.5517	0.054
H25F	0.5839	0.1990	0.5045	0.054
H26A	0.3838	0.0637	0.4667	0.056
H26B	0.4230	0.1481	0.4741	0.056
H26C	0.3455	0.1189	0.5216	0.056
H27A	0.3489	0.0168	0.6394	0.057
H27B	0.4109	-0.0598	0.6425	0.057
H27C	0.3546	-0.0255	0.5660	0.057
H28A	0.6478	-0.0872	0.6797	0.054
H28B	0.5686	-0.0621	0.7277	0.054
H28C	0.6832	-0.0292	0.7446	0.054
H29A	0.7978	0.0168	0.6312	0.058
H29B	0.7939	0.0639	0.7022	0.058
H29C	0.8015	0.1057	0.6290	0.058

trans-{Cp*Ta[N(iPr)C(Ph)N(iPr](μ-N)}$_2$ (*trans*-3b)



A dark red prism-like specimen of $C_{46}H_{68}N_6Ta_2$, approximate dimensions 0.14 mm x 0.17 mm x 0.17 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker Smart Apex2, CCD system equipped with a graphite monochromator and a CuK_α fine focus sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 12.63 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 68126 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 6299 were independent (average redundancy 10.815, completeness = 100.0%, R_{int} = 2.60%, R_{sig} = 1.22%) and 5387 (85.52%) were greater than $2\sigma(F^2)$. The final cell constants of a = 16.4902(11) Å, b = 15.3364(10) Å, c = 17.0776(11) Å, volume = 4318.9(5) $Å^3$, are based upon the refinement of the XYZ-centroids of 9819 reflections above 20 σ(I) with 4.341° < 2θ < 62.18°. Data were corrected for absorption effects using the integration method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.4775 and 0.5290.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P b c a, with Z = 4 for the formula unit, $C_{46}H_{68}N_6Ta_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 269 variables converged at R1 = 1.52%, for the observed data and wR2 = 3.11% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.685 $e^-/Å^3$ and the largest hole was -0.351 $e^-/Å^3$ with an RMS deviation of 0.074 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.641 g/cm^3 and F(000), 2128 e^-.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)

XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2008/4 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for *trans*-3b.

Identification code	***trans*-3b**	
Chemical formula	$C_{46}H_{68}N_6Ta_2$	
Formula weight	1066.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.14 x 0.17 x 0.17 mm	
Crystal habit	dark red prism	
Crystal system	orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 16.4902(11) Å	α = 90°
	b = 15.3364(10) Å	β = 90°
	c = 17.0776(11) Å	γ = 90°
Volume	4318.9(5) $Å^3$	
Z	4	
Density (calculated)	1.641 Mg/cm^3	
Absorption coefficient	5.102 mm^{-1}	
F(000)	2128	

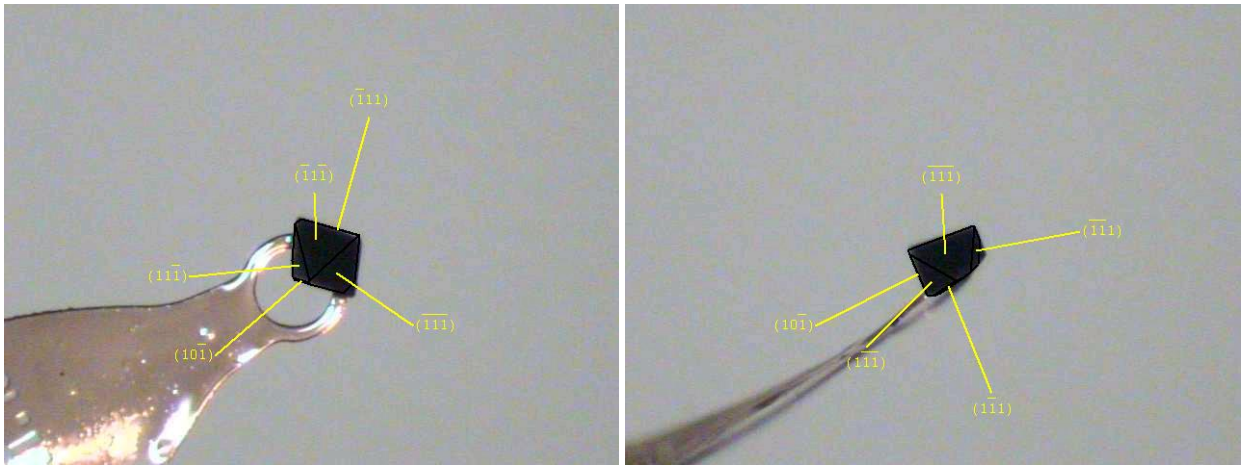


Table 2. Data collection and structure refinement for *trans*-3b.

Diffractometer	Bruker Smart Apex2, CCD
Radiation source	fine focus sealed tube, CuK_α
Theta range for data collection	2.17 to 30.00°
Index ranges	-23<=h<=23, -21<=k<=21, -24<=l<=24
Reflections collected	68126

Independent reflections	6299 [R(int) = 0.0260]
Coverage of independent reflections	100.0%
Absorption correction	integration
Max. and min. transmission	0.5290 and 0.4775
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	6299 / 0 / 269
Goodness-of-fit on F^2	1.000
Δ/σ_{max}	0.003
Final R indices	5387 data; I>2σ(I) $R_1 = 0.0152$, $wR_2 = 0.0297$
	all data $R_1 = 0.0211$, $wR_2 = 0.0311$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.003P)^2+6.5P]$, $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.685 and -0.351 eÅ^{-3}
R.M.S. deviation from mean	0.074 eÅ^{-3}

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$ $\quad R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$

GOOF = S = $\{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$ $\quad wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for *trans*-3b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ta1	0.039891(4)	0.434118(4)	0.041222(4)	0.01667(2)
N1	0.93088(10)	0.45992(11)	0.01144(11)	0.0322(4)
C10	0.07444(12)	0.34268(13)	0.93226(11)	0.0251(4)
C11	0.15178(12)	0.35951(12)	0.96672(11)	0.0251(4)
C12	0.15402(11)	0.31662(12)	0.03973(11)	0.0238(4)
C13	0.07911(12)	0.27136(11)	0.05018(11)	0.0230(4)
C14	0.03049(12)	0.28604(12)	0.98331(11)	0.0240(4)
C15	0.05151(14)	0.36478(14)	0.84925(11)	0.0307(4)
C16	0.21874(13)	0.40903(15)	0.92710(13)	0.0350(5)
C17	0.22483(12)	0.30701(14)	0.09411(13)	0.0321(4)
C18	0.06305(13)	0.21012(13)	0.11700(12)	0.0308(4)
C19	0.95064(12)	0.24419(13)	0.96299(13)	0.0316(4)
N21	0.10770(10)	0.47817(10)	0.14783(9)	0.0233(3)
N22	0.99507(10)	0.40342(11)	0.16383(9)	0.0236(3)
C20	0.05890(11)	0.43871(12)	0.19861(10)	0.0211(3)
C21	0.07686(11)	0.43342(13)	0.28452(11)	0.0243(4)
C22	0.04890(15)	0.49651(14)	0.33643(12)	0.0348(5)
C23	0.06894(17)	0.49170(17)	0.41522(13)	0.0434(6)
C24	0.11637(16)	0.42481(17)	0.44238(13)	0.0444(6)
C25	0.14462(14)	0.36203(16)	0.39197(14)	0.0392(5)

	x/a	y/b	z/c	U(eq)
C26	0.12500(13)	0.36595(14)	0.31270(12)	0.0301(4)
C27	0.18170(12)	0.52451(13)	0.17222(11)	0.0249(4)
C28	0.23835(13)	0.53555(15)	0.10293(13)	0.0336(5)
C29	0.16483(14)	0.61424(14)	0.20704(13)	0.0344(5)
C30	0.92853(12)	0.36105(13)	0.20667(12)	0.0280(4)
C31	0.87602(14)	0.30897(16)	0.15058(14)	0.0409(5)
C32	0.87430(16)	0.42578(18)	0.24846(17)	0.0511(7)

Table 4. Bond lengths (Å) for *trans*-3b.

Ta1-N1	1.9096(17)	Ta1-N1#1	1.9188(16)
Ta1-N21	2.2408(15)	Ta1-N22	2.2699(15)
Ta1-C10	2.3988(19)	Ta1-C14	2.4819(18)
Ta1-C11	2.5164(19)	Ta1-C13	2.5830(17)
Ta1-C12	2.6057(17)	Ta1-Ta1#1	2.79226(17)
N1-Ta1#1	1.9188(16)	C10-C14	1.428(3)
C10-C11	1.428(3)	C10-C15	1.506(3)
C11-C12	1.410(3)	C11-C16	1.501(3)
C12-C13	1.428(3)	C12-C17	1.499(3)
C13-C14	1.413(3)	C13-C18	1.502(3)
C14-C19	1.505(3)	C15-H15A	0.98
C15-H15B	0.98	C15-H15C	0.98
C16-H16A	0.98	C16-H16B	0.98
C16-H16C	0.98	C17-H17A	0.98
C17-H17B	0.98	C17-H17C	0.98
C18-H18A	0.98	C18-H18B	0.98
C18-H18C	0.98	C19-H19A	0.98
C19-H19B	0.98	C19-H19C	0.98
N21-C20	1.329(2)	N21-C27	1.472(2)
N22-C20	1.324(2)	N22-C30	1.470(2)
C20-C21	1.499(2)	C21-C26	1.390(3)
C21-C22	1.391(3)	C22-C23	1.387(3)
C22-H22	0.95	C23-C24	1.371(4)
C23-H23	0.95	C24-C25	1.373(4)
C24-H24	0.95	C25-C26	1.393(3)
C25-H25	0.95	C26-H26	0.95
C27-C28	1.517(3)	C27-C29	1.525(3)
C27-H27	1.0	C28-H28A	0.98
C28-H28B	0.98	C28-H28C	0.98
C29-H29A	0.98	C29-H29B	0.98
C29-H29C	0.98	C30-C32	1.515(3)
C30-C31	1.518(3)	C30-H30	1.0
C31-H31A	0.98	C31-H31B	0.98

C31-H31C	0.98	C32-H32A	0.98
C32-H32B	0.98	C32-H32C	0.98

Symmetry transformations used to generate equivalent atoms:
#1 -x, -y+1, -z

Table 5. Bond angles (°) for *trans*-3b.

N1-Ta1-N1#1	86.33(7)	N1-Ta1-N21	128.58(8)
N1#1-Ta1-N21	90.01(7)	N1-Ta1-N22	88.98(7)
N1#1-Ta1-N22	133.61(7)	N21-Ta1-N22	58.37(6)
N1-Ta1-C10	97.94(8)	N1#1-Ta1-C10	94.12(8)
N21-Ta1-C10	133.48(6)	N22-Ta1-C10	132.20(6)
N1-Ta1-C14	91.41(7)	N1#1-Ta1-C14	127.15(8)
N21-Ta1-C14	129.11(6)	N22-Ta1-C14	99.06(6)
C10-Ta1-C14	33.98(6)	N1-Ta1-C11	130.52(8)
N1#1-Ta1-C11	87.93(7)	N21-Ta1-C11	100.49(6)
N22-Ta1-C11	127.65(6)	C10-Ta1-C11	33.68(6)
C14-Ta1-C11	55.13(6)	N1-Ta1-C13	116.86(7)
N1#1-Ta1-C13	141.56(7)	N21-Ta1-C13	96.79(6)
N22-Ta1-C13	80.01(6)	C10-Ta1-C13	54.66(6)
C14-Ta1-C13	32.33(6)	C11-Ta1-C13	53.63(6)
N1-Ta1-C12	145.14(7)	N1#1-Ta1-C12	113.56(7)
N21-Ta1-C12	81.73(6)	N22-Ta1-C12	95.78(6)
C10-Ta1-C12	54.31(6)	C14-Ta1-C12	53.73(6)
C11-Ta1-C12	31.90(6)	C13-Ta1-C12	31.95(6)
N1-Ta1-Ta1#1	43.30(5)	N1#1-Ta1-Ta1#1	43.04(5)
N21-Ta1-Ta1#1	115.25(4)	N22-Ta1-Ta1#1	117.50(4)
C10-Ta1-Ta1#1	98.27(5)	C14-Ta1-Ta1#1	115.58(4)
C11-Ta1-Ta1#1	114.81(5)	C13-Ta1-Ta1#1	147.91(4)
C12-Ta1-Ta1#1	146.71(4)	Ta1-N1-Ta1#1	93.67(7)
C14-C10-C11	108.16(17)	C14-C10-C15	125.74(18)
C11-C10-C15	124.85(18)	C14-C10-Ta1	76.20(11)
C11-C10-Ta1	77.69(11)	C15-C10-Ta1	122.62(13)
C12-C11-C10	107.65(17)	C12-C11-C16	127.97(18)
C10-C11-C16	124.23(18)	C12-C11-Ta1	77.54(11)
C10-C11-Ta1	68.64(10)	C16-C11-Ta1	122.49(14)
C11-C12-C13	108.34(16)	C11-C12-C17	127.87(18)
C13-C12-C17	123.26(18)	C11-C12-Ta1	70.56(10)
C13-C12-Ta1	73.15(10)	C17-C12-Ta1	128.64(13)
C14-C13-C12	108.19(16)	C14-C13-C18	127.85(18)
C12-C13-C18	123.48(17)	C14-C13-Ta1	69.89(10)
C12-C13-Ta1	74.90(10)	C18-C13-Ta1	127.25(13)
C13-C14-C10	107.59(17)	C13-C14-C19	127.92(18)
C10-C14-C19	124.23(17)	C13-C14-Ta1	77.78(10)
C10-C14-Ta1	69.82(10)	C19-C14-Ta1	122.45(13)

C10-C15-H15A	109.5	C10-C15-H15B	109.5
H15A-C15-H15B	109.5	C10-C15-H15C	109.5
H15A-C15-H15C	109.5	H15B-C15-H15C	109.5
C11-C16-H16A	109.5	C11-C16-H16B	109.5
H16A-C16-H16B	109.5	C11-C16-H16C	109.5
H16A-C16-H16C	109.5	H16B-C16-H16C	109.5
C12-C17-H17A	109.5	C12-C17-H17B	109.5
H17A-C17-H17B	109.5	C12-C17-H17C	109.5
H17A-C17-H17C	109.5	H17B-C17-H17C	109.5
C13-C18-H18A	109.5	C13-C18-H18B	109.5
H18A-C18-H18B	109.5	C13-C18-H18C	109.5
H18A-C18-H18C	109.5	H18B-C18-H18C	109.5
C14-C19-H19A	109.5	C14-C19-H19B	109.5
H19A-C19-H19B	109.5	C14-C19-H19C	109.5
H19A-C19-H19C	109.5	H19B-C19-H19C	109.5
C20-N21-C27	122.49(16)	C20-N21-Ta1	95.21(11)
C27-N21-Ta1	142.09(12)	C20-N22-C30	123.42(16)
C20-N22-Ta1	94.02(11)	C30-N22-Ta1	142.53(13)
N22-C20-N21	112.01(16)	N22-C20-C21	125.02(16)
N21-C20-C21	122.94(17)	C26-C21-C22	119.10(19)
C26-C21-C20	119.47(18)	C22-C21-C20	121.38(18)
C23-C22-C21	120.1(2)	C23-C22-H22	119.9
C21-C22-H22	119.9	C24-C23-C22	120.3(2)
C24-C23-H23	119.9	C22-C23-H23	119.9
C23-C24-C25	120.4(2)	C23-C24-H24	119.8
C25-C24-H24	119.8	C24-C25-C26	120.0(2)
C24-C25-H25	120.0	C26-C25-H25	120.0
C21-C26-C25	120.1(2)	C21-C26-H26	120.0
C25-C26-H26	120.0	N21-C27-C28	110.09(16)
N21-C27-C29	113.24(17)	C28-C27-C29	108.41(17)
N21-C27-H27	108.3	C28-C27-H27	108.3
C29-C27-H27	108.3	C27-C28-H28A	109.5
C27-C28-H28B	109.5	H28A-C28-H28B	109.5
C27-C28-H28C	109.5	H28A-C28-H28C	109.5
H28B-C28-H28C	109.5	C27-C29-H29A	109.5
C27-C29-H29B	109.5	H29A-C29-H29B	109.5
C27-C29-H29C	109.5	H29A-C29-H29C	109.5
H29B-C29-H29C	109.5	N22-C30-C32	112.66(17)
N22-C30-C31	110.13(17)	C32-C30-C31	107.79(19)
N22-C30-H30	108.7	C32-C30-H30	108.7
C31-C30-H30	108.7	C30-C31-H31A	109.5
C30-C31-H31B	109.5	H31A-C31-H31B	109.5
C30-C31-H31C	109.5	H31A-C31-H31C	109.5
H31B-C31-H31C	109.5	C30-C32-H32A	109.5

C30-C32-H32B	109.5	H32A-C32-H32B	109.5
C30-C32-H32C	109.5	H32A-C32-H32C	109.5
H32B-C32-H32C	109.5		

Symmetry transformations used to generate equivalent atoms:
#1 -x, -y+1, -z

Table 6. Torsion angles (°) for *trans*-3b.

N1#1-Ta1-N1-Ta1#1	0	N21-Ta1-N1-Ta1#1	87.08(9)
N22-Ta1-N1-Ta1#1	133.82(8)	C10-Ta1-N1-Ta1#1	-93.66(8)
C14-Ta1-N1-Ta1#1	-127.13(8)	C11-Ta1-N1-Ta1#1	-84.13(10)
C13-Ta1-N1-Ta1#1	-147.92(6)	C12-Ta1-N1-Ta1#1	-127.50(10)
N1-Ta1-C10-C14	-80.66(12)	N1#1-Ta1-C10-C14	-167.52(12)
N21-Ta1-C10-C14	98.55(13)	N22-Ta1-C10-C14	15.20(15)
C11-Ta1-C10-C14	112.46(16)	C13-Ta1-C10-C14	36.75(11)
C12-Ta1-C10-C14	76.27(12)	Ta1#1-Ta1-C10-C14	-124.41(10)
N1-Ta1-C10-C11	166.88(11)	N1#1-Ta1-C10-C11	80.01(12)
N21-Ta1-C10-C11	-13.91(15)	N22-Ta1-C10-C11	-97.26(13)
C14-Ta1-C10-C11	-112.46(16)	C13-Ta1-C10-C11	-75.71(12)
C12-Ta1-C10-C11	-36.19(11)	Ta1#1-Ta1-C10-C11	123.13(11)
N1-Ta1-C10-C15	43.19(17)	N1#1-Ta1-C10-C15	-43.68(17)
N21-Ta1-C10-C15	-137.61(15)	N22-Ta1-C10-C15	139.05(15)
C14-Ta1-C10-C15	123.8(2)	C11-Ta1-C10-C15	-123.7(2)
C13-Ta1-C10-C15	160.59(19)	C12-Ta1-C10-C15	-159.89(19)
Ta1#1-Ta1-C10-C15	-0.57(17)	C14-C10-C11-C12	-2.4(2)
C15-C10-C11-C12	-170.21(18)	Ta1-C10-C11-C12	68.43(13)
C14-C10-C11-C16	173.61(18)	C15-C10-C11-C16	5.8(3)
Ta1-C10-C11-C16	-115.57(19)	C14-C10-C11-Ta1	-70.82(13)
C15-C10-C11-Ta1	121.36(19)	N1-Ta1-C11-C12	-132.03(11)
N1#1-Ta1-C11-C12	144.57(12)	N21-Ta1-C11-C12	54.95(12)
N22-Ta1-C11-C12	-2.99(14)	C10-Ta1-C11-C12	-114.83(16)
C14-Ta1-C11-C12	-75.82(12)	C13-Ta1-C11-C12	-35.80(10)
Ta1#1-Ta1-C11-C12	179.25(9)	N1-Ta1-C11-C10	-17.20(15)
N1#1-Ta1-C11-C10	-100.60(12)	N21-Ta1-C11-C10	169.78(11)
N22-Ta1-C11-C10	111.84(12)	C14-Ta1-C11-C10	39.01(11)
C13-Ta1-C11-C10	79.03(12)	C12-Ta1-C11-C10	114.83(16)
Ta1#1-Ta1-C11-C10	-65.92(12)	N1-Ta1-C11-C16	100.64(17)
N1#1-Ta1-C11-C16	17.25(17)	N21-Ta1-C11-C16	-72.37(17)
N22-Ta1-C11-C16	-130.31(15)	C10-Ta1-C11-C16	117.8(2)
C14-Ta1-C11-C16	156.86(19)	C13-Ta1-C11-C16	-163.12(19)
C12-Ta1-C11-C16	-127.3(2)	Ta1#1-Ta1-C11-C16	51.92(17)
C10-C11-C12-C13	1.3(2)	C16-C11-C12-C13	-174.46(19)
Ta1-C11-C12-C13	63.84(13)	C10-C11-C12-C17	173.14(18)
C16-C11-C12-C17	-2.7(3)	Ta1-C11-C12-C17	-124.36(19)
C10-C11-C12-Ta1	-62.50(13)	C16-C11-C12-Ta1	121.7(2)

N1-Ta1-C12-C11	81.07(16)	N1#1-Ta1-C12-C11	-39.20(13)
N21-Ta1-C12-C11	-125.57(12)	N22-Ta1-C12-C11	177.62(11)
C10-Ta1-C12-C11	38.29(11)	C14-Ta1-C12-C11	80.61(12)
C13-Ta1-C12-C11	117.10(16)	Ta1#1-Ta1-C12-C11	-1.25(15)
N1-Ta1-C12-C13	-36.03(18)	N1#1-Ta1-C12-C13	-156.30(11)
N21-Ta1-C12-C13	117.33(11)	N22-Ta1-C12-C13	60.52(11)
C10-Ta1-C12-C13	-78.81(12)	C14-Ta1-C12-C13	-36.49(10)
C11-Ta1-C12-C13	-117.10(16)	Ta1#1-Ta1-C12-C13	-118.35(10)
N1-Ta1-C12-C17	-155.48(17)	N1#1-Ta1-C12-C17	84.25(19)
N21-Ta1-C12-C17	-2.12(17)	N22-Ta1-C12-C17	-58.92(18)
C10-Ta1-C12-C17	161.7(2)	C14-Ta1-C12-C17	-155.9(2)
C11-Ta1-C12-C17	123.5(2)	C13-Ta1-C12-C17	-119.4(2)
Ta1#1-Ta1-C12-C17	122.20(16)	C11-C12-C13-C14	0.2(2)
C17-C12-C13-C14	-172.05(17)	Ta1-C12-C13-C14	62.39(12)
C11-C12-C13-C18	172.85(17)	C17-C12-C13-C18	0.6(3)
Ta1-C12-C13-C18	-124.98(18)	C11-C12-C13-Ta1	-62.18(13)
C17-C12-C13-Ta1	125.57(18)	N1-Ta1-C13-C14	41.56(14)
N1#1-Ta1-C13-C14	-79.96(15)	N21-Ta1-C13-C14	-178.60(11)
N22-Ta1-C13-C14	125.27(12)	C10-Ta1-C13-C14	-38.69(11)
C11-Ta1-C13-C14	-80.56(12)	C12-Ta1-C13-C14	-116.31(16)
Ta1#1-Ta1-C13-C14	-1.71(16)	N1-Ta1-C13-C12	157.86(11)
N1#1-Ta1-C13-C12	36.35(16)	N21-Ta1-C13-C12	-62.29(11)
N22-Ta1-C13-C12	-118.42(11)	C10-Ta1-C13-C12	77.61(12)
C14-Ta1-C13-C12	116.31(16)	C11-Ta1-C13-C12	35.75(11)
Ta1#1-Ta1-C13-C12	114.59(11)	N1-Ta1-C13-C18	-81.30(18)
N1#1-Ta1-C13-C18	157.19(16)	N21-Ta1-C13-C18	58.54(17)
N22-Ta1-C13-C18	2.42(16)	C10-Ta1-C13-C18	-161.6(2)
C14-Ta1-C13-C18	-122.9(2)	C11-Ta1-C13-C18	156.6(2)
C12-Ta1-C13-C18	120.8(2)	Ta1#1-Ta1-C13-C18	-124.57(15)
C12-C13-C14-C10	-1.7(2)	C18-C13-C14-C10	-173.90(18)
Ta1-C13-C14-C10	63.96(13)	C12-C13-C14-C19	172.53(18)
C18-C13-C14-C19	0.3(3)	Ta1-C13-C14-C19	-121.8(2)
C12-C13-C14-Ta1	-65.65(13)	C18-C13-C14-Ta1	122.13(19)
C11-C10-C14-C13	2.5(2)	C15-C10-C14-C13	170.21(18)
Ta1-C10-C14-C13	-69.32(13)	C11-C10-C14-C19	-171.96(18)
C15-C10-C14-C19	-4.3(3)	Ta1-C10-C14-C19	116.20(18)
C11-C10-C14-Ta1	71.84(13)	C15-C10-C14-Ta1	-120.5(2)
N1-Ta1-C14-C13	-143.70(12)	N1#1-Ta1-C14-C13	129.83(12)
N21-Ta1-C14-C13	1.79(14)	N22-Ta1-C14-C13	-54.51(12)
C10-Ta1-C14-C13	114.15(17)	C11-Ta1-C14-C13	75.49(12)
C12-Ta1-C14-C13	36.04(11)	Ta1#1-Ta1-C14-C13	178.99(9)
N1-Ta1-C14-C10	102.16(12)	N1#1-Ta1-C14-C10	15.68(14)
N21-Ta1-C14-C10	-112.35(12)	N22-Ta1-C14-C10	-168.65(11)
C11-Ta1-C14-C10	-38.65(11)	C13-Ta1-C14-C10	-114.15(17)

C12-Ta1-C14-C10	-78.11(12)	Ta1#1-Ta1-C14-C10	64.85(12)
N1-Ta1-C14-C19	-16.30(16)	N1#1-Ta1-C14-C19	-102.77(16)
N21-Ta1-C14-C19	129.19(15)	N22-Ta1-C14-C19	72.89(16)
C10-Ta1-C14-C19	-118.5(2)	C11-Ta1-C14-C19	-157.11(18)
C13-Ta1-C14-C19	127.4(2)	C12-Ta1-C14-C19	163.44(18)
Ta1#1-Ta1-C14-C19	-53.61(16)	N1-Ta1-N21-C20	62.59(13)
N1#1-Ta1-N21-C20	147.91(12)	N22-Ta1-N21-C20	3.80(10)
C10-Ta1-N21-C20	-116.40(12)	C14-Ta1-N21-C20	-70.98(13)
C11-Ta1-N21-C20	-124.19(11)	C13-Ta1-N21-C20	-70.02(12)
C12-Ta1-N21-C20	-98.27(12)	Ta1#1-Ta1-N21-C20	111.81(10)
N1-Ta1-N21-C27	-123.3(2)	N1#1-Ta1-N21-C27	-38.0(2)
N22-Ta1-N21-C27	177.9(2)	C10-Ta1-N21-C27	57.7(2)
C14-Ta1-N21-C27	103.1(2)	C11-Ta1-N21-C27	49.9(2)
C13-Ta1-N21-C27	104.1(2)	C12-Ta1-N21-C27	75.9(2)
Ta1#1-Ta1-N21-C27	-74.1(2)	N1-Ta1-N22-C20	-141.84(12)
N1#1-Ta1-N22-C20	-57.89(14)	N21-Ta1-N22-C20	-3.81(10)
C10-Ta1-N22-C20	118.35(12)	C14-Ta1-N22-C20	126.89(11)
C11-Ta1-N22-C20	74.34(13)	C13-Ta1-N22-C20	100.65(12)
C12-Ta1-N22-C20	72.76(11)	Ta1#1-Ta1-N22-C20	-107.94(10)
N1-Ta1-N22-C30	40.2(2)	N1#1-Ta1-N22-C30	124.2(2)
N21-Ta1-N22-C30	178.3(2)	C10-Ta1-N22-C30	-59.6(2)
C14-Ta1-N22-C30	-51.0(2)	C11-Ta1-N22-C30	-103.6(2)
C13-Ta1-N22-C30	-77.3(2)	C12-Ta1-N22-C30	-105.2(2)
Ta1#1-Ta1-N22-C30	74.1(2)	C30-N22-C20-N21	-175.61(17)
Ta1-N22-C20-N21	5.91(16)	C30-N22-C20-C21	6.2(3)
Ta1-N22-C20-C21	-172.31(16)	C27-N21-C20-N22	178.28(16)
Ta1-N21-C20-N22	-5.99(16)	C27-N21-C20-C21	-3.5(3)
Ta1-N21-C20-C21	172.27(15)	N22-C20-C21-C26	91.8(2)
N21-C20-C21-C26	-86.2(2)	N22-C20-C21-C22	-90.6(3)
N21-C20-C21-C22	91.3(2)	C26-C21-C22-C23	-0.1(3)
C20-C21-C22-C23	-177.6(2)	C21-C22-C23-C24	0.0(4)
C22-C23-C24-C25	0.1(4)	C23-C24-C25-C26	-0.1(4)
C22-C21-C26-C25	0.1(3)	C20-C21-C26-C25	177.66(19)
C24-C25-C26-C21	0.0(3)	C20-N21-C27-C28	160.81(18)
Ta1-N21-C27-C28	-12.3(3)	C20-N21-C27-C29	-77.6(2)
Ta1-N21-C27-C29	109.3(2)	C20-N22-C30-C32	73.2(3)
Ta1-N22-C30-C32	-109.3(2)	C20-N22-C30-C31	-166.39(18)
Ta1-N22-C30-C31	11.1(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y+1, -z

Table 7. Anisotropic atomic displacement parameters (Å^2) for *trans*-3b.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.01705(3)	0.01593(3)	0.01703(3)	0.00182(3)	-0.00019(3)	0.00166(3)
N1	0.0195(8)	0.0310(9)	0.0460(10)	0.0210(8)	-0.0065(7)	-0.0040(7)
C10	0.0285(10)	0.0262(9)	0.0206(8)	-0.0026(7)	-0.0001(7)	0.0015(8)
C11	0.0240(9)	0.0269(9)	0.0245(9)	-0.0036(7)	0.0029(7)	0.0018(7)
C12	0.0236(9)	0.0231(8)	0.0247(8)	-0.0040(7)	-0.0032(8)	0.0062(7)
C13	0.0276(9)	0.0182(8)	0.0233(9)	-0.0005(7)	-0.0018(7)	0.0050(7)
C14	0.0274(10)	0.0214(8)	0.0234(8)	-0.0026(7)	-0.0021(7)	0.0004(7)
C15	0.0390(12)	0.0311(10)	0.0220(9)	0.0002(8)	-0.0014(8)	0.0036(9)
C16	0.0282(11)	0.0444(12)	0.0325(11)	-0.0025(9)	0.0077(9)	-0.0032(9)
C17	0.0281(10)	0.0310(10)	0.0373(11)	-0.0003(9)	-0.0076(9)	0.0086(8)
C18	0.0378(11)	0.0235(9)	0.0312(10)	0.0055(8)	-0.0007(9)	0.0048(8)
C19	0.0341(11)	0.0284(9)	0.0321(10)	0.0003(8)	-0.0074(9)	-0.0071(8)
N21	0.0244(8)	0.0258(8)	0.0198(7)	0.0005(6)	-0.0003(6)	-0.0041(6)
N22	0.0210(8)	0.0283(8)	0.0217(7)	0.0010(6)	0.0026(6)	-0.0017(6)
C20	0.0236(9)	0.0202(8)	0.0195(8)	-0.0001(7)	0.0014(6)	0.0038(7)
C21	0.0259(9)	0.0257(8)	0.0211(8)	0.0033(7)	0.0001(7)	-0.0023(8)
C22	0.0474(14)	0.0322(11)	0.0249(10)	0.0003(8)	0.0035(9)	0.0005(10)
C23	0.0616(16)	0.0444(13)	0.0243(11)	-0.0037(10)	0.0056(11)	-0.0142(12)
C24	0.0527(15)	0.0553(15)	0.0253(10)	0.0108(10)	-0.0083(10)	-0.0268(13)
C25	0.0347(12)	0.0458(13)	0.0371(12)	0.0187(10)	-0.0108(10)	-0.0105(10)
C26	0.0277(10)	0.0312(10)	0.0315(10)	0.0076(8)	-0.0016(8)	-0.0010(8)
C27	0.0246(9)	0.0261(9)	0.0241(9)	0.0022(7)	-0.0027(7)	-0.0036(7)
C28	0.0295(11)	0.0352(11)	0.0360(11)	-0.0043(9)	0.0043(9)	-0.0089(9)
C29	0.0393(12)	0.0318(11)	0.0320(11)	-0.0052(9)	0.0003(9)	-0.0092(9)
C30	0.0235(9)	0.0325(10)	0.0279(10)	0.0087(8)	0.0040(8)	-0.0005(8)
C31	0.0276(11)	0.0492(14)	0.0458(13)	0.0029(11)	0.0054(10)	-0.0127(10)
C32	0.0365(13)	0.0547(15)	0.0620(16)	-0.0067(14)	0.0250(12)	-0.0039(12)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for *trans*-3b.

	x/a	y/b	z/c	U(eq)
H15A	0.0674	0.3169	-0.1855	0.077(6)
H15B	0.0794	0.4183	-0.1668	0.077(6)
H15C	-0.0073	0.3736	-0.1540	0.077(6)
H16A	0.2035	0.4706	-0.0772	0.050(4)
H16B	0.2278	0.3850	-0.1253	0.050(4)
H16C	0.2686	0.4038	-0.0420	0.050(4)
H17A	0.2725	0.3354	0.0712	0.045(4)
H17B	0.2363	0.2450	0.1023	0.045(4)
H17C	0.2120	0.3344	0.1444	0.045(4)
H18A	0.0594	0.2433	0.1659	0.054(5)
H18B	0.1074	0.1678	0.1208	0.054(5)
H18C	0.0119	0.1792	0.1079	0.054(5)

	x/a	y/b	z/c	U(eq)
H19A	-0.0913	0.2892	-0.0410	0.045(4)
H19B	-0.0642	0.2024	0.0040	0.045(4)
H19C	-0.0445	0.2137	-0.0872	0.045(4)
H22	0.0160	0.5430	0.3179	0.042(7)
H23	0.0497	0.5349	0.4505	0.060(9)
H24	0.1298	0.4219	0.4964	0.064(9)
H25	0.1775	0.3159	0.4111	0.051(8)
H26	0.1445	0.3225	0.2779	0.028(6)
H27	0.2099	0.4885	0.2127	0.029(6)
H28A	0.2528	0.4781	0.0821	0.043(4)
H28B	0.2876	0.5660	0.1198	0.043(4)
H28C	0.2112	0.5697	0.0621	0.043(4)
H29A	0.1385	0.6511	0.1676	0.045(4)
H29B	0.2160	0.6412	0.2232	0.045(4)
H29C	0.1291	0.6082	0.2526	0.045(4)
H30	-0.0478	0.3203	0.2463	0.035(6)
H31A	-0.1456	0.3478	0.1101	0.057(5)
H31B	-0.1690	0.2823	0.1795	0.057(5)
H31C	-0.0913	0.2632	0.1260	0.057(5)
H32A	-0.0932	0.4606	0.2849	0.069(6)
H32B	-0.1677	0.3943	0.2775	0.069(6)
H32C	-0.1513	0.4644	0.2099	0.069(6)

Table 9. Data collection details for *trans*-3b.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s
Omega	50.346	-31.50	-31.50	0.00	54.71	0.30	610	15.00
Omega	50.346	-31.50	-31.50	120.00	54.71	0.30	610	15.00
Omega	50.346	-31.50	-31.50	240.00	54.71	0.30	610	15.00
Phi	50.346	-31.50	-211.50	0.00	54.71	0.30	1200	15.00

Table 10. Data collection details for *trans*-3b.

```
#==============================================================================
# PLATON/CHECK-(160910) versus check.def version of 160910  for entry: 2058
# Data From: 2058.cif - Data Type: CIF          Bond Precision   C-C = 0.0030 A
# Refl Data: 2058.fcf - Data Type: SHELXL                          Temp = 150 K
#
# UCL 16.4902(11) 15.3364(10) 17.0776(11)           90           90          90
# WaveLength 0.71073    Volume Reported     4318.9(5)  Calculated     4318.9(5)
# SpaceGroup from Symmetry P b c a       Hall: -P 2ac 2ab
#                 Reported Pbca                -P 2ac 2ab
# MoietyFormula C46 H68 N6 Ta2
#      Reported C46 H68 N6 Ta2
#    SumFormula C46 H68 N6 Ta2
#      Reported C46 H68 N6 Ta2
# Mr        =   1066.96[Calc],   1066.96[Rep]
# Dx,gcm-3  =     1.641[Calc],     1.641[Rep]
```

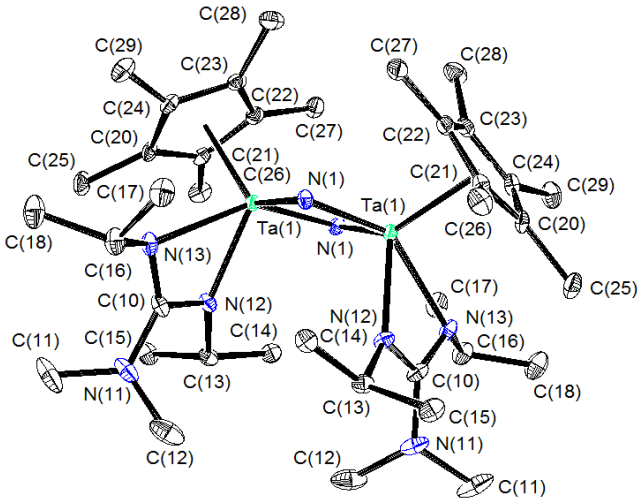
```
# Z         =         4[Calc],         4[Rep]
# Mu (mm-1) =     5.102[Calc],     5.102[Rep]
# F000      =    2128.0[Calc],    2128.0[Rep]  or F000' =   2123.10[Calc]
# Reported   T Limits: Tmin=0.383               Tmax=0.482  AbsCorr=INTEGRATION
# Calculated T Limits: Tmin=0.437 Tmin'=0.404   Tmax=0.482
# Reported   Hmax= 23, Kmax= 21, Lmax= 24, Nref=  6299        , Th(max)= 30.000
# Obs in FCF Hmax= 23, Kmax= 21, Lmax= 24, Nref=  6299        , Th(max)= 29.999
# Calculated Hmax= 23, Kmax= 21, Lmax= 24, Nref=  6299        , Ratio  =  1.000
# Reported   Rho(min) = -0.35, Rho(max) =  0.69 e/Ang**3 (From CIF)
# Calculated Rho(min) = -0.38, Rho(max) =  0.69 e/Ang**3 (From CIF+FCF data)
# w=1/[sigma**2(Fo**2)+(0.0030P)**2+  6.5000P], P=(Fo**2+2*Fc**2)/3
# R= 0.0152(  5387), wR2= 0.0310(  6299), S = 0.998      (From CIF+FCF data)
# R= 0.0152(  5387), wR2= 0.0310(  6299), S = 0.998      (From FCF data only)
# R= 0.0152(  5387), wR2= 0.0311(  6299), S = 1.000, Npar= 269
#===============================================================================

==================================================================================
>>> The Following Model and Quality ALERTS were generated     - (Acta-Mode) <<<
==================================================================================
083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       6.50
#===============================================================================

==================================================================================
>>> The Following Improvement and Query ALERTS were generated - (Acta-Mode) <<<
==================================================================================
764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
#===============================================================================

#===============================================================================
!! Congratulations !! : No (A,B,C) ALERT Conditions were Detected
#===============================================================================
```

cis-{Cp*Ta[N(iPr)C(NMe$_2$)N(iPr](μ-N)}$_2$ (*cis*-3c)



A yellow prism-like specimen of $C_{38}H_{70}N_8Ta_2$, approximate dimensions 0.29 mm × 0.29 mm × 0.34 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 3.37 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a tetragonal unit cell yielded a total of 54593 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 5986 were independent (average redundancy 9.120, completeness = 100.0%, R_{int} = 2.68%) and 5882 (98.26%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.3498(6) Å, b = 11.3498(6) Å, c = 31.8364(17) Å, V = 4101.1(5) Å^3, are based upon the refinement of the XYZ-centroids of 9921 reflections above 20 σ(I) with 5.234° < 2θ < 64.10°. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.1440 and 0.2110. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P4_12_12$, with Z = 4 for the formula unit, $C_{38}H_{70}N_8Ta_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 243 variables converged at R_1 = 1.39%, for the observed data and wR_2 = 3.14% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.720 e$^-$/Å^3 and the largest hole was -0.443 e$^-$/Å^3 with an RMS deviation of 0.062 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.621 g/cm^3 and F(000), 2000 e$^-$.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 3c.

Identification code	**3c**	
Chemical formula	$C_{38}H_{70}N_8Ta_2$	
Formula weight	1000.92	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.29 × 0.29 × 0.34 mm	
Crystal habit	yellow prism	
Crystal system	tetragonal	
Space group	P41212	
Unit cell dimensions	a = 11.3498(6) Å	α = 90°
	b = 11.3498(6) Å	β = 90°
	c = 31.8364(17) Å	γ = 90°
Volume	4101.1(5) Å^3	
Z	4	
Density (calculated)	1.621 Mg/cm^3	
Absorption coefficient	5.368 mm^{-1}	
F(000)	2000	

Table 2. Data collection and structure refinement for 3c.

Diffractometer	Bruker APEX-II CCD	
Radiation source	sealed tube, MoKα	
Theta range for data collection	1.91 to 30.00°	
Index ranges	$-15 \le h \le 15$, $-15 \le k \le 15$, $-44 \le l \le 44$	
Reflections collected	54593	
Independent reflections	5986 [R(int) = 0.0268]	
Coverage of independent reflections	100.0%	
Absorption correction	multi-scan	
Max. and min. transmission	0.2110 and 0.1440	
Structure solution technique	direct methods	
Structure solution program	ShelXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	ShelXL-2012 (Sheldrick, 2012)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5986 / 0 / 243	
Goodness-of-fit on F^2	1.000	
Δ/σ_{max}	0.003	
Final R indices	5882 data; $I>2\sigma(I)$	$R_1 = 0.0139$, $wR_2 = 0.0312$
	all data	$R_1 = 0.0145$, $wR_2 = 0.0314$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0100P)^2+4.7100P]$, $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	-0.013(3)	
Extinction coefficient	0.0003(0)	
Largest diff. peak and hole	0.720 and -0.443 eÅ^{-3}	
R.M.S. deviation from mean	0.062 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$

$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 3c.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ta1	0.56927(2)	0.47287(2)	0.46311(2)	0.01588(3)
N1	0.5833(2)	0.4478(2)	0.52155(7)	0.0179(4)
C10	0.7971(3)	0.5452(3)	0.45156(9)	0.0239(7)
N11	0.9041(2)	0.6076(3)	0.45058(10)	0.0339(7)
C11	0.0054(3)	0.5620(5)	0.42877(16)	0.0549(13)
C12	0.9278(4)	0.7000(4)	0.48047(13)	0.0488(11)
N12	0.6946(2)	0.6036(2)	0.44457(8)	0.0208(5)
C13	0.6975(3)	0.7196(3)	0.42356(10)	0.0230(6)
C14	0.5799(3)	0.7830(3)	0.42835(10)	0.0256(6)
N13	0.7840(2)	0.4329(2)	0.45934(8)	0.0225(5)
C15	0.7326(3)	0.7094(3)	0.37725(10)	0.0293(7)
C16	0.8797(3)	0.3683(3)	0.48107(11)	0.0293(7)
C17	0.8316(3)	0.2995(3)	0.51875(11)	0.0333(8)
C18	0.9469(4)	0.2833(4)	0.45205(13)	0.0425(10)
C20	0.5890(3)	0.3721(3)	0.38952(8)	0.0225(6)
C21	0.4842(3)	0.4385(3)	0.38684(8)	0.0224(5)
C22	0.4027(3)	0.3950(3)	0.41679(9)	0.0230(6)
C23	0.4582(3)	0.2993(3)	0.43853(9)	0.0229(6)
C24	0.5729(3)	0.2850(3)	0.42110(9)	0.0239(6)
C25	0.6953(3)	0.3834(3)	0.36172(10)	0.0329(8)
C26	0.4563(3)	0.5329(3)	0.35501(10)	0.0319(7)
C27	0.2802(3)	0.4405(3)	0.42231(11)	0.0295(7)
C28	0.4023(3)	0.2095(3)	0.46695(11)	0.0332(8)
C29	0.6509(4)	0.1812(3)	0.42972(12)	0.0353(8)

Table 4. Bond lengths (Å) for 3c.

Ta1-N1	1.889(2)	Ta1-N1	1.926(2)
Ta1-N12	2.138(2)	Ta1-C23	2.467(3)
Ta1-N13	2.482(2)	Ta1-C24	2.517(3)
Ta1-C22	2.555(3)	Ta1-C20	2.616(3)

Ta1-C21	2.642(3)	N1-Ta1	1.926(2)
C10-N13	1.308(4)	C10-N12	1.358(4)
C10-N11	1.406(4)	N11-C11	1.440(5)
N11-C12	1.441(6)	C11-H11A	0.98
C11-H11B	0.98	C11-H11C	0.98
C12-H12A	0.98	C12-H12B	0.98
C12-H12C	0.98	N12-C13	1.477(4)
C13-C14	1.524(5)	C13-C15	1.531(4)
C13-H13	1.0	C14-H14A	0.98
C14-H14B	0.98	C14-H14C	0.98
N13-C16	1.482(4)	C15-H15A	0.98
C15-H15B	0.98	C15-H15C	0.98
C16-C17	1.532(5)	C16-C18	1.538(5)
C16-H16	1.0	C17-H17A	0.98
C17-H17B	0.98	C17-H17C	0.98
C18-H18A	0.98	C18-H18B	0.98
C18-H18C	0.98	C20-C21	1.411(4)
C20-C24	1.422(4)	C20-C25	1.501(4)
C21-C22	1.417(4)	C21-C26	1.508(4)
C22-C23	1.434(4)	C22-C27	1.494(4)
C23-C24	1.424(5)	C23-C28	1.503(4)
C24-C29	1.500(5)	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C25-H25D	0.98	C25-H25E	0.98
C25-H25F	0.98	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C28-H28A	0.98
C28-H28B	0.98	C28-H28C	0.98
C29-H29A	0.98	C29-H29B	0.98
C29-H29C	0.98		

Table 5. Bond angles (°) for 3c.

N1-Ta1-N1	84.75(10)	N1-Ta1-N12	108.69(10)
N1-Ta1-N12	95.42(11)	N1-Ta1-C23	103.60(10)
N1-Ta1-C23	103.55(11)	N12-Ta1-C23	143.78(10)
N1-Ta1-N13	86.41(9)	N1-Ta1-N13	146.54(10)

N12-Ta1-N13	57.37(10)	C23-Ta1-N13	109.90(10)
N1-Ta1-C24	113.23(10)	N1-Ta1-C24	134.22(11)
N12-Ta1-C24	115.49(11)	C23-Ta1-C24	33.19(11)
N13-Ta1-C24	78.66(11)	N1-Ta1-C22	125.35(10)
N1-Ta1-C22	80.90(10)	N12-Ta1-C22	124.94(10)
C23-Ta1-C22	33.12(10)	N13-Ta1-C22	129.43(9)
C24-Ta1-C22	54.00(11)	N1-Ta1-C20	143.98(10)
N1-Ta1-C20	124.94(9)	N12-Ta1-C20	89.95(10)
C23-Ta1-C20	53.89(10)	N13-Ta1-C20	78.03(9)
C24-Ta1-C20	32.08(10)	C22-Ta1-C20	52.81(10)
N1-Ta1-C21	156.03(10)	N1-Ta1-C21	93.87(9)
N12-Ta1-C21	95.27(9)	C23-Ta1-C21	53.40(9)
N13-Ta1-C21	106.70(9)	C24-Ta1-C21	52.59(10)
C22-Ta1-C21	31.59(9)	C20-Ta1-C21	31.13(9)
Ta1-N1-Ta1	95.00(10)	N13-C10-N12	114.2(3)
N13-C10-N11	126.4(3)	N12-C10-N11	119.4(3)
C10-N11-C11	121.3(4)	C10-N11-C12	120.9(3)
C11-N11-C12	115.5(4)	N11-C11-H11A	109.5
N11-C11-H11B	109.5	H11A-C11-H11B	109.5
N11-C11-H11C	109.5	H11A-C11-H11C	109.5
H11B-C11-H11C	109.5	N11-C12-H12A	109.5
N11-C12-H12B	109.5	H12A-C12-H12B	109.5
N11-C12-H12C	109.5	H12A-C12-H12C	109.5
H12B-C12-H12C	109.5	C10-N12-C13	119.3(2)
C10-N12-Ta1	100.73(19)	C13-N12-Ta1	139.3(2)
N12-C13-C14	110.8(2)	N12-C13-C15	112.0(3)
C14-C13-C15	111.1(3)	N12-C13-H13	107.6
C14-C13-H13	107.6	C15-C13-H13	107.6
C13-C14-H14A	109.5	C13-C14-H14B	109.5
H14A-C14-H14B	109.5	C13-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
C10-N13-C16	119.1(3)	C10-N13-Ta1	86.71(18)
C16-N13-Ta1	142.0(2)	C13-C15-H15A	109.5
C13-C15-H15B	109.5	H15A-C15-H15B	109.5
C13-C15-H15C	109.5	H15A-C15-H15C	109.5
H15B-C15-H15C	109.5	N13-C16-C17	110.9(3)
N13-C16-C18	113.1(3)	C17-C16-C18	109.1(3)
N13-C16-H16	107.9	C17-C16-H16	107.9

C18-C16-H16	107.9	C16-C17-H17A	109.5
C16-C17-H17B	109.5	H17A-C17-H17B	109.5
C16-C17-H17C	109.5	H17A-C17-H17C	109.5
H17B-C17-H17C	109.5	C16-C18-H18A	109.5
C16-C18-H18B	109.5	H18A-C18-H18B	109.5
C16-C18-H18C	109.5	H18A-C18-H18C	109.5
H18B-C18-H18C	109.5	C21-C20-C24	107.8(3)
C21-C20-C25	126.6(3)	C24-C20-C25	125.4(3)
C21-C20-Ta1	75.43(15)	C24-C20-Ta1	70.10(15)
C25-C20-Ta1	124.0(2)	C20-C21-C22	108.9(3)
C20-C21-C26	126.6(3)	C22-C21-C26	124.3(3)
C20-C21-Ta1	73.44(16)	C22-C21-Ta1	70.84(16)
C26-C21-Ta1	126.10(19)	C21-C22-C23	107.6(3)
C21-C22-C27	124.5(3)	C23-C22-C27	127.9(3)
C21-C22-Ta1	77.57(17)	C23-C22-Ta1	70.04(16)
C27-C22-Ta1	120.1(2)	C24-C23-C22	107.4(3)
C24-C23-C28	122.9(3)	C22-C23-C28	128.2(3)
C24-C23-Ta1	75.34(17)	C22-C23-Ta1	76.84(17)
C28-C23-Ta1	124.5(2)	C20-C24-C23	108.4(3)
C20-C24-C29	126.8(3)	C23-C24-C29	123.9(3)
C20-C24-Ta1	77.82(17)	C23-C24-Ta1	71.47(16)
C29-C24-Ta1	125.3(2)	C20-C25-H25A	109.5
C20-C25-H25B	109.5	H25A-C25-H25B	109.5
C20-C25-H25C	109.5	H25A-C25-H25C	109.5
H25B-C25-H25C	109.5	C20-C25-H25D	109.5
H25A-C25-H25D	141.1	H25B-C25-H25D	56.3
H25C-C25-H25D	56.3	C20-C25-H25E	109.5
H25A-C25-H25E	56.3	H25B-C25-H25E	141.1
H25C-C25-H25E	56.3	H25D-C25-H25E	109.5
C20-C25-H25F	109.5	H25A-C25-H25F	56.3
H25B-C25-H25F	56.3	H25C-C25-H25F	141.1
H25D-C25-H25F	109.5	H25E-C25-H25F	109.5
C21-C26-H26A	109.5	C21-C26-H26B	109.5
H26A-C26-H26B	109.5	C21-C26-H26C	109.5
H26A-C26-H26C	109.5	H26B-C26-H26C	109.5
C22-C27-H27A	109.5	C22-C27-H27B	109.5
H27A-C27-H27B	109.5	C22-C27-H27C	109.5
H27A-C27-H27C	109.5	H27B-C27-H27C	109.5

C23-C28-H28A	109.5	C23-C28-H28B	109.5
H28A-C28-H28B	109.5	C23-C28-H28C	109.5
H28A-C28-H28C	109.5	H28B-C28-H28C	109.5
C24-C29-H29A	109.5	C24-C29-H29B	109.5
H29A-C29-H29B	109.5	C24-C29-H29C	109.5
H29A-C29-H29C	109.5	H29B-C29-H29C	109.5

Table 6. Torsion angles (°) for 3c.

N1-Ta1-N1-Ta1	-5.30(15)	N12-Ta1-N1-Ta1	88.66(11)
C23-Ta1-N1-Ta1	-108.00(11)	N13-Ta1-N1-Ta1	142.38(11)
C24-Ta1-N1-Ta1	-141.58(11)	C22-Ta1-N1-Ta1	-80.25(13)
C20-Ta1-N1-Ta1	-153.71(13)	C21-Ta1-N1-Ta1	-93.0(2)
N13-C10-N11-C11	46.1(5)	N12-C10-N11-C11	-135.0(3)
N13-C10-N11-C12	-115.8(4)	N12-C10-N11-C12	63.1(4)
N13-C10-N12-C13	-162.1(3)	N11-C10-N12-C13	18.8(4)
N13-C10-N12-Ta1	10.6(3)	N11-C10-N12-Ta1	-168.4(2)
C10-N12-C13-C14	-166.0(3)	Ta1-N12-C13-C14	25.0(4)
C10-N12-C13-C15	69.3(4)	Ta1-N12-C13-C15	-99.7(3)
N12-C10-N13-C16	-159.6(3)	N11-C10-N13-C16	19.3(5)
N12-C10-N13-Ta1	-9.0(2)	N11-C10-N13-Ta1	170.0(3)
C10-N13-C16-C17	128.9(3)	Ta1-N13-C16-C17	1.6(5)
C10-N13-C16-C18	-108.2(4)	Ta1-N13-C16-C18	124.5(3)
C24-C20-C21-C22	0.7(3)	C25-C20-C21-C22	175.8(3)
Ta1-C20-C21-C22	-62.4(2)	C24-C20-C21-C26	-173.9(3)
C25-C20-C21-C26	1.2(5)	Ta1-C20-C21-C26	123.0(3)
C24-C20-C21-Ta1	63.1(2)	C25-C20-C21-Ta1	-121.8(3)
C20-C21-C22-C23	-0.1(3)	C26-C21-C22-C23	174.7(3)
Ta1-C21-C22-C23	-64.11(19)	C20-C21-C22-C27	-177.9(3)
C26-C21-C22-C27	-3.1(5)	Ta1-C21-C22-C27	118.1(3)
C20-C21-C22-Ta1	64.1(2)	C26-C21-C22-Ta1	-121.2(3)
C21-C22-C23-C24	-0.6(3)	C27-C22-C23-C24	177.1(3)
Ta1-C22-C23-C24	-69.8(2)	C21-C22-C23-C28	-167.0(3)
C27-C22-C23-C28	10.7(5)	Ta1-C22-C23-C28	123.8(3)
C21-C22-C23-Ta1	69.2(2)	C27-C22-C23-Ta1	-113.1(3)
C21-C20-C24-C23	-1.1(3)	C25-C20-C24-C23	-176.2(3)
Ta1-C20-C24-C23	65.5(2)	C21-C20-C24-C29	168.1(3)
C25-C20-C24-C29	-7.0(5)	Ta1-C20-C24-C29	-125.3(4)

C21-C20-C24-Ta1	-66.6(2)	C25-C20-C24-Ta1	118.2(3)
C22-C23-C24-C20	1.0(3)	C28-C23-C24-C20	168.4(3)
Ta1-C23-C24-C20	-69.8(2)	C22-C23-C24-C29	-168.6(3)
C28-C23-C24-C29	-1.2(5)	Ta1-C23-C24-C29	120.6(3)
C22-C23-C24-Ta1	70.8(2)	C28-C23-C24-Ta1	-121.9(3)

Table 7. Anisotropic atomic displacement parameters ($Å^2$) for 3c.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.01694(5)	0.01615(5)	0.01454(4)	-0.00105(4)	0.00160(4)	0.00090(4)
N1	0.0183(11)	0.0204(12)	0.0151(9)	0.0016(8)	0.0017(8)	0.0029(8)
C10	0.0170(13)	0.0347(19)	0.0200(13)	0.0058(11)	0.0033(10)	0.0014(12)
N11	0.0171(13)	0.0427(17)	0.0419(17)	0.0151(13)	0.0038(11)	-0.0017(12)
C11	0.0236(19)	0.075(3)	0.066(3)	0.030(3)	0.0167(18)	0.006(2)
C12	0.032(2)	0.068(3)	0.046(2)	0.018(2)	-0.0145(18)	-0.020(2)
N12	0.0171(12)	0.0233(13)	0.0218(11)	0.0057(9)	0.0027(9)	0.0006(9)
C13	0.0226(15)	0.0241(15)	0.0221(13)	0.0055(11)	-0.0009(11)	-0.0025(11)
C14	0.0297(16)	0.0212(14)	0.0260(15)	0.0041(11)	-0.0024(13)	0.0020(13)
N13	0.0220(11)	0.0291(12)	0.0164(11)	0.0037(11)	0.0035(9)	0.0066(10)
C15	0.0306(17)	0.0353(18)	0.0221(14)	0.0091(13)	0.0022(12)	0.0002(14)
C16	0.0239(16)	0.0347(18)	0.0293(16)	0.0039(14)	-0.0016(13)	0.0105(14)
C17	0.040(2)	0.0316(18)	0.0285(16)	0.0089(14)	-0.0004(14)	0.0118(16)
C18	0.034(2)	0.050(2)	0.044(2)	0.0017(17)	0.0062(16)	0.0199(17)
C20	0.0293(17)	0.0241(14)	0.0141(11)	-0.0052(10)	0.0036(11)	0.0032(11)
C21	0.0268(14)	0.0204(13)	0.0201(11)	-0.0045(10)	-0.0030(10)	0.0016(11)
C22	0.0240(15)	0.0231(14)	0.0218(13)	-0.0054(11)	-0.0026(10)	-0.0010(11)
C23	0.0286(17)	0.0199(13)	0.0202(13)	-0.0040(10)	-0.0011(11)	-0.0037(11)
C24	0.0321(16)	0.0197(13)	0.0200(13)	-0.0050(10)	-0.0001(12)	0.0043(13)
C25	0.039(2)	0.0363(19)	0.0230(14)	-0.0039(13)	0.0115(14)	0.0042(15)
C26	0.0402(19)	0.0292(15)	0.0262(14)	0.0014(12)	-0.0077(12)	0.0013(14)
C27	0.0222(14)	0.0353(18)	0.0309(16)	-0.0102(14)	-0.0043(12)	0.0007(13)
C28	0.043(2)	0.0283(16)	0.0287(17)	0.0012(14)	-0.0005(15)	-0.0116(14)
C29	0.044(2)	0.0246(17)	0.0372(19)	-0.0038(14)	-0.0021(16)	0.0101(15)

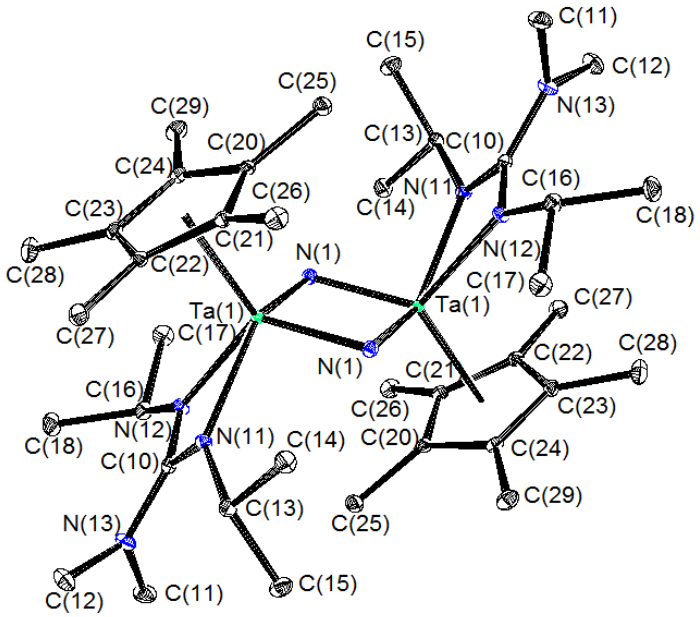
Table 8. Hydrogen atomic coordinates and isotropic

atomic displacement parameters (Å^2) for 3c.

	x/a	y/b	z/c	U(eq)
H11A	1.0563	0.5201	0.4487	0.061(9)
H11B	1.0494	0.6272	0.4161	0.061(9)
H11C	0.9796	0.5075	0.4067	0.061(9)
H12A	0.8555	0.7190	0.4959	0.062(9)
H12B	0.9558	0.7703	0.4656	0.062(9)
H12C	0.9884	0.6736	0.5003	0.062(9)
H13	0.7588	0.7684	0.4379	0.023(9)
H14A	0.5187	0.7394	0.4132	0.037(6)
H14B	0.5863	0.8627	0.4168	0.037(6)
H14C	0.5591	0.7876	0.4582	0.037(6)
H15A	0.8087	0.6690	0.3751	0.036(6)
H15B	0.7391	0.7883	0.3650	0.036(6)
H15C	0.6725	0.6643	0.3621	0.036(6)
H16	0.9373	0.4277	0.4919	0.027(9)
H17A	0.7901	0.3535	0.5377	0.040(7)
H17B	0.8970	0.2623	0.5338	0.040(7)
H17C	0.7769	0.2387	0.5089	0.040(7)
H18A	0.8971	0.2149	0.4458	0.051(8)
H18B	1.0192	0.2570	0.4660	0.051(8)
H18C	0.9670	0.3237	0.4258	0.051(8)
H25A	0.6702	0.3857	0.3323	0.042(11)
H25B	0.7473	0.3156	0.3661	0.042(11)
H25C	0.7376	0.4561	0.3686	0.042(11)
H25D	0.7665	0.3859	0.3791	0.042(11)
H25E	0.6894	0.4560	0.3452	0.042(11)
H25F	0.6992	0.3155	0.3427	0.042(11)
H26A	0.5246	0.5449	0.3366	0.055(8)
H26B	0.4379	0.6067	0.3696	0.055(8)
H26C	0.3884	0.5085	0.3381	0.055(8)
H27A	0.2821	0.5126	0.4393	0.047(8)
H27B	0.2322	0.3809	0.4365	0.047(8)
H27C	0.2460	0.4580	0.3947	0.047(8)
H28A	0.3950	0.1344	0.4520	0.047(8)
H28B	0.3240	0.2370	0.4754	0.047(8)
H28C	0.4516	0.1987	0.4919	0.047(8)
H29A	0.6603	0.1715	0.4601	0.051(8)

	x/a	y/b	z/c	U(eq)
H29B	0.7282	0.1942	0.4168	0.051(8)
H29C	0.6151	0.1100	0.4179	0.051(8)

trans-{Cp*Ta[N(iPr)C(NMe$_2$)N(iPr](μ-N)}$_2$ (*trans*-3c)



A brown prism of $C_{38}H_{70}N_8Ta_2$, approximate dimensions 0.18×0.21×0.28 mm^3, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 100(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoKα fine-focus sealed tube (λ= 0.71073 Å) . The detector was placed at a distance of 5.0000 cm from the crystal.

A total of 1830 frames were collected with a scan width of -0.30° an exposure time of 5 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 5.6 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of the data using a Monoclinic unit cell yielded a total of 22594 reflections to a maximum θ angle of 30.00°, of which 5734 were independent (completeness = 99.9%, R_{int} = 1.88%, R_{sig} = 1.58%) and 5513 were greater than 2σ(I). The final cell dimensions of a = 11.1501(7) Å, b = 11.8403(8) Å, c = 14.9152(10) Å, α = 90°, β = 90.4380(10)°, γ = 90°, V = 1969.1(2) Å^3, are based upon the refinement of the XYZ-centroids of 16923 reflections with 2.2 < θ < 32.4° using Apex2 software. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.272 and 0.366.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group $P2_1/n$ with Z = 2 for the formula unit $C_{38}H_{70}N_8Ta_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 241 variables converged at R_1 = 1.48 % for the observed data and wR_2 = 3.50 % for all data. The goodness-of-fit was 1.000. The largest peak on the final difference map was 1.129 $\bar{e}$/Å^3 and the largest hole was -0.681 $\bar{e}$/Å^3. On the basis of the final model, the calculated density was 1.688 g/cm^3 and F(000), 1000 $\bar{e}$.

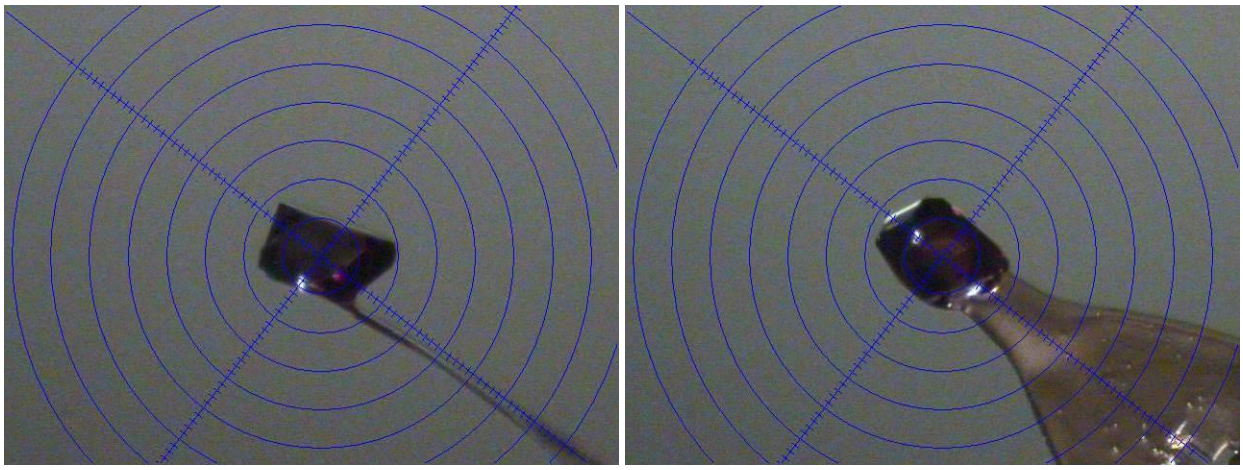


Table 1. Crystal data and structure refinement for ***trans*-3c**.

X-ray lab book No.		***trans*-3c**
Crystal ID		***trans*-3c**
Empirical formula		$C_{38}H_{70}N_8Ta_2$
Formula weight		1000.92
Temperature		100(2) K
Wavelength		0.71073 Å
Crystal size		0.28×0.21×0.18 mm^3
Crystal habit		brown prism
Crystal system		Monoclinic
Space group		$P2_1/n$
Unit cell dimensions		a = 11.1501(7) Å α = 90°
		b = 11.8403(8) Å β = 90.4380(10)°
		c = 14.9152(10) Å γ = 90°
Volume		1969.1(2) $Å^3$
Z		2
Density, ρ_{calc}		1.688 g/cm^3
Absorption coefficient, μ		5.590 mm^{-1}
F(000)		1000 $\bar{e}$
Diffractometer		Bruker Smart Apex II CCD area detector
Radiation source		fine-focus sealed tube, MoKα
Detector distance		5.00 cm
Data collection method		ω scans
Total frames		1830
Frame size		512 pixels
Frame width		-0.30°
Exposure per frame		5 sec
Total measurement time		5.6 hours
θ range for data collection		2.20 to 30.00°
Index ranges		$-15 \le h \le 15$, $-16 \le k \le 16$, $-20 \le l \le 20$
Reflections collected		22594
Independent reflections		5734
Observed reflection, I>2σ(I)		5513
Coverage of independent reflections		99.9 %
Variation in check reflections		0 %
Absorption correction		Semi-empirical from equivalents
		SADABS (Sheldrick, 1996)
Max. and min. transmission		0.366 and 0.272
Structure solution technique		direct
Structure solution program		SHELXS-97 (Sheldrick, 1990)
Refinement technique		Full-matrix least-squares on F^2
Refinement program		SHELXL-97 (Sheldrick, 1997)
Function minimized		$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters		5734 / 0 / 241
Goodness-of-fit on F^2		1.000
Δ/σ_{max}		0.002
Final R indices:	R_1, I>2σ(I)	0.0148
	wR_2, all data	0.0350
	R_{int}	0.0188
	R_{sig}	0.0158
Weighting scheme		$w = 1/[\sigma^2(F_o^2)+ (0.01P)^2 + 2.41P]$, $P = [\max(F_o^2, 0) + 2F_o^2]/3$
Largest diff. peak and hole		1.129 and -0.681 $\bar{e}/Å^3$

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table 2. Atomic coordinates and equivalent* isotropic atomic displacement parameters (Å^2) for ***trans*-3c**.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Ta1	0.463683(5)	0.592129(5)	0.053643(4)	0.00762(2)
N1	0.43657(13)	0.42927(12)	0.04602(9)	0.0108(2)
N11	0.40000(12)	0.76060(12)	-0.00427(9)	0.0108(2)
N12	0.27047(12)	0.62702(12)	0.03137(10)	0.0109(3)
N13	0.19172(13)	0.79786(13)	-0.03536(10)	0.0148(3)
C10	0.28498(15)	0.73070(14)	-0.00384(11)	0.0114(3)
C11	0.10019(17)	0.75621(17)	-0.09668(13)	0.0202(4)
C12	0.18961(18)	0.91826(15)	-0.01888(14)	0.0203(4)
C13	0.44589(15)	0.84825(14)	-0.06509(11)	0.0125(3)
C14	0.58269(16)	0.84957(15)	-0.06154(12)	0.0164(3)
C15	0.40578(18)	0.83284(16)	-0.16306(12)	0.0178(3)
C16	0.15286(15)	0.57662(15)	0.05121(12)	0.0139(3)
C17	0.16968(16)	0.46426(16)	0.09944(13)	0.0187(3)
C18	0.06862(16)	0.65170(18)	0.10651(13)	0.0208(4)
C20	0.60222(15)	0.56328(14)	0.17875(11)	0.0114(3)
C21	0.61730(15)	0.67948(14)	0.15476(11)	0.0112(3)
C22	0.51100(15)	0.73732(14)	0.17923(11)	0.0120(3)
C23	0.43122(15)	0.65819(15)	0.21906(11)	0.0127(3)
C24	0.48803(15)	0.55111(14)	0.22034(11)	0.0120(3)
C25	0.69882(16)	0.47504(15)	0.17638(12)	0.0160(3)
C26	0.73304(16)	0.72991(16)	0.12206(12)	0.0170(3)
C27	0.48931(17)	0.86243(15)	0.17583(12)	0.0175(3)
C28	0.31503(17)	0.68923(17)	0.26265(13)	0.0204(4)
C29	0.44118(17)	0.44401(16)	0.26069(12)	0.0179(3)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic atomic displacement parameters* ($Å^2$) for ***trans*-3c**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.00809(3)	0.00747(3)	0.00729(3)	-0.00037(2)	-0.00009(2)	-0.00013(2)
N1	0.0114(6)	0.0106(6)	0.0103(6)	0.0004(5)	0.0010(5)	-0.0006(5)
N11	0.0122(6)	0.0089(6)	0.0114(6)	0.0021(5)	0.0004(5)	0.0004(5)
N12	0.0090(6)	0.0102(6)	0.0135(6)	0.0009(5)	0.0001(5)	0.0000(5)
N13	0.0133(7)	0.0127(7)	0.0183(7)	0.0004(5)	-0.0044(5)	0.0024(5)
C10	0.0130(7)	0.0120(7)	0.0093(7)	-0.0015(6)	-0.0005(5)	0.0026(6)
C11	0.0174(8)	0.0224(9)	0.0207(9)	0.0001(7)	-0.0076(7)	0.0021(7)
C12	0.0195(9)	0.0146(8)	0.0268(10)	-0.0012(7)	-0.0010(7)	0.0053(7)
C13	0.0167(8)	0.0086(7)	0.0121(7)	0.0009(6)	0.0015(6)	0.0005(6)
C14	0.0152(8)	0.0150(8)	0.0192(8)	0.0030(6)	0.0037(6)	-0.0017(6)
C15	0.0254(9)	0.0147(8)	0.0132(8)	0.0023(6)	-0.0001(6)	-0.0021(7)
C16	0.0113(7)	0.0165(8)	0.0139(7)	0.0002(6)	0.0013(6)	-0.0026(6)
C17	0.0145(8)	0.0190(9)	0.0227(9)	0.0032(7)	0.0035(7)	-0.0047(7)
C18	0.0124(8)	0.0272(10)	0.0228(9)	-0.0018(7)	0.0048(7)	0.0011(7)
C20	0.0132(7)	0.0120(7)	0.0089(7)	-0.0008(5)	-0.0018(5)	0.0005(6)
C21	0.0122(7)	0.0118(7)	0.0098(7)	-0.0009(5)	-0.0018(5)	-0.0019(6)
C22	0.0161(7)	0.0107(7)	0.0093(7)	-0.0017(5)	-0.0023(6)	0.0005(6)
C23	0.0135(7)	0.0149(8)	0.0098(7)	-0.0026(6)	-0.0003(6)	0.0004(6)
C24	0.0155(7)	0.0123(7)	0.0081(7)	-0.0001(6)	-0.0006(5)	-0.0017(6)
C25	0.0177(8)	0.0150(8)	0.0151(8)	-0.0022(6)	-0.0024(6)	0.0038(6)
C26	0.0145(8)	0.0190(8)	0.0176(8)	0.0002(7)	-0.0010(6)	-0.0048(6)
C27	0.0250(9)	0.0112(8)	0.0162(8)	-0.0028(6)	-0.0009(7)	0.0018(7)
C28	0.0161(8)	0.0263(9)	0.0188(8)	-0.0079(7)	0.0034(6)	-0.0003(7)
C29	0.0231(9)	0.0160(8)	0.0147(8)	0.0027(6)	0.0017(6)	-0.0040(7)

* The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Table 4. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å^2) for ***trans*-3c**.

Atom	*x/a*	*y/b*	*z/c*	U_{iso}
H11A	0.1203	0.6792	-0.1153	0.034(4)
H11B	0.0961	0.8053	-0.1495	0.034(4)
H11C	0.0223	0.7561	-0.0666	0.034(4)
H12A	0.2474	0.9369	0.0287	0.031(4)
H12B	0.1090	0.9409	-0.0003	0.031(4)
H12C	0.2110	0.9586	-0.0739	0.031(4)
H13	0.4162	0.9232	-0.0438	0.013(5)
H14A	0.6096	0.8667	-0.0003	0.021(3)
H14B	0.6129	0.9074	-0.1026	0.021(3)
H14C	0.6135	0.7754	-0.0794	0.021(3)
H15A	0.4370	0.7611	-0.1860	0.031(4)
H15B	0.4368	0.8953	-0.1993	0.031(4)
H15C	0.3180	0.8323	-0.1664	0.031(4)
H16	0.1120	0.5607	-0.0074	0.014(5)
H17A	0.2207	0.4148	0.0634	0.025(4)
H17B	0.0914	0.4284	0.1080	0.025(4)
H17C	0.2077	0.4774	0.1580	0.025(4)
H18A	0.1015	0.6609	0.1672	0.032(4)
H18B	-0.0106	0.6162	0.1098	0.032(4)
H18C	0.0612	0.7259	0.0778	0.032(4)
H25A	0.7376	0.4699	0.2354	0.034(4)
H25B	0.7586	0.4958	0.1314	0.034(4)
H25C	0.6634	0.4018	0.1607	0.034(4)
H26A	0.7249	0.8122	0.1183	0.029(4)
H26B	0.7515	0.6995	0.0626	0.029(4)
H26C	0.7980	0.7108	0.1640	0.029(4)
H27A	0.4941	0.8937	0.2366	0.050(5)
H27B	0.4095	0.8771	0.1505	0.050(5)
H27C	0.5502	0.8982	0.1382	0.050(5)
H28A	0.2649	0.6217	0.2684	0.031(4)
H28B	0.2731	0.7455	0.2258	0.031(4)
H28C	0.3312	0.7208	0.3223	0.031(4)
H29A	0.3670	0.4599	0.2931	0.029(4)
H29B	0.5011	0.4130	0.3023	0.029(4)
H29C	0.4249	0.3891	0.2130	0.029(4)

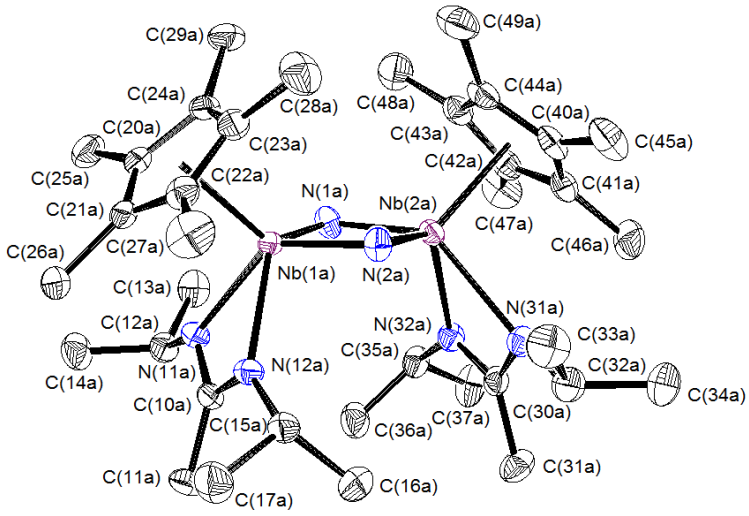
Table 5. Bond lengths (Å), valence and torsion angles (°) for ***trans*-3c**.

Ta1-N1#1	1.8805(14)	Ta1-N1	1.9550(14)	Ta1-N12	2.2162(14)
Ta1-N11	2.2847(14)	Ta1-C20	2.4374(16)	Ta1-C21	2.4977(16)
Ta1-C24	2.5458(16)	Ta1-C22	2.5937(16)	Ta1-C23	2.6160(16)
Ta1-Ta1#1	2.82778(18)	N1-Ta1#1	1.8805(14)	N11-C10	1.330(2)
N11-C13	1.473(2)	N12-C10	1.345(2)	N12-C16	1.473(2)
N13-C10	1.388(2)	N13-C12	1.447(2)	N13-C11	1.452(2)
C13-C14	1.526(2)	C13-C15	1.536(2)	C16-C17	1.523(3)
C16-C18	1.538(3)	C20-C24	1.428(2)	C20-C21	1.432(2)
C20-C25	1.501(2)	C21-C22	1.419(2)	C21-C26	1.506(2)
C22-C23	1.425(2)	C22-C27	1.502(2)	C23-C24	1.417(2)
C23-C28	1.500(2)	C24-C29	1.499(2)		
N1#1-Ta1-N1	85.02(6)	N1#1-Ta1-N12	119.13(6)	N1-Ta1-N12	91.46(6)
N1#1-Ta1-N11	90.16(6)	N1-Ta1-N11	142.34(5)	N12-Ta1-N11	58.77(5)
N1#1-Ta1-C20	102.19(6)	N1-Ta1-C20	90.18(6)	N12-Ta1-C20	138.64(5)
N11-Ta1-C20	127.24(5)	N1#1-Ta1-C21	97.25(6)	N1-Ta1-C21	123.27(6)
N12-Ta1-C21	132.43(5)	N11-Ta1-C21	94.38(5)	C20-Ta1-C21	33.70(5)
N1#1-Ta1-C24	133.40(6)	N1-Ta1-C24	83.33(6)	N12-Ta1-C24	106.16(5)
N11-Ta1-C24	124.49(5)	C20-Ta1-C24	33.21(5)	C21-Ta1-C24	54.67(5)
N1#1-Ta1-C22	122.82(6)	N1-Ta1-C22	136.57(6)	N12-Ta1-C22	100.19(5)
N11-Ta1-C22	75.83(5)	C20-Ta1-C22	54.25(5)	C21-Ta1-C22	32.30(5)
C24-Ta1-C22	53.24(5)	N1#1-Ta1-C23	150.78(6)	N1-Ta1-C23	109.11(6)
N12-Ta1-C23	86.81(5)	N11-Ta1-C23	92.90(5)	C20-Ta1-C23	53.94(5)
C21-Ta1-C23	53.55(5)	C24-Ta1-C23	31.84(5)	C22-Ta1-C23	31.74(5)
N1#1-Ta1-Ta1#1	43.53(4)	N1-Ta1-Ta1#1	41.49(4)	N12-Ta1-Ta1#1	109.95(4)
N11-Ta1-Ta1#1	123.31(4)	C20-Ta1-Ta1#1	98.20(4)	C21-Ta1-Ta1#1	117.59(4)
C24-Ta1-Ta1#1	112.13(4)	C22-Ta1-Ta1#1	149.60(4)	C23-Ta1-Ta1#1	143.77(4)
Ta1#1-N1-Ta1	94.98(6)	C10-N11-C13	122.00(14)	C10-N11-Ta1	93.60(10)
C13-N11-Ta1	137.70(11)	C10-N12-C16	123.92(14)	C10-N12-Ta1	96.25(10)
C16-N12-Ta1	139.49(11)	C10-N13-C12	121.33(15)	C10-N13-C11	122.68(15)
C12-N13-C11	115.44(15)	N11-C10-N12	111.31(14)	N11-C10-N13	124.44(15)
N12-C10-N13	124.25(15)	N11-C13-C14	109.74(13)	N11-C13-C15	113.72(14)
C14-C13-C15	108.55(14)	N12-C16-C17	110.01(14)	N12-C16-C18	114.96(15)
C17-C16-C18	108.96(15)	C24-C20-C21	108.20(15)	C24-C20-C25	125.62(15)
C21-C20-C25	125.26(15)	C24-C20-Ta1	77.57(9)	C21-C20-Ta1	75.46(9)
C25-C20-Ta1	122.01(11)	C22-C21-C20	107.43(14)	C22-C21-C26	127.68(15)
C20-C21-C26	124.35(15)	C22-C21-Ta1	77.58(9)	C20-C21-Ta1	70.84(9)
C26-C21-Ta1	123.63(11)	C21-C22-C23	108.37(14)	C21-C22-C27	127.01(16)
C23-C22-C27	124.18(15)	C21-C22-Ta1	70.13(9)	C23-C22-Ta1	74.99(9)
C27-C22-Ta1	126.70(11)	C24-C23-C22	108.27(15)	C24-C23-C28	126.93(16)
C22-C23-C28	124.32(16)	C24-C23-Ta1	71.35(9)	C22-C23-Ta1	73.27(9)
C28-C23-Ta1	127.47(12)	C23-C24-C20	107.69(15)	C23-C24-C29	127.23(16)
C20-C24-C29	125.05(16)	C23-C24-Ta1	76.81(9)	C20-C24-Ta1	69.22(9)
C29-C24-Ta1	121.23(11)				
N1#1-Ta1-N1-Ta1#1	0.0	N12-Ta1-N1-Ta1#1	119.11(6)	N11-Ta1-N1-Ta1#1	83.78(10)
C20-Ta1-N1-Ta1#1	-102.22(6)	C21-Ta1-N1-Ta1#1	-95.41(7)	C24-Ta1-N1-Ta1#1	-134.79(6)
C22-Ta1-N1-Ta1#1	-134.38(6)	C23-Ta1-N1-Ta1#1	-153.76(5)	N1#1-Ta1-N11-C10	123.01(10)
N1-Ta1-N11-C10	40.97(14)	N12-Ta1-N11-C10	-1.57(9)	C20-Ta1-N11-C10	-131.48(10)
C21-Ta1-N11-C10	-139.71(10)	C24-Ta1-N11-C10	-90.32(11)	C22-Ta1-N11-C10	-113.05(10)
C23-Ta1-N11-C10	-86.06(10)	Ta1#1-Ta1-N11-C10	92.97(9)	N1#1-Ta1-N11-C13	-26.09(16)
N1-Ta1-N11-C13	-108.13(16)	N12-Ta1-N11-C13	-150.66(17)	C20-Ta1-N11-C13	79.42(17)
C21-Ta1-N11-C13	71.19(16)	C24-Ta1-N11-C13	120.58(15)	C22-Ta1-N11-C13	97.85(16)
C23-Ta1-N11-C13	124.84(16)	Ta1#1-Ta1-N11-C13	-56.12(17)	N1#1-Ta1-N12-C10	-68.93(11)
N1-Ta1-N12-C10	-154.04(10)	N11-Ta1-N12-C10	1.55(9)	C20-Ta1-N12-C10	114.03(11)
C21-Ta1-N12-C10	65.90(12)	C24-Ta1-N12-C10	122.47(10)	C22-Ta1-N12-C10	67.99(10)
C23-Ta1-N12-C10	96.90(10)	Ta1#1-Ta1-N12-C10	-116.04(9)	N1#1-Ta1-N12-C16	118.07(17)
N1-Ta1-N12-C16	32.96(17)	N11-Ta1-N12-C16	-171.44(19)	C20-Ta1-N12-C16	-59.0(2)
C21-Ta1-N12-C16	-107.10(17)	C24-Ta1-N12-C16	-50.52(18)	C22-Ta1-N12-C16	-105.00(17)
C23-Ta1-N12-C16	-76.10(17)	Ta1#1-Ta1-N12-C16	70.96(17)	C13-N11-C10-N12	158.32(14)

Ta1-N11-C10-N12	2.37(14)	C13-N11-C10-N13	-21.9(2)	Ta1-N11-C10-N13	-177.83(14)
C16-N12-C10-N11	172.07(14)	Ta1-N12-C10-N11	-2.45(14)	C16-N12-C10-N13	-7.7(3)
Ta1-N12-C10-N13	177.74(14)	C12-N13-C10-N11	-40.2(3)	C11-N13-C10-N11	130.96(18)
C12-N13-C10-N12	139.63(18)	C11-N13-C10-N12	-49.3(2)	C10-N11-C13-C14	-170.34(15)
Ta1-N11-C13-C14	-27.5(2)	C10-N11-C13-C15	-48.6(2)	Ta1-N11-C13-C15	94.26(18)
C10-N12-C16-C17	-174.01(15)	Ta1-N12-C16-C17	-2.4(2)	C10-N12-C16-C18	-50.6(2)
Ta1-N12-C16-C18	121.03(17)	N1#1-Ta1-C20-C24	-162.43(10)	N1-Ta1-C20-C24	-77.49(10)
N12-Ta1-C20-C24	14.92(14)	N11-Ta1-C20-C24	97.91(10)	C21-Ta1-C20-C24	112.80(14)
C22-Ta1-C20-C24	75.72(10)	C23-Ta1-C20-C24	36.26(9)	Ta1#1-Ta1-C20-C24	-118.34(9)
N1#1-Ta1-C20-C21	84.77(10)	N1-Ta1-C20-C21	169.71(10)	N12-Ta1-C20-C21	-97.88(11)
N11-Ta1-C20-C21	-14.89(12)	C24-Ta1-C20-C21	-112.80(14)	C22-Ta1-C20-C21	-37.08(9)
C23-Ta1-C20-C21	-76.55(10)	Ta1#1-Ta1-C20-C21	128.85(9)	N1#1-Ta1-C20-C25	-37.99(14)
N1-Ta1-C20-C25	46.95(14)	N12-Ta1-C20-C25	139.36(12)	N11-Ta1-C20-C25	-137.65(13)
C21-Ta1-C20-C25	-122.76(18)	C24-Ta1-C20-C25	124.44(18)	C22-Ta1-C20-C25	-159.84(16)
C23-Ta1-C20-C25	160.69(16)	Ta1#1-Ta1-C20-C25	6.09(14)	C24-C20-C21-C22	-1.73(18)
C25-C20-C21-C22	-171.20(15)	Ta1-C20-C21-C22	69.64(11)	C24-C20-C21-C26	170.42(15)
C25-C20-C21-C26	1.0(3)	Ta1-C20-C21-C26	-118.21(16)	C24-C20-C21-Ta1	-71.37(11)
C25-C20-C21-Ta1	119.16(16)	N1#1-Ta1-C21-C22	145.22(10)	N1-Ta1-C21-C22	-126.00(10)
N12-Ta1-C21-C22	3.87(13)	N11-Ta1-C21-C22	54.50(10)	C20-Ta1-C21-C22	-113.66(14)
C24-Ta1-C21-C22	-75.43(10)	C23-Ta1-C21-C22	-35.88(9)	Ta1#1-Ta1-C21-C22	-174.08(8)
N1#1-Ta1-C21-C20	-101.12(10)	N1-Ta1-C21-C20	-12.34(12)	N12-Ta1-C21-C20	117.53(10)
N11-Ta1-C21-C20	168.16(10)	C24-Ta1-C21-C20	38.23(9)	C22-Ta1-C21-C20	113.66(14)
C23-Ta1-C21-C20	77.78(10)	Ta1#1-Ta1-C21-C20	-60.42(10)	N1#1-Ta1-C21-C26	17.98(15)
N1-Ta1-C21-C26	106.76(14)	N12-Ta1-C21-C26	-123.38(13)	N11-Ta1-C21-C26	-72.75(14)
C20-Ta1-C21-C26	119.10(18)	C24-Ta1-C21-C26	157.33(16)	C22-Ta1-C21-C26	-127.24(18)
C23-Ta1-C21-C26	-163.12(16)	Ta1#1-Ta1-C21-C26	58.67(14)	C20-C21-C22-C23	0.71(18)
C26-C21-C22-C23	-171.09(16)	Ta1-C21-C22-C23	65.78(11)	C20-C21-C22-C27	173.37(16)
C26-C21-C22-C27	1.6(3)	Ta1-C21-C22-C27	-121.56(16)	C20-C21-C22-Ta1	-65.07(11)
C26-C21-C22-Ta1	123.12(17)	N1#1-Ta1-C22-C21	-42.33(12)	N1-Ta1-C22-C21	79.75(12)
N12-Ta1-C22-C21	-177.10(10)	N11-Ta1-C22-C21	-123.16(10)	C20-Ta1-C22-C21	38.78(9)
C24-Ta1-C22-C21	80.27(10)	C23-Ta1-C22-C21	116.35(14)	Ta1#1-Ta1-C22-C21	10.40(14)
N1#1-Ta1-C22-C23	-158.68(10)	N1-Ta1-C22-C23	-36.60(13)	N12-Ta1-C22-C23	66.55(10)
N11-Ta1-C22-C23	120.49(10)	C20-Ta1-C22-C23	-77.58(10)	C21-Ta1-C22-C23	-116.35(14)
C24-Ta1-C22-C23	-36.08(9)	Ta1#1-Ta1-C22-C23	-105.95(10)	N1#1-Ta1-C22-C27	79.61(16)
N1-Ta1-C22-C27	-158.31(13)	N12-Ta1-C22-C27	-55.17(15)	N11-Ta1-C22-C27	-1.22(14)
C20-Ta1-C22-C27	160.71(17)	C21-Ta1-C22-C27	121.93(19)	C24-Ta1-C22-C27	-157.80(17)
C23-Ta1-C22-C27	-121.71(19)	Ta1#1-Ta1-C22-C27	132.33(12)	C21-C22-C23-C24	0.58(18)
C27-C22-C23-C24	-172.33(15)	Ta1-C22-C23-C24	63.20(11)	C21-C22-C23-C28	173.05(16)
C27-C22-C23-C28	0.1(3)	Ta1-C22-C23-C28	-124.33(16)	C21-C22-C23-Ta1	-62.62(11)
C27-C22-C23-Ta1	124.47(16)	N1#1-Ta1-C23-C24	-77.80(15)	N1-Ta1-C23-C24	37.74(11)
N12-Ta1-C23-C24	128.18(10)	N11-Ta1-C23-C24	-173.33(10)	C20-Ta1-C23-C24	-37.89(10)
C21-Ta1-C23-C24	-80.02(11)	C22-Ta1-C23-C24	-116.55(14)	Ta1#1-Ta1-C23-C24	8.04(13)
N1#1-Ta1-C23-C22	38.75(17)	N1-Ta1-C23-C22	154.29(10)	N12-Ta1-C23-C22	-115.27(10)
N11-Ta1-C23-C22	-56.78(10)	C20-Ta1-C23-C22	78.66(10)	C21-Ta1-C23-C22	36.53(9)
C24-Ta1-C23-C22	116.55(14)	Ta1#1-Ta1-C23-C22	124.59(9)	N1#1-Ta1-C23-C28	159.50(15)
N1-Ta1-C23-C28	-84.96(16)	N12-Ta1-C23-C28	5.48(15)	N11-Ta1-C23-C28	63.97(16)
C20-Ta1-C23-C28	-160.59(18)	C21-Ta1-C23-C28	157.27(18)	C24-Ta1-C23-C28	-122.7(2)
C22-Ta1-C23-C28	120.7(2)	Ta1#1-Ta1-C23-C28	-114.67(14)	C22-C23-C24-C20	-1.64(18)
C28-C23-C24-C20	-173.86(16)	Ta1-C23-C24-C20	62.80(11)	C22-C23-C24-C29	176.17(16)
C28-C23-C24-C29	3.9(3)	Ta1-C23-C24-C29	-119.39(17)	C22-C23-C24-Ta1	-64.44(11)
C28-C23-C24-Ta1	123.34(17)	C21-C20-C24-C23	2.08(18)	C25-C20-C24-C23	171.50(15)
Ta1-C20-C24-C23	-67.85(11)	C21-C20-C24-C29	-175.78(15)	C25-C20-C24-C29	-6.4(3)
Ta1-C20-C24-C29	114.28(16)	C21-C20-C24-Ta1	69.93(11)	C25-C20-C24-Ta1	-120.65(16)
N1#1-Ta1-C24-C23	138.96(10)	N1-Ta1-C24-C23	-144.38(11)	N12-Ta1-C24-C23	-54.80(11)
N11-Ta1-C24-C23	8.09(12)	C20-Ta1-C24-C23	115.00(14)	C21-Ta1-C24-C23	76.17(10)
C22-Ta1-C24-C23	35.97(9)	Ta1#1-Ta1-C24-C23	-174.88(8)	N1#1-Ta1-C24-C20	23.96(13)
N1-Ta1-C24-C20	100.62(10)	N12-Ta1-C24-C20	-169.79(9)	N11-Ta1-C24-C20	-106.91(10)
C21-Ta1-C24-C20	-38.83(9)	C22-Ta1-C24-C20	-79.03(10)	C23-Ta1-C24-C20	-115.00(14)
Ta1#1-Ta1-C24-C20	70.12(10)	N1#1-Ta1-C24-C29	-95.26(15)	N1-Ta1-C24-C29	-18.61(14)
N12-Ta1-C24-C29	70.98(14)	N11-Ta1-C24-C29	133.87(13)	C20-Ta1-C24-C29	-119.22(18)
C21-Ta1-C24-C29	-158.05(16)	C22-Ta1-C24-C29	161.75(16)	C23-Ta1-C24-C29	125.78(18)
Ta1#1-Ta1-C24-C29	-49.11(14)				

Symmetry transformation codes:#1 -x+1,-y+1,-z

cis-{Cp*Nb[N(iPr)C(Me)N(iPr](μ-N)}$_2$ (*cis*-4a)



A red prism-like specimen of $C_{36}H_{64}N_6Nb_2$, approximate dimensions 0.14 mm × 0.18 mm × 0.25 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker Smart Apex2, CCD system equipped with a graphite monochromator and a MoKα fine focus sealed tube (λ = 0.71073 Å). Data collection temperature was 295 K.

The total exposure time was 12.63 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 55595 reflections to a maximum θ angle of 27.50° (0.77 Å resolution), of which 17869 were independent (average redundancy 3.111, completeness = 99.9%, R_{int} = 2.93%, R_{sig} = 3.19%) and 14751 (82.55%) were greater than $2\sigma(F^2)$. The final cell constants of *a* = 11.9347(14) Å, *b* = 19.054(2) Å, *c* = 19.120(2) Å, α = 112.5059(17)°, β = 90.9022(17)°, γ = 102.7028(17)°, *V* = 3894.3(8) Å^3, are based upon the refinement of the XYZ-centroids of 9513 reflections above 20 σ(I) with 4.425° < 2θ < 60.01°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8220 and 0.9170.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 4 for the formula unit, $C_{36}H_{64}N_6Nb_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 833 variables converged at R_1 = 3.00%, for the observed data and wR_2 = 6.03% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.402 e$^-$/Å^3 and the largest hole was -0.294 e$^-$/Å^3 with an RMS deviation of 0.061 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.308 g/cm^3 and F(000), 1616 e$^-$

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APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)

SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2008/4 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for *cis*-4a.

Identification code	***cis*-4a**	
Chemical formula	$C_{36}H_{64}N_6Nb_2$	
Formula weight	766.75	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal size	0.14 × 0.18 × 0.25 mm	
Crystal habit	red prism	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.9347(14) Å	α = 112.5059(17)°
	b = 19.054(2) Å	β = 90.9022(17)°
	c = 19.120(2) Å	γ = 102.7028(17)°
Volume	3894.3(8) $Å^3$	
Z	4	
Density (calculated)	1.308 Mg/cm^3	
Absorption coefficient	0.620 mm^{-1}	
F(000)	1616	

Table 2. Data collection and structure refinement for *cis*-4a.

Diffractometer	Bruker Smart Apex2, CCD
Radiation source	fine focus sealed tube, MoKα
Theta range for data collection	1.87 to 27.50°
Index ranges	$-15 \le h \le 15$, $-24 \le k \le 24$, $-24 \le l \le 24$
Reflections collected	55595
Independent reflections	17869 [R(int) = 0.0293]
Coverage of independent reflections	99.9%
Absorption correction	multi-scan
Max. and min.	0.9170 and 0.8220

transmission		
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	17869 / 0 / 833	
Goodness-of-fit on F^2	1.000	
Δ/σ_{max}	0.003	
Final R indices	14751 data; $I>2\sigma(I)$	$R_1 = 0.0300$, $wR_2 = 0.0573$
	all data	$R_1 = 0.0415$, $wR_2 = 0.0603$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.01P)^2+2.925P]$, $P=(\max(F_o^2,0)+2F_c^2)/3$	
Largest diff. peak and hole	0.402 and -0.294 eÅ^{-3}	
R.M.S. deviation from mean	0.061 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for *cis*-4a.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Nb1A	0.106252(15)	0.255895(11)	0.781891(10)	0.03022(5)
Nb2A	0.90612(16)	0.250721(12)	0.857311(11)	0.03385(5)
N1A	0.99796(16)	0.18047(10)	0.80437(11)	0.0411(4)
N2A	0.02164(15)	0.32775(10)	0.84289(11)	0.0402(4)
N11A	0.08412(15)	0.16803(11)	0.65521(10)	0.0384(4)
N12A	0.07089(16)	0.28880(11)	0.68634(10)	0.0392(4)
C10A	0.05628(18)	0.21828(14)	0.63016(12)	0.0400(5)

	x/a	y/b	z/c	U(eq)
C11A	0.0132(2)	0.19762(17)	0.54823(14)	0.0594(7)
C12A	0.0651(2)	0.08454(14)	0.60565(13)	0.0467(6)
C13A	0.0376(2)	0.03449(15)	0.65186(16)	0.0596(7)
C14A	0.1665(2)	0.06730(17)	0.55950(15)	0.0639(8)
C15A	0.0409(2)	0.35747(15)	0.68133(14)	0.0472(6)
C16A	0.9114(2)	0.34619(19)	0.66394(17)	0.0674(8)
C17A	0.1109(3)	0.38928(17)	0.62843(17)	0.0666(8)
C20A	0.30675(17)	0.23035(14)	0.78332(13)	0.0387(5)
C21A	0.31899(17)	0.28801(14)	0.75247(13)	0.0406(5)
C22A	0.30227(18)	0.35731(14)	0.80987(14)	0.0441(6)
C23A	0.27811(19)	0.34245(14)	0.87527(13)	0.0447(6)
C24A	0.27926(18)	0.26339(14)	0.85866(13)	0.0407(5)
C25A	0.3337(2)	0.15167(16)	0.74940(16)	0.0592(7)
C26A	0.3497(2)	0.27957(18)	0.67410(14)	0.0572(7)
C27A	0.3125(3)	0.43491(16)	0.80457(19)	0.0731(9)
C28A	0.2689(3)	0.40474(17)	0.95077(16)	0.0708(9)
C29A	0.2774(2)	0.22394(18)	0.91353(15)	0.0632(8)
N31A	0.76817(15)	0.31338(11)	0.82640(11)	0.0404(4)
N32A	0.76155(15)	0.18798(11)	0.76833(10)	0.0399(4)
C30A	0.72008(18)	0.24795(14)	0.76854(13)	0.0389(5)
C31A	0.6297(2)	0.24196(16)	0.70889(16)	0.0580(7)
C32A	0.7451(2)	0.38789(14)	0.83171(15)	0.0519(6)
C33A	0.8520(3)	0.45462(15)	0.86742(17)	0.0669(8)
C34A	0.6406(3)	0.40498(18)	0.87457(18)	0.0714(9)
C35A	0.72921(19)	0.10734(14)	0.71093(14)	0.0460(6)
C36A	0.7667(2)	0.10009(17)	0.63331(15)	0.0638(8)
C37A	0.6011(2)	0.06560(16)	0.70475(19)	0.0696(9)
C40A	0.8498(2)	0.30288(15)	0.99015(13)	0.0494(6)
C41A	0.7542(2)	0.23937(16)	0.95139(14)	0.0500(6)
C42A	0.7922(2)	0.16945(15)	0.93023(14)	0.0485(6)
C43A	0.9104(2)	0.18913(15)	0.95503(14)	0.0480(6)
C44A	0.9470(2)	0.27214(15)	0.99170(13)	0.0487(6)
C45A	0.8498(3)	0.38810(17)	0.02974(16)	0.0745(9)
C46A	0.6311(2)	0.2423(2)	0.93874(18)	0.0731(9)
C47A	0.7176(3)	0.08737(17)	0.89310(19)	0.0764(9)
C48A	0.9816(3)	0.13124(18)	0.94810(18)	0.0715(8)
C49A	0.0588(3)	0.31742(19)	0.04177(16)	0.0741(9)

	x/a	y/b	z/c	U(eq)
Nb1B	0.644242(16)	0.237145(12)	0.338356(11)	0.03360(5)
Nb2B	0.42504(15)	0.257863(12)	0.307593(11)	0.03233(5)
N1B	0.49589(15)	0.17297(11)	0.29402(11)	0.0392(4)
N2B	0.57018(15)	0.32152(11)	0.35945(11)	0.0431(5)
N11B	0.72339(15)	0.15446(11)	0.23123(10)	0.0390(4)
N12B	0.76088(16)	0.28224(11)	0.26970(11)	0.0421(4)
C10B	0.76844(18)	0.21490(14)	0.21461(13)	0.0386(5)
C11B	0.8201(2)	0.20816(16)	0.14129(14)	0.0547(7)
C12B	0.7111(2)	0.07409(14)	0.17501(15)	0.0482(6)
C13B	0.6048(2)	0.01961(16)	0.18558(18)	0.0656(8)
C14B	0.8187(2)	0.04403(17)	0.17852(18)	0.0683(8)
C15B	0.7943(2)	0.36045(15)	0.26804(17)	0.0543(7)
C16B	0.7217(3)	0.3681(2)	0.2066(2)	0.0780(10)
C17B	0.9238(2)	0.39000(18)	0.2657(2)	0.0829(10)
C20B	0.7418(2)	0.18069(16)	0.41489(13)	0.0462(6)
C21B	0.8334(2)	0.23825(17)	0.40871(14)	0.0504(6)
C22B	0.8107(2)	0.31248(17)	0.44991(15)	0.0572(7)
C23B	0.7059(2)	0.30059(18)	0.48055(14)	0.0570(7)
C24B	0.6622(2)	0.21959(18)	0.45878(14)	0.0513(6)
C25B	0.7344(3)	0.09506(18)	0.38956(18)	0.0734(9)
C26B	0.9397(2)	0.2242(2)	0.36995(17)	0.0731(9)
C27B	0.8874(3)	0.3916(2)	0.4623(2)	0.0986(13)
C28B	0.6574(3)	0.3655(2)	0.53372(18)	0.0922(12)
C29B	0.5634(3)	0.1787(2)	0.48915(18)	0.0821(11)
N31B	0.42195(16)	0.34747(12)	0.24987(11)	0.0430(5)
N32B	0.39617(16)	0.22116(12)	0.18445(10)	0.0434(5)
C30B	0.4133(2)	0.29136(16)	0.18169(14)	0.0458(6)
C31B	0.4227(3)	0.3058(2)	0.10912(16)	0.0728(9)
C32B	0.4577(2)	0.43077(16)	0.26247(16)	0.0576(7)
C33B	0.5234(3)	0.47905(16)	0.34074(18)	0.0696(8)
C34B	0.3556(3)	0.4632(2)	0.2500(2)	0.0880(11)
C35B	0.3857(2)	0.14516(16)	0.12101(14)	0.0542(7)
C36B	0.4979(3)	0.1369(2)	0.08557(17)	0.0759(9)
C37B	0.2833(3)	0.1208(2)	0.06010(17)	0.0836(10)
C40B	0.2577(2)	0.30903(15)	0.37094(15)	0.0493(6)
C41B	0.20529(19)	0.25209(16)	0.29878(15)	0.0495(6)
C42B	0.21260(19)	0.17839(16)	0.29582(15)	0.0507(6)

	x/a	y/b	z/c	U(eq)
C43B	0.2715(2)	0.18934(16)	0.36483(16)	0.0519(6)
C44B	0.3012(2)	0.27032(17)	0.41125(14)	0.0492(6)
C45B	0.2534(3)	0.39372(18)	0.4053(2)	0.0817(10)
C46B	0.1451(2)	0.2663(2)	0.23754(18)	0.0766(10)
C47B	0.1629(3)	0.10005(19)	0.2325(2)	0.0867(11)
C48B	0.2870(3)	0.1232(2)	0.3854(2)	0.0830(10)
C49B	0.3452(3)	0.3078(2)	0.49448(16)	0.0844(11)

Table 4. Bond lengths (Å) for *cis*-4a.

Nb1A-N1A	1.8959(18)	Nb1A-N2A	1.9176(18)
Nb1A-N12A	2.2085(17)	Nb1A-N11A	2.3282(18)
Nb1A-C24A	2.460(2)	Nb1A-C23A	2.502(2)
Nb1A-C20A	2.546(2)	Nb1A-C22A	2.583(2)
Nb1A-C21A	2.601(2)	Nb1A-Nb2A	2.8121(3)
Nb2A-N2A	1.8875(18)	Nb2A-N1A	1.9133(18)
Nb2A-N32A	2.1781(18)	Nb2A-N31A	2.4206(18)
Nb2A-C44A	2.465(2)	Nb2A-C40A	2.511(2)
Nb2A-C43A	2.564(2)	Nb2A-C41A	2.607(2)
Nb2A-C42A	2.641(2)	N11A-C10A	1.320(3)
N11A-C12A	1.470(3)	N12A-C10A	1.333(3)
N12A-C15A	1.466(3)	C10A-C11A	1.512(3)
C11A-H11A	0.96	C11A-H11B	0.96
C11A-H11C	0.96	C12A-C13A	1.521(4)
C12A-C14A	1.528(3)	C12A-H12A	0.98
C13A-H13A	0.96	C13A-H13B	0.96
C13A-H13C	0.96	C14A-H14A	0.96
C14A-H14B	0.96	C14A-H14C	0.96
C15A-C16A	1.525(3)	C15A-C17A	1.537(3)
C15A-H15A	0.98	C16A-H16A	0.96
C16A-H16B	0.96	C16A-H16C	0.96
C17A-H17A	0.96	C17A-H17B	0.96
C17A-H17C	0.96	C20A-C24A	1.411(3)
C20A-C21A	1.416(3)	C20A-C25A	1.498(3)
C21A-C22A	1.415(3)	C21A-C26A	1.505(3)
C22A-C23A	1.405(3)	C22A-C27A	1.499(3)
C23A-C24A	1.419(3)	C23A-C28A	1.502(3)

C24A-C29A	1.504(3)	C25A-H25A	0.96
C25A-H25B	0.96	C25A-H25C	0.96
C26A-H26A	0.96	C26A-H26B	0.96
C26A-H26C	0.96	C27A-H27A	0.96
C27A-H27B	0.96	C27A-H27C	0.96
C28A-H28A	0.96	C28A-H28B	0.96
C28A-H28C	0.96	C29A-H29A	0.96
C29A-H29B	0.96	C29A-H29C	0.96
N31A-C30A	1.310(3)	N31A-C32A	1.471(3)
N32A-C30A	1.340(3)	N32A-C35A	1.466(3)
C30A-C31A	1.512(3)	C31A-H31A	0.96
C31A-H31B	0.96	C31A-H31C	0.96
C32A-C33A	1.518(4)	C32A-C34A	1.529(4)
C32A-H32A	0.98	C33A-H33A	0.96
C33A-H33B	0.96	C33A-H33C	0.96
C34A-H34A	0.96	C34A-H34B	0.96
C34A-H34C	0.96	C35A-C36A	1.521(4)
C35A-C37A	1.540(3)	C35A-H35A	0.98
C36A-H36A	0.96	C36A-H36B	0.96
C36A-H36C	0.96	C37A-H37A	0.96
C37A-H37B	0.96	C37A-H37C	0.96
C40A-C41A	1.412(4)	C40A-C44A	1.415(4)
C40A-C45A	1.506(4)	C41A-C42A	1.415(4)
C41A-C46A	1.502(4)	C42A-C43A	1.401(3)
C42A-C47A	1.503(4)	C43A-C44A	1.422(4)
C43A-C48A	1.504(4)	C44A-C49A	1.504(4)
C45A-H45A	0.96	C45A-H45B	0.96
C45A-H45C	0.96	C46A-H46A	0.96
C46A-H46B	0.96	C46A-H46C	0.96
C47A-H47A	0.96	C47A-H47B	0.96
C47A-H47C	0.96	C48A-H48A	0.96
C48A-H48B	0.96	C48A-H48C	0.96
C49A-H49A	0.96	C49A-H49B	0.96
C49A-H49C	0.96	Nb1B-N1B	1.8857(18)
Nb1B-N2B	1.9153(18)	Nb1B-N12B	2.1895(18)
Nb1B-N11B	2.4114(18)	Nb1B-C24B	2.463(2)
Nb1B-C20B	2.521(2)	Nb1B-C23B	2.535(2)
Nb1B-C21B	2.602(2)	Nb1B-C22B	2.612(2)

Nb1B-Nb2B	2.8159(4)	Nb2B-N2B	1.8857(18)
Nb2B-N1B	1.9198(18)	Nb2B-N32B	2.1815(18)
Nb2B-N31B	2.3672(18)	Nb2B-C44B	2.461(2)
Nb2B-C43B	2.523(2)	Nb2B-C40B	2.537(2)
Nb2B-C41B	2.601(2)	Nb2B-C42B	2.609(2)
N11B-C10B	1.315(3)	N11B-C12B	1.469(3)
N12B-C10B	1.335(3)	N12B-C15B	1.468(3)
C10B-C11B	1.512(3)	C11B-H11D	0.96
C11B-H11E	0.96	C11B-H11F	0.96
C12B-C13B	1.522(3)	C12B-C14B	1.527(3)
C12B-H12B	0.98	C13B-H13D	0.96
C13B-H13E	0.96	C13B-H13F	0.96
C14B-H14D	0.96	C14B-H14E	0.96
C14B-H14F	0.96	C15B-C16B	1.517(4)
C15B-C17B	1.532(4)	C15B-H15B	0.98
C16B-H16D	0.96	C16B-H16E	0.96
C16B-H16F	0.96	C17B-H17D	0.96
C17B-H17E	0.96	C17B-H17F	0.96
C20B-C21B	1.410(3)	C20B-C24B	1.419(3)
C20B-C25B	1.495(4)	C21B-C22B	1.420(4)
C21B-C26B	1.502(3)	C22B-C23B	1.399(4)
C22B-C27B	1.511(4)	C23B-C24B	1.405(4)
C23B-C28B	1.507(4)	C24B-C29B	1.516(4)
C25B-H25D	0.96	C25B-H25E	0.96
C25B-H25F	0.96	C26B-H26D	0.96
C26B-H26E	0.96	C26B-H26F	0.96
C27B-H27D	0.96	C27B-H27E	0.96
C27B-H27F	0.96	C28B-H28D	0.96
C28B-H28E	0.96	C28B-H28F	0.96
C29B-H29D	0.96	C29B-H29E	0.96
C29B-H29F	0.96	N31B-C30B	1.317(3)
N31B-C32B	1.472(3)	N32B-C30B	1.329(3)
N32B-C35B	1.468(3)	C30B-C31B	1.515(3)
C31B-H31D	0.96	C31B-H31E	0.96
C31B-H31F	0.96	C32B-C33B	1.514(4)
C32B-C34B	1.535(4)	C32B-H32B	0.98
C33B-H33D	0.96	C33B-H33E	0.96
C33B-H33F	0.96	C34B-H34D	0.96

C34B-H34E	0.96	C34B-H34F	0.96
C35B-C36B	1.522(4)	C35B-C37B	1.536(4)
C35B-H35B	0.98	C36B-H36D	0.96
C36B-H36E	0.96	C36B-H36F	0.96
C37B-H37D	0.96	C37B-H37E	0.96
C37B-H37F	0.96	C40B-C44B	1.414(4)
C40B-C41B	1.414(4)	C40B-C45B	1.505(4)
C41B-C42B	1.406(4)	C41B-C46B	1.503(4)
C42B-C43B	1.405(4)	C42B-C47B	1.500(4)
C43B-C44B	1.413(4)	C43B-C48B	1.503(4)
C44B-C49B	1.502(4)	C45B-H45D	0.96
C45B-H45E	0.96	C45B-H45F	0.96
C46B-H46D	0.96	C46B-H46E	0.96
C46B-H46F	0.96	C47B-H47D	0.96
C47B-H47E	0.96	C47B-H47F	0.96
C48B-H48D	0.96	C48B-H48E	0.96
C48B-H48F	0.96	C49B-H49D	0.96
C49B-H49E	0.96	C49B-H49F	0.96

Table 5. Bond angles (°) for *cis*-4a.

N1A-Nb1A-N2A	84.38(8)	N1A-Nb1A-N12A	122.32(8)
N2A-Nb1A-N12A	88.97(7)	N1A-Nb1A-N11A	89.45(7)
N2A-Nb1A-N11A	135.05(7)	N12A-Nb1A-N11A	57.60(7)
N1A-Nb1A-C24A	99.25(8)	N2A-Nb1A-C24A	110.02(8)
N12A-Nb1A-C24A	136.15(7)	N11A-Nb1A-C24A	114.92(7)
N1A-Nb1A-C23A	120.45(8)	N2A-Nb1A-C23A	85.98(8)
N12A-Nb1A-C23A	116.07(8)	N11A-Nb1A-C23A	133.62(7)
C24A-Nb1A-C23A	33.22(8)	N1A-Nb1A-C20A	110.42(8)
N2A-Nb1A-C20A	139.62(8)	N12A-Nb1A-C20A	111.03(7)
N11A-Nb1A-C20A	83.93(7)	C24A-Nb1A-C20A	32.68(7)
C23A-Nb1A-C20A	53.90(8)	N1A-Nb1A-C22A	151.66(8)
N2A-Nb1A-C22A	96.32(8)	N12A-Nb1A-C22A	86.01(7)
N11A-Nb1A-C22A	108.91(7)	C24A-Nb1A-C22A	53.79(8)
C23A-Nb1A-C22A	32.03(7)	C20A-Nb1A-C22A	52.94(8)
N1A-Nb1A-C21A	141.63(8)	N2A-Nb1A-C21A	127.63(8)
N12A-Nb1A-C21A	83.21(7)	N11A-Nb1A-C21A	81.08(7)
C24A-Nb1A-C21A	53.64(7)	C23A-Nb1A-C21A	53.17(7)

C20A-Nb1A-C21A	31.91(7)	C22A-Nb1A-C21A	31.67(7)
N1A-Nb1A-Nb2A	42.66(6)	N2A-Nb1A-Nb2A	41.94(5)
N12A-Nb1A-Nb2A	107.25(5)	N11A-Nb1A-Nb2A	115.65(5)
C24A-Nb1A-Nb2A	113.19(5)	C23A-Nb1A-Nb2A	109.94(6)
C20A-Nb1A-Nb2A	141.65(5)	C22A-Nb1A-Nb2A	133.72(6)
C21A-Nb1A-Nb2A	163.11(5)	N2A-Nb2A-N1A	84.73(8)
N2A-Nb2A-N32A	117.31(8)	N1A-Nb2A-N32A	91.67(8)
N2A-Nb2A-N31A	86.51(7)	N1A-Nb2A-N31A	137.84(7)
N32A-Nb2A-N31A	56.81(7)	N2A-Nb2A-C44A	104.58(8)
N1A-Nb2A-C44A	103.84(9)	N32A-Nb2A-C44A	136.49(8)
N31A-Nb2A-C44A	118.27(8)	N2A-Nb2A-C40A	110.16(8)
N1A-Nb2A-C40A	135.79(8)	N32A-Nb2A-C40A	114.72(8)
N31A-Nb2A-C40A	85.73(8)	C44A-Nb2A-C40A	33.03(8)
N2A-Nb2A-C43A	128.95(8)	N1A-Nb2A-C43A	84.10(8)
N32A-Nb2A-C43A	112.67(8)	N31A-Nb2A-C43A	131.32(7)
C44A-Nb2A-C43A	32.77(8)	C40A-Nb2A-C43A	53.73(8)
N2A-Nb2A-C41A	139.51(8)	N1A-Nb2A-C41A	130.23(8)
N32A-Nb2A-C41A	85.45(8)	N31A-Nb2A-C41A	78.86(7)
C44A-Nb2A-C41A	53.47(8)	C40A-Nb2A-C41A	31.95(8)
C43A-Nb2A-C41A	52.46(8)	N2A-Nb2A-C42A	157.50(8)
N1A-Nb2A-C42A	98.95(8)	N32A-Nb2A-C42A	84.90(8)
N31A-Nb2A-C42A	104.52(7)	C44A-Nb2A-C42A	52.94(8)
C40A-Nb2A-C42A	52.60(8)	C43A-Nb2A-C42A	31.19(8)
C41A-Nb2A-C42A	31.28(8)	N2A-Nb2A-Nb1A	42.76(5)
N1A-Nb2A-Nb1A	42.18(5)	N32A-Nb2A-Nb1A	106.03(5)
N31A-Nb2A-Nb1A	115.10(5)	C44A-Nb2A-Nb1A	112.75(6)
C40A-Nb2A-Nb1A	139.09(6)	C43A-Nb2A-Nb1A	113.38(6)
C41A-Nb2A-Nb1A	165.20(6)	C42A-Nb2A-Nb1A	138.44(6)
Nb1A-N1A-Nb2A	95.16(8)	Nb2A-N2A-Nb1A	95.30(8)
C10A-N11A-C12A	121.49(19)	C10A-N11A-Nb1A	92.70(14)
C12A-N11A-Nb1A	143.40(15)	C10A-N12A-C15A	126.63(19)
C10A-N12A-Nb1A	97.80(14)	C15A-N12A-Nb1A	133.87(15)
N11A-C10A-N12A	111.16(19)	N11A-C10A-C11A	123.9(2)
N12A-C10A-C11A	124.9(2)	C10A-C11A-H11A	109.5
C10A-C11A-H11B	109.5	H11A-C11A-H11B	109.5
C10A-C11A-H11C	109.5	H11A-C11A-H11C	109.5
H11B-C11A-H11C	109.5	N11A-C12A-C13A	110.47(19)
N11A-C12A-C14A	112.2(2)	C13A-C12A-C14A	111.9(2)

N11A-C12A-H12A	107.3	C13A-C12A-H12A	107.3
C14A-C12A-H12A	107.3	C12A-C13A-H13A	109.5
C12A-C13A-H13B	109.5	H13A-C13A-H13B	109.5
C12A-C13A-H13C	109.5	H13A-C13A-H13C	109.5
H13B-C13A-H13C	109.5	C12A-C14A-H14A	109.5
C12A-C14A-H14B	109.5	H14A-C14A-H14B	109.5
C12A-C14A-H14C	109.5	H14A-C14A-H14C	109.5
H14B-C14A-H14C	109.5	N12A-C15A-C16A	113.3(2)
N12A-C15A-C17A	114.2(2)	C16A-C15A-C17A	111.7(2)
N12A-C15A-H15A	105.6	C16A-C15A-H15A	105.6
C17A-C15A-H15A	105.6	C15A-C16A-H16A	109.5
C15A-C16A-H16B	109.5	H16A-C16A-H16B	109.5
C15A-C16A-H16C	109.5	H16A-C16A-H16C	109.5
H16B-C16A-H16C	109.5	C15A-C17A-H17A	109.5
C15A-C17A-H17B	109.5	H17A-C17A-H17B	109.5
C15A-C17A-H17C	109.5	H17A-C17A-H17C	109.5
H17B-C17A-H17C	109.5	C24A-C20A-C21A	108.0(2)
C24A-C20A-C25A	123.4(2)	C21A-C20A-C25A	128.1(2)
C24A-C20A-Nb1A	70.30(12)	C21A-C20A-Nb1A	76.15(12)
C25A-C20A-Nb1A	125.63(16)	C22A-C21A-C20A	107.8(2)
C22A-C21A-C26A	125.3(2)	C20A-C21A-C26A	126.9(2)
C22A-C21A-Nb1A	73.50(12)	C20A-C21A-Nb1A	71.94(11)
C26A-C21A-Nb1A	122.39(15)	C23A-C22A-C21A	108.3(2)
C23A-C22A-C27A	124.8(2)	C21A-C22A-C27A	126.9(2)
C23A-C22A-Nb1A	70.78(12)	C21A-C22A-Nb1A	74.83(12)
C27A-C22A-Nb1A	121.99(17)	C22A-C23A-C24A	108.0(2)
C22A-C23A-C28A	123.6(2)	C24A-C23A-C28A	128.0(2)
C22A-C23A-Nb1A	77.20(13)	C24A-C23A-Nb1A	71.79(12)
C28A-C23A-Nb1A	123.04(17)	C20A-C24A-C23A	107.9(2)
C20A-C24A-C29A	123.2(2)	C23A-C24A-C29A	127.8(2)
C20A-C24A-Nb1A	77.02(12)	C23A-C24A-Nb1A	74.99(13)
C29A-C24A-Nb1A	123.83(16)	C20A-C25A-H25A	109.5
C20A-C25A-H25B	109.5	H25A-C25A-H25B	109.5
C20A-C25A-H25C	109.5	H25A-C25A-H25C	109.5
H25B-C25A-H25C	109.5	C21A-C26A-H26A	109.5
C21A-C26A-H26B	109.5	H26A-C26A-H26B	109.5
C21A-C26A-H26C	109.5	H26A-C26A-H26C	109.5
H26B-C26A-H26C	109.5	C22A-C27A-H27A	109.5

C22A-C27A-H27B	109.5	H27A-C27A-H27B	109.5
C22A-C27A-H27C	109.5	H27A-C27A-H27C	109.5
H27B-C27A-H27C	109.5	C23A-C28A-H28A	109.5
C23A-C28A-H28B	109.5	H28A-C28A-H28B	109.5
C23A-C28A-H28C	109.5	H28A-C28A-H28C	109.5
H28B-C28A-H28C	109.5	C24A-C29A-H29A	109.5
C24A-C29A-H29B	109.5	H29A-C29A-H29B	109.5
C24A-C29A-H29C	109.5	H29A-C29A-H29C	109.5
H29B-C29A-H29C	109.5	C30A-N31A-C32A	120.4(2)
C30A-N31A-Nb2A	89.98(13)	C32A-N31A-Nb2A	145.92(15)
C30A-N32A-C35A	126.4(2)	C30A-N32A-Nb2A	100.21(14)
C35A-N32A-Nb2A	132.15(15)	N31A-C30A-N32A	112.1(2)
N31A-C30A-C31A	123.4(2)	N32A-C30A-C31A	124.5(2)
C30A-C31A-H31A	109.5	C30A-C31A-H31B	109.5
H31A-C31A-H31B	109.5	C30A-C31A-H31C	109.5
H31A-C31A-H31C	109.5	H31B-C31A-H31C	109.5
N31A-C32A-C33A	110.5(2)	N31A-C32A-C34A	112.1(2)
C33A-C32A-C34A	111.4(2)	N31A-C32A-H32A	107.6
C33A-C32A-H32A	107.6	C34A-C32A-H32A	107.6
C32A-C33A-H33A	109.5	C32A-C33A-H33B	109.5
H33A-C33A-H33B	109.5	C32A-C33A-H33C	109.5
H33A-C33A-H33C	109.5	H33B-C33A-H33C	109.5
C32A-C34A-H34A	109.5	C32A-C34A-H34B	109.5
H34A-C34A-H34B	109.5	C32A-C34A-H34C	109.5
H34A-C34A-H34C	109.5	H34B-C34A-H34C	109.5
N32A-C35A-C36A	113.1(2)	N32A-C35A-C37A	114.24(19)
C36A-C35A-C37A	111.5(2)	N32A-C35A-H35A	105.7
C36A-C35A-H35A	105.7	C37A-C35A-H35A	105.7
C35A-C36A-H36A	109.5	C35A-C36A-H36B	109.5
H36A-C36A-H36B	109.5	C35A-C36A-H36C	109.5
H36A-C36A-H36C	109.5	H36B-C36A-H36C	109.5
C35A-C37A-H37A	109.5	C35A-C37A-H37B	109.5
H37A-C37A-H37B	109.5	C35A-C37A-H37C	109.5
H37A-C37A-H37C	109.5	H37B-C37A-H37C	109.5
C41A-C40A-C44A	107.9(2)	C41A-C40A-C45A	127.5(3)
C44A-C40A-C45A	124.4(3)	C41A-C40A-Nb2A	77.76(13)
C44A-C40A-Nb2A	71.70(13)	C45A-C40A-Nb2A	120.46(17)
C40A-C41A-C42A	107.9(2)	C40A-C41A-C46A	127.6(3)

C42A-C41A-C46A	124.4(3)	C40A-C41A-Nb2A	70.29(13)
C42A-C41A-Nb2A	75.70(13)	C46A-C41A-Nb2A	123.24(17)
C43A-C42A-C41A	108.5(2)	C43A-C42A-C47A	125.1(3)
C41A-C42A-C47A	126.2(3)	C43A-C42A-Nb2A	71.34(13)
C41A-C42A-Nb2A	73.02(13)	C47A-C42A-Nb2A	125.21(18)
C42A-C43A-C44A	107.8(2)	C42A-C43A-C48A	125.1(3)
C44A-C43A-C48A	127.0(3)	C42A-C43A-Nb2A	77.47(14)
C44A-C43A-Nb2A	69.81(13)	C48A-C43A-Nb2A	121.70(17)
C40A-C44A-C43A	107.9(2)	C40A-C44A-C49A	124.6(3)
C43A-C44A-C49A	125.5(3)	C40A-C44A-Nb2A	75.27(14)
C43A-C44A-Nb2A	77.42(14)	C49A-C44A-Nb2A	126.24(17)
C40A-C45A-H45A	109.5	C40A-C45A-H45B	109.5
H45A-C45A-H45B	109.5	C40A-C45A-H45C	109.5
H45A-C45A-H45C	109.5	H45B-C45A-H45C	109.5
C41A-C46A-H46A	109.5	C41A-C46A-H46B	109.5
H46A-C46A-H46B	109.5	C41A-C46A-H46C	109.5
H46A-C46A-H46C	109.5	H46B-C46A-H46C	109.5
C42A-C47A-H47A	109.5	C42A-C47A-H47B	109.5
H47A-C47A-H47B	109.5	C42A-C47A-H47C	109.5
H47A-C47A-H47C	109.5	H47B-C47A-H47C	109.5
C43A-C48A-H48A	109.5	C43A-C48A-H48B	109.5
H48A-C48A-H48B	109.5	C43A-C48A-H48C	109.5
H48A-C48A-H48C	109.5	H48B-C48A-H48C	109.5
C44A-C49A-H49A	109.5	C44A-C49A-H49B	109.5
H49A-C49A-H49B	109.5	C44A-C49A-H49C	109.5
H49A-C49A-H49C	109.5	H49B-C49A-H49C	109.5
N1B-Nb1B-N2B	84.35(8)	N1B-Nb1B-N12B	119.73(8)
N2B-Nb1B-N12B	90.76(8)	N1B-Nb1B-N11B	88.53(7)
N2B-Nb1B-N11B	136.76(7)	N12B-Nb1B-N11B	56.68(7)
N1B-Nb1B-C24B	101.91(9)	N2B-Nb1B-C24B	105.67(9)
N12B-Nb1B-C24B	136.65(8)	N11B-Nb1B-C24B	117.52(8)
N1B-Nb1B-C20B	110.95(8)	N2B-Nb1B-C20B	136.63(8)
N12B-Nb1B-C20B	112.87(7)	N11B-Nb1B-C20B	85.48(7)
C24B-Nb1B-C20B	33.07(8)	N1B-Nb1B-C23B	123.92(9)
N2B-Nb1B-C23B	83.65(8)	N12B-Nb1B-C23B	115.00(9)
N11B-Nb1B-C23B	133.45(7)	C24B-Nb1B-C23B	32.62(9)
C20B-Nb1B-C23B	53.78(8)	N1B-Nb1B-C21B	141.59(8)
N2B-Nb1B-C21B	127.60(8)	N12B-Nb1B-C21B	84.49(8)

N11B-Nb1B-C21B	80.80(7)	C24B-Nb1B-C21B	53.56(8)
C20B-Nb1B-C21B	31.90(8)	C23B-Nb1B-C21B	52.83(8)
N1B-Nb1B-C22B	154.26(9)	N2B-Nb1B-C22B	96.06(9)
N12B-Nb1B-C22B	86.01(8)	N11B-Nb1B-C22B	107.74(8)
C24B-Nb1B-C22B	53.09(9)	C20B-Nb1B-C22B	52.80(9)
C23B-Nb1B-C22B	31.50(9)	C21B-Nb1B-C22B	31.61(8)
N1B-Nb1B-Nb2B	42.74(5)	N2B-Nb1B-Nb2B	41.79(5)
N12B-Nb1B-Nb2B	107.04(5)	N11B-Nb1B-Nb2B	116.20(4)
C24B-Nb1B-Nb2B	111.88(6)	C20B-Nb1B-Nb2B	140.06(6)
C23B-Nb1B-Nb2B	109.96(6)	C21B-Nb1B-Nb2B	162.72(6)
C22B-Nb1B-Nb2B	134.15(7)	N2B-Nb2B-N1B	84.23(8)
N2B-Nb2B-N32B	118.98(8)	N1B-Nb2B-N32B	90.54(8)
N2B-Nb2B-N31B	87.85(7)	N1B-Nb2B-N31B	137.23(7)
N32B-Nb2B-N31B	57.47(7)	N2B-Nb2B-C44B	103.01(9)
N1B-Nb2B-C44B	108.51(8)	N32B-Nb2B-C44B	135.54(8)
N31B-Nb2B-C44B	114.23(8)	N2B-Nb2B-C43B	124.58(9)
N1B-Nb2B-C43B	85.32(8)	N32B-Nb2B-C43B	115.38(9)
N31B-Nb2B-C43B	131.92(7)	C44B-Nb2B-C43B	32.90(8)
N2B-Nb2B-C40B	112.75(9)	N1B-Nb2B-C40B	138.53(8)
N32B-Nb2B-C40B	110.55(8)	N31B-Nb2B-C40B	82.87(7)
C44B-Nb2B-C40B	32.82(8)	C43B-Nb2B-C40B	53.59(8)
N2B-Nb2B-C41B	143.38(9)	N1B-Nb2B-C41B	127.39(8)
N32B-Nb2B-C41B	82.68(8)	N31B-Nb2B-C41B	79.74(7)
C44B-Nb2B-C41B	53.64(8)	C43B-Nb2B-C41B	52.77(8)
C40B-Nb2B-C41B	31.92(8)	N2B-Nb2B-C42B	155.43(9)
N1B-Nb2B-C42B	96.34(8)	N32B-Nb2B-C42B	85.59(8)
N31B-Nb2B-C42B	107.34(8)	C44B-Nb2B-C42B	53.42(8)
C43B-Nb2B-C42B	31.73(8)	C40B-Nb2B-C42B	52.58(8)
C41B-Nb2B-C42B	31.31(8)	N2B-Nb2B-Nb1B	42.60(6)
N1B-Nb2B-Nb1B	41.81(5)	N32B-Nb2B-Nb1B	106.42(5)
N31B-Nb2B-Nb1B	115.89(5)	C44B-Nb2B-Nb1B	114.57(6)
C43B-Nb2B-Nb1B	111.57(6)	C40B-Nb2B-Nb1B	142.94(6)
C41B-Nb2B-Nb1B	164.31(6)	C42B-Nb2B-Nb1B	134.81(6)
Nb1B-N1B-Nb2B	95.45(8)	Nb2B-N2B-Nb1B	95.60(8)
C10B-N11B-C12B	120.72(19)	C10B-N11B-Nb1B	90.45(13)
C12B-N11B-Nb1B	145.10(14)	C10B-N12B-C15B	126.6(2)
C10B-N12B-Nb1B	100.01(14)	C15B-N12B-Nb1B	131.10(15)
N11B-C10B-N12B	111.65(19)	N11B-C10B-C11B	123.8(2)

N12B-C10B-C11B	124.6(2)	C10B-C11B-H11D	109.5
C10B-C11B-H11E	109.5	H11D-C11B-H11E	109.5
C10B-C11B-H11F	109.5	H11D-C11B-H11F	109.5
H11E-C11B-H11F	109.5	N11B-C12B-C13B	110.1(2)
N11B-C12B-C14B	112.4(2)	C13B-C12B-C14B	110.6(2)
N11B-C12B-H12B	107.8	C13B-C12B-H12B	107.8
C14B-C12B-H12B	107.8	C12B-C13B-H13D	109.5
C12B-C13B-H13E	109.5	H13D-C13B-H13E	109.5
C12B-C13B-H13F	109.5	H13D-C13B-H13F	109.5
H13E-C13B-H13F	109.5	C12B-C14B-H14D	109.5
C12B-C14B-H14E	109.5	H14D-C14B-H14E	109.5
C12B-C14B-H14F	109.5	H14D-C14B-H14F	109.5
H14E-C14B-H14F	109.5	N12B-C15B-C16B	112.6(2)
N12B-C15B-C17B	114.5(2)	C16B-C15B-C17B	111.8(2)
N12B-C15B-H15B	105.7	C16B-C15B-H15B	105.7
C17B-C15B-H15B	105.7	C15B-C16B-H16D	109.5
C15B-C16B-H16E	109.5	H16D-C16B-H16E	109.5
C15B-C16B-H16F	109.5	H16D-C16B-H16F	109.5
H16E-C16B-H16F	109.5	C15B-C17B-H17D	109.5
C15B-C17B-H17E	109.5	H17D-C17B-H17E	109.5
C15B-C17B-H17F	109.5	H17D-C17B-H17F	109.5
H17E-C17B-H17F	109.5	C21B-C20B-C24B	107.7(2)
C21B-C20B-C25B	127.3(2)	C24B-C20B-C25B	124.5(3)
C21B-C20B-Nb1B	77.20(13)	C24B-C20B-Nb1B	71.21(13)
C25B-C20B-Nb1B	123.25(17)	C20B-C21B-C22B	107.6(2)
C20B-C21B-C26B	126.3(3)	C22B-C21B-C26B	126.0(3)
C20B-C21B-Nb1B	70.89(12)	C22B-C21B-Nb1B	74.61(13)
C26B-C21B-Nb1B	123.04(17)	C23B-C22B-C21B	108.3(2)
C23B-C22B-C27B	124.9(3)	C21B-C22B-C27B	126.7(3)
C23B-C22B-Nb1B	71.18(14)	C21B-C22B-Nb1B	73.78(14)
C27B-C22B-Nb1B	122.85(19)	C22B-C23B-C24B	108.2(2)
C22B-C23B-C28B	124.2(3)	C24B-C23B-C28B	127.3(3)
C22B-C23B-Nb1B	77.31(15)	C24B-C23B-Nb1B	70.87(14)
C28B-C23B-Nb1B	122.32(18)	C23B-C24B-C20B	108.1(2)
C23B-C24B-C29B	127.7(3)	C20B-C24B-C29B	122.9(3)
C23B-C24B-Nb1B	76.51(15)	C20B-C24B-Nb1B	75.72(13)
C29B-C24B-Nb1B	124.16(17)	C20B-C25B-H25D	109.5
C20B-C25B-H25E	109.5	H25D-C25B-H25E	109.5

C20B-C25B-H25F	109.5	H25D-C25B-H25F	109.5
H25E-C25B-H25F	109.5	C21B-C26B-H26D	109.5
C21B-C26B-H26E	109.5	H26D-C26B-H26E	109.5
C21B-C26B-H26F	109.5	H26D-C26B-H26F	109.5
H26E-C26B-H26F	109.5	C22B-C27B-H27D	109.5
C22B-C27B-H27E	109.5	H27D-C27B-H27E	109.5
C22B-C27B-H27F	109.5	H27D-C27B-H27F	109.5
H27E-C27B-H27F	109.5	C23B-C28B-H28D	109.5
C23B-C28B-H28E	109.5	H28D-C28B-H28E	109.5
C23B-C28B-H28F	109.5	H28D-C28B-H28F	109.5
H28E-C28B-H28F	109.5	C24B-C29B-H29D	109.5
C24B-C29B-H29E	109.5	H29D-C29B-H29E	109.5
C24B-C29B-H29F	109.5	H29D-C29B-H29F	109.5
H29E-C29B-H29F	109.5	C30B-N31B-C32B	121.7(2)
C30B-N31B-Nb2B	90.82(14)	C32B-N31B-Nb2B	143.55(16)
C30B-N32B-C35B	128.0(2)	C30B-N32B-Nb2B	98.93(15)
C35B-N32B-Nb2B	131.97(16)	N31B-C30B-N32B	111.9(2)
N31B-C30B-C31B	123.7(2)	N32B-C30B-C31B	124.4(2)
C30B-C31B-H31D	109.5	C30B-C31B-H31E	109.5
H31D-C31B-H31E	109.5	C30B-C31B-H31F	109.5
H31D-C31B-H31F	109.5	H31E-C31B-H31F	109.5
N31B-C32B-C33B	110.7(2)	N31B-C32B-C34B	112.5(2)
C33B-C32B-C34B	111.2(3)	N31B-C32B-H32B	107.4
C33B-C32B-H32B	107.4	C34B-C32B-H32B	107.4
C32B-C33B-H33D	109.5	C32B-C33B-H33E	109.5
H33D-C33B-H33E	109.5	C32B-C33B-H33F	109.5
H33D-C33B-H33F	109.5	H33E-C33B-H33F	109.5
C32B-C34B-H34D	109.5	C32B-C34B-H34E	109.5
H34D-C34B-H34E	109.5	C32B-C34B-H34F	109.5
H34D-C34B-H34F	109.5	H34E-C34B-H34F	109.5
N32B-C35B-C36B	113.2(2)	N32B-C35B-C37B	114.8(2)
C36B-C35B-C37B	111.6(2)	N32B-C35B-H35B	105.4
C36B-C35B-H35B	105.4	C37B-C35B-H35B	105.4
C35B-C36B-H36D	109.5	C35B-C36B-H36E	109.5
H36D-C36B-H36E	109.5	C35B-C36B-H36F	109.5
H36D-C36B-H36F	109.5	H36E-C36B-H36F	109.5
C35B-C37B-H37D	109.5	C35B-C37B-H37E	109.5
H37D-C37B-H37E	109.5	C35B-C37B-H37F	109.5

H37D-C37B-H37F	109.5	H37E-C37B-H37F	109.5
C44B-C40B-C41B	107.9(2)	C44B-C40B-C45B	124.2(3)
C41B-C40B-C45B	127.2(3)	C44B-C40B-Nb2B	70.62(12)
C41B-C40B-Nb2B	76.52(13)	C45B-C40B-Nb2B	125.55(17)
C42B-C41B-C40B	107.9(2)	C42B-C41B-C46B	125.4(3)
C40B-C41B-C46B	126.6(3)	C42B-C41B-Nb2B	74.65(13)
C40B-C41B-Nb2B	71.56(13)	C46B-C41B-Nb2B	122.60(17)
C43B-C42B-C41B	108.3(2)	C43B-C42B-C47B	124.4(3)
C41B-C42B-C47B	127.3(3)	C43B-C42B-Nb2B	70.78(13)
C41B-C42B-Nb2B	74.04(13)	C47B-C42B-Nb2B	122.94(17)
C42B-C43B-C44B	108.2(2)	C42B-C43B-C48B	123.6(3)
C44B-C43B-C48B	127.9(3)	C42B-C43B-Nb2B	77.50(14)
C44B-C43B-Nb2B	71.13(13)	C48B-C43B-Nb2B	122.09(17)
C43B-C44B-C40B	107.6(2)	C43B-C44B-C49B	126.7(3)
C40B-C44B-C49B	124.3(3)	C43B-C44B-Nb2B	75.97(13)
C40B-C44B-Nb2B	76.55(13)	C49B-C44B-Nb2B	124.36(17)
C40B-C45B-H45D	109.5	C40B-C45B-H45E	109.5
H45D-C45B-H45E	109.5	C40B-C45B-H45F	109.5
H45D-C45B-H45F	109.5	H45E-C45B-H45F	109.5
C41B-C46B-H46D	109.5	C41B-C46B-H46E	109.5
H46D-C46B-H46E	109.5	C41B-C46B-H46F	109.5
H46D-C46B-H46F	109.5	H46E-C46B-H46F	109.5
C42B-C47B-H47D	109.5	C42B-C47B-H47E	109.5
H47D-C47B-H47E	109.5	C42B-C47B-H47F	109.5
H47D-C47B-H47F	109.5	H47E-C47B-H47F	109.5
C43B-C48B-H48D	109.5	C43B-C48B-H48E	109.5
H48D-C48B-H48E	109.5	C43B-C48B-H48F	109.5
H48D-C48B-H48F	109.5	H48E-C48B-H48F	109.5
C44B-C49B-H49D	109.5	C44B-C49B-H49E	109.5
H49D-C49B-H49E	109.5	C44B-C49B-H49F	109.5
H49D-C49B-H49F	109.5	H49E-C49B-H49F	109.5

Table 6. Torsion angles (°) for *cis*-4a.

N1A-Nb1A-Nb2A-N2A	172.67(12)	N12A-Nb1A-Nb2A-N2A	-68.05(10)
N11A-Nb1A-Nb2A-N2A	-129.80(10)	C24A-Nb1A-Nb2A-N2A	94.61(11)
C23A-Nb1A-Nb2A-N2A	58.98(11)	C20A-Nb1A-Nb2A-N2A	115.49(12)
C22A-Nb1A-Nb2A-N2A	33.26(11)	C21A-Nb1A-Nb2A-N2A	58.6(2)

N2A-Nb1A-Nb2A-N1A	-172.67(12)	N12A-Nb1A-Nb2A-N1A	119.28(10)
N11A-Nb1A-Nb2A-N1A	57.52(10)	C24A-Nb1A-Nb2A-N1A	-78.06(11)
C23A-Nb1A-Nb2A-N1A	-113.70(11)	C20A-Nb1A-Nb2A-N1A	-57.18(12)
C22A-Nb1A-Nb2A-N1A	-139.41(11)	C21A-Nb1A-Nb2A-N1A	-114.1(2)
N1A-Nb1A-Nb2A-N32A	-74.22(10)	N2A-Nb1A-Nb2A-N32A	113.10(10)
N12A-Nb1A-Nb2A-N32A	45.06(7)	N11A-Nb1A-Nb2A-N32A	-16.70(7)
C24A-Nb1A-Nb2A-N32A	-152.29(8)	C23A-Nb1A-Nb2A-N32A	172.08(8)
C20A-Nb1A-Nb2A-N32A	-131.41(10)	C22A-Nb1A-Nb2A-N32A	146.36(9)
C21A-Nb1A-Nb2A-N32A	171.71(19)	N1A-Nb1A-Nb2A-N31A	-134.60(10)
N2A-Nb1A-Nb2A-N31A	52.73(10)	N12A-Nb1A-Nb2A-N31A	-15.32(7)
N11A-Nb1A-Nb2A-N31A	-77.08(7)	C24A-Nb1A-Nb2A-N31A	147.34(8)
C23A-Nb1A-Nb2A-N31A	111.70(8)	C20A-Nb1A-Nb2A-N31A	168.22(10)
C22A-Nb1A-Nb2A-N31A	85.99(9)	C21A-Nb1A-Nb2A-N31A	111.33(19)
N1A-Nb1A-Nb2A-C44A	85.61(11)	N2A-Nb1A-Nb2A-C44A	-87.06(11)
N12A-Nb1A-Nb2A-C44A	-155.11(9)	N11A-Nb1A-Nb2A-C44A	143.14(9)
C24A-Nb1A-Nb2A-C44A	7.55(9)	C23A-Nb1A-Nb2A-C44A	-28.08(9)
C20A-Nb1A-Nb2A-C44A	28.43(11)	C22A-Nb1A-Nb2A-C44A	-53.80(10)
C21A-Nb1A-Nb2A-C44A	-28.5(2)	N1A-Nb1A-Nb2A-C40A	110.88(13)
N2A-Nb1A-Nb2A-C40A	-61.79(13)	N12A-Nb1A-Nb2A-C40A	-129.83(11)
N11A-Nb1A-Nb2A-C40A	168.41(10)	C24A-Nb1A-Nb2A-C40A	32.82(11)
C23A-Nb1A-Nb2A-C40A	-2.81(11)	C20A-Nb1A-Nb2A-C40A	53.70(13)
C22A-Nb1A-Nb2A-C40A	-28.53(12)	C21A-Nb1A-Nb2A-C40A	-3.2(2)
N1A-Nb1A-Nb2A-C43A	49.91(11)	N2A-Nb1A-Nb2A-C43A	-122.77(11)
N12A-Nb1A-Nb2A-C43A	169.19(8)	N11A-Nb1A-Nb2A-C43A	107.43(8)
C24A-Nb1A-Nb2A-C43A	-28.15(9)	C23A-Nb1A-Nb2A-C43A	-63.79(9)
C20A-Nb1A-Nb2A-C43A	-7.28(11)	C22A-Nb1A-Nb2A-C43A	-89.51(10)
C21A-Nb1A-Nb2A-C43A	-64.16(19)	N1A-Nb1A-Nb2A-C41A	65.7(3)
N2A-Nb1A-Nb2A-C41A	-107.0(3)	N12A-Nb1A-Nb2A-C41A	-175.0(2)
N11A-Nb1A-Nb2A-C41A	123.2(2)	C24A-Nb1A-Nb2A-C41A	-12.4(3)
C23A-Nb1A-Nb2A-C41A	-48.0(3)	C20A-Nb1A-Nb2A-C41A	8.5(3)
C22A-Nb1A-Nb2A-C41A	-73.7(3)	C21A-Nb1A-Nb2A-C41A	-48.4(3)
N1A-Nb1A-Nb2A-C42A	26.42(12)	N2A-Nb1A-Nb2A-C42A	-146.25(12)
N12A-Nb1A-Nb2A-C42A	145.70(10)	N11A-Nb1A-Nb2A-C42A	83.95(10)
C24A-Nb1A-Nb2A-C42A	-51.64(11)	C23A-Nb1A-Nb2A-C42A	-87.27(11)
C20A-Nb1A-Nb2A-C42A	-30.76(12)	C22A-Nb1A-Nb2A-C42A	-112.99(11)
C21A-Nb1A-Nb2A-C42A	-87.6(2)	N2A-Nb1A-N1A-Nb2A	4.91(8)
N12A-Nb1A-N1A-Nb2A	-80.29(10)	N11A-Nb1A-N1A-Nb2A	-130.49(8)
C24A-Nb1A-N1A-Nb2A	114.33(8)	C23A-Nb1A-N1A-Nb2A	86.89(10)

C20A-Nb1A-N1A-Nb2A	146.19(7)	C22A-Nb1A-N1A-Nb2A	97.83(17)
C21A-Nb1A-N1A-Nb2A	154.70(9)	N2A-Nb2A-N1A-Nb1A	-4.99(8)
N32A-Nb2A-N1A-Nb1A	112.28(8)	N31A-Nb2A-N1A-Nb1A	73.88(12)
C44A-Nb2A-N1A-Nb1A	-108.74(9)	C40A-Nb2A-N1A-Nb1A	-118.66(10)
C43A-Nb2A-N1A-Nb1A	-135.10(9)	C41A-Nb2A-N1A-Nb1A	-162.25(8)
C42A-Nb2A-N1A-Nb1A	-162.61(8)	N1A-Nb2A-N2A-Nb1A	4.93(8)
N32A-Nb2A-N2A-Nb1A	-84.23(9)	N31A-Nb2A-N2A-Nb1A	-133.78(8)
C44A-Nb2A-N2A-Nb1A	107.89(9)	C40A-Nb2A-N2A-Nb1A	142.07(8)
C43A-Nb2A-N2A-Nb1A	82.97(11)	C41A-Nb2A-N2A-Nb1A	157.91(9)
C42A-Nb2A-N2A-Nb1A	105.6(2)	N1A-Nb1A-N2A-Nb2A	-4.98(8)
N12A-Nb1A-N2A-Nb2A	117.64(8)	N11A-Nb1A-N2A-Nb2A	78.58(11)
C24A-Nb1A-N2A-Nb2A	-102.80(8)	C23A-Nb1A-N2A-Nb2A	-126.14(9)
C20A-Nb1A-N2A-Nb2A	-120.16(10)	C22A-Nb1A-N2A-Nb2A	-156.49(8)
C21A-Nb1A-N2A-Nb2A	-161.75(7)	N1A-Nb1A-N11A-C10A	124.48(14)
N2A-Nb1A-N11A-C10A	43.00(17)	N12A-Nb1A-N11A-C10A	-5.26(12)
C24A-Nb1A-N11A-C10A	-135.57(13)	C23A-Nb1A-N11A-C10A	-101.82(15)
C20A-Nb1A-N11A-C10A	-124.92(14)	C22A-Nb1A-N11A-C10A	-77.53(14)
C21A-Nb1A-N11A-C10A	-92.85(14)	Nb2A-Nb1A-N11A-C10A	89.61(13)
N1A-Nb1A-N11A-C12A	-35.7(2)	N2A-Nb1A-N11A-C12A	-117.2(2)
N12A-Nb1A-N11A-C12A	-165.4(3)	C24A-Nb1A-N11A-C12A	64.3(3)
C23A-Nb1A-N11A-C12A	98.0(2)	C20A-Nb1A-N11A-C12A	74.9(2)
C22A-Nb1A-N11A-C12A	122.3(2)	C21A-Nb1A-N11A-C12A	107.0(2)
Nb2A-Nb1A-N11A-C12A	-70.5(2)	N1A-Nb1A-N12A-C10A	-60.23(15)
N2A-Nb1A-N12A-C10A	-142.93(14)	N11A-Nb1A-N12A-C10A	5.25(12)
C24A-Nb1A-N12A-C10A	98.68(16)	C23A-Nb1A-N12A-C10A	132.06(13)
C20A-Nb1A-N12A-C10A	73.04(14)	C22A-Nb1A-N12A-C10A	120.66(14)
C21A-Nb1A-N12A-C10A	88.97(14)	Nb2A-Nb1A-N12A-C10A	-104.61(12)
N1A-Nb1A-N12A-C15A	105.0(2)	N2A-Nb1A-N12A-C15A	22.3(2)
N11A-Nb1A-N12A-C15A	170.5(2)	C24A-Nb1A-N12A-C15A	-96.1(2)
C23A-Nb1A-N12A-C15A	-62.7(2)	C20A-Nb1A-N12A-C15A	-121.7(2)
C22A-Nb1A-N12A-C15A	-74.1(2)	C21A-Nb1A-N12A-C15A	-105.8(2)
Nb2A-Nb1A-N12A-C15A	60.6(2)	C12A-N11A-C10A-N12A	174.17(19)
Nb1A-N11A-C10A-N12A	7.91(18)	C12A-N11A-C10A-C11A	-5.6(3)
Nb1A-N11A-C10A-C11A	-171.9(2)	C15A-N12A-C10A-N11A	-175.2(2)
Nb1A-N12A-C10A-N11A	-8.41(19)	C15A-N12A-C10A-C11A	4.6(4)
Nb1A-N12A-C10A-C11A	171.4(2)	C10A-N11A-C12A-C13A	-147.8(2)
Nb1A-N11A-C12A-C13A	8.8(3)	C10A-N11A-C12A-C14A	86.6(3)
Nb1A-N11A-C12A-C14A	-116.8(2)	C10A-N12A-C15A-C16A	64.5(3)

Nb1A-N12A-C15A-C16A	-97.1(3)	C10A-N12A-C15A-C17A	-64.8(3)
Nb1A-N12A-C15A-C17A	133.5(2)	N1A-Nb1A-C20A-C24A	-74.78(15)
N2A-Nb1A-C20A-C24A	31.28(19)	N12A-Nb1A-C20A-C24A	146.26(13)
N11A-Nb1A-C20A-C24A	-161.92(14)	C23A-Nb1A-C20A-C24A	38.66(14)
C22A-Nb1A-C20A-C24A	78.83(15)	C21A-Nb1A-C20A-C24A	115.2(2)
Nb2A-Nb1A-C20A-C24A	-37.36(18)	N1A-Nb1A-C20A-C21A	170.00(13)
N2A-Nb1A-C20A-C21A	-83.95(17)	N12A-Nb1A-C20A-C21A	31.03(15)
N11A-Nb1A-C20A-C21A	82.86(14)	C24A-Nb1A-C20A-C21A	-115.2(2)
C23A-Nb1A-C20A-C21A	-76.56(15)	C22A-Nb1A-C20A-C21A	-36.40(13)
Nb2A-Nb1A-C20A-C21A	-152.58(11)	N1A-Nb1A-C20A-C25A	42.8(2)
N2A-Nb1A-C20A-C25A	148.85(19)	N12A-Nb1A-C20A-C25A	-96.2(2)
N11A-Nb1A-C20A-C25A	-44.3(2)	C24A-Nb1A-C20A-C25A	117.6(3)
C23A-Nb1A-C20A-C25A	156.2(2)	C22A-Nb1A-C20A-C25A	-163.6(2)
C21A-Nb1A-C20A-C25A	-127.2(3)	Nb2A-Nb1A-C20A-C25A	80.2(2)
C24A-C20A-C21A-C22A	1.7(2)	C25A-C20A-C21A-C22A	-170.1(2)
Nb1A-C20A-C21A-C22A	65.26(15)	C24A-C20A-C21A-C26A	179.1(2)
C25A-C20A-C21A-C26A	7.3(4)	Nb1A-C20A-C21A-C26A	-117.4(2)
C24A-C20A-C21A-Nb1A	-63.57(14)	C25A-C20A-C21A-Nb1A	124.7(2)
N1A-Nb1A-C21A-C22A	-130.79(15)	N2A-Nb1A-C21A-C22A	9.98(17)
N12A-Nb1A-C21A-C22A	93.40(14)	N11A-Nb1A-C21A-C22A	151.56(14)
C24A-Nb1A-C21A-C22A	-78.25(15)	C23A-Nb1A-C21A-C22A	-36.54(13)
C20A-Nb1A-C21A-C22A	-115.6(2)	Nb2A-Nb1A-C21A-C22A	-36.1(3)
N1A-Nb1A-C21A-C20A	-15.2(2)	N2A-Nb1A-C21A-C20A	125.57(14)
N12A-Nb1A-C21A-C20A	-151.01(14)	N11A-Nb1A-C21A-C20A	-92.85(14)
C24A-Nb1A-C21A-C20A	37.34(13)	C23A-Nb1A-C21A-C20A	79.05(15)
C22A-Nb1A-C21A-C20A	115.6(2)	Nb2A-Nb1A-C21A-C20A	79.5(2)
N1A-Nb1A-C21A-C26A	107.5(2)	N2A-Nb1A-C21A-C26A	-111.7(2)
N12A-Nb1A-C21A-C26A	-28.3(2)	N11A-Nb1A-C21A-C26A	29.9(2)
C24A-Nb1A-C21A-C26A	160.0(2)	C23A-Nb1A-C21A-C26A	-158.2(2)
C20A-Nb1A-C21A-C26A	122.7(3)	C22A-Nb1A-C21A-C26A	-121.7(3)
Nb2A-Nb1A-C21A-C26A	-157.81(15)	C20A-C21A-C22A-C23A	-0.9(2)
C26A-C21A-C22A-C23A	-178.3(2)	Nb1A-C21A-C22A-C23A	63.33(15)
C20A-C21A-C22A-C27A	176.9(2)	C26A-C21A-C22A-C27A	-0.5(4)
Nb1A-C21A-C22A-C27A	-118.9(2)	C20A-C21A-C22A-Nb1A	-64.23(14)
C26A-C21A-C22A-Nb1A	118.3(2)	N1A-Nb1A-C22A-C23A	-18.0(2)
N2A-Nb1A-C22A-C23A	71.92(15)	N12A-Nb1A-C22A-C23A	160.44(15)
N11A-Nb1A-C22A-C23A	-145.83(14)	C24A-Nb1A-C22A-C23A	-38.30(14)
C20A-Nb1A-C22A-C23A	-79.33(15)	C21A-Nb1A-C22A-C23A	-116.0(2)

Nb2A-Nb1A-C22A-C23A	50.28(17)	N1A-Nb1A-C22A-C21A	98.1(2)
N2A-Nb1A-C22A-C21A	-172.06(14)	N12A-Nb1A-C22A-C21A	-83.54(14)
N11A-Nb1A-C22A-C21A	-29.82(15)	C24A-Nb1A-C22A-C21A	77.71(14)
C23A-Nb1A-C22A-C21A	116.0(2)	C20A-Nb1A-C22A-C21A	36.69(13)
Nb2A-Nb1A-C22A-C21A	166.30(10)	N1A-Nb1A-C22A-C27A	-137.6(2)
N2A-Nb1A-C22A-C27A	-47.7(2)	N12A-Nb1A-C22A-C27A	40.8(2)
N11A-Nb1A-C22A-C27A	94.5(2)	C24A-Nb1A-C22A-C27A	-157.9(3)
C23A-Nb1A-C22A-C27A	-119.6(3)	C20A-Nb1A-C22A-C27A	161.0(3)
C21A-Nb1A-C22A-C27A	124.4(3)	Nb2A-Nb1A-C22A-C27A	-69.3(2)
C21A-C22A-C23A-C24A	-0.2(2)	C27A-C22A-C23A-C24A	-178.1(2)
Nb1A-C22A-C23A-C24A	65.75(15)	C21A-C22A-C23A-C28A	172.7(2)
C27A-C22A-C23A-C28A	-5.2(4)	Nb1A-C22A-C23A-C28A	-121.3(2)
C21A-C22A-C23A-Nb1A	-65.98(15)	C27A-C22A-C23A-Nb1A	116.2(2)
N1A-Nb1A-C23A-C22A	170.22(14)	N2A-Nb1A-C23A-C22A	-108.70(15)
N12A-Nb1A-C23A-C22A	-21.83(17)	N11A-Nb1A-C23A-C22A	47.21(18)
C24A-Nb1A-C23A-C22A	114.1(2)	C20A-Nb1A-C23A-C22A	76.09(15)
C21A-Nb1A-C23A-C22A	36.12(13)	Nb2A-Nb1A-C23A-C22A	-143.74(13)
N1A-Nb1A-C23A-C24A	56.13(16)	N2A-Nb1A-C23A-C24A	137.21(14)
N12A-Nb1A-C23A-C24A	-135.91(13)	N11A-Nb1A-C23A-C24A	-66.87(16)
C20A-Nb1A-C23A-C24A	-38.00(13)	C22A-Nb1A-C23A-C24A	-114.1(2)
C21A-Nb1A-C23A-C24A	-77.97(14)	Nb2A-Nb1A-C23A-C24A	102.17(13)
N1A-Nb1A-C23A-C28A	-67.9(2)	N2A-Nb1A-C23A-C28A	13.2(2)
N12A-Nb1A-C23A-C28A	100.1(2)	N11A-Nb1A-C23A-C28A	169.11(19)
C24A-Nb1A-C23A-C28A	-124.0(3)	C20A-Nb1A-C23A-C28A	-162.0(3)
C22A-Nb1A-C23A-C28A	121.9(3)	C21A-Nb1A-C23A-C28A	158.0(3)
Nb2A-Nb1A-C23A-C28A	-21.8(2)	C21A-C20A-C24A-C23A	-1.8(2)
C25A-C20A-C24A-C23A	170.4(2)	Nb1A-C20A-C24A-C23A	-69.28(15)
C21A-C20A-C24A-C29A	-170.4(2)	C25A-C20A-C24A-C29A	1.8(3)
Nb1A-C20A-C24A-C29A	122.1(2)	C21A-C20A-C24A-Nb1A	67.44(15)
C25A-C20A-C24A-Nb1A	-120.3(2)	C22A-C23A-C24A-C20A	1.3(2)
C28A-C23A-C24A-C20A	-171.2(2)	Nb1A-C23A-C24A-C20A	70.67(15)
C22A-C23A-C24A-C29A	169.2(2)	C28A-C23A-C24A-C29A	-3.3(4)
Nb1A-C23A-C24A-C29A	-121.4(2)	C22A-C23A-C24A-Nb1A	-69.39(16)
C28A-C23A-C24A-Nb1A	118.1(2)	N1A-Nb1A-C24A-C20A	113.62(14)
N2A-Nb1A-C24A-C20A	-159.02(13)	N12A-Nb1A-C24A-C20A	-48.44(18)
N11A-Nb1A-C24A-C20A	19.90(16)	C23A-Nb1A-C24A-C20A	-112.87(19)
C22A-Nb1A-C24A-C20A	-76.00(15)	C21A-Nb1A-C24A-C20A	-36.43(13)
Nb2A-Nb1A-C24A-C20A	155.82(12)	N1A-Nb1A-C24A-C23A	-133.51(14)

N2A-Nb1A-C24A-C23A	-46.16(15)	N12A-Nb1A-C24A-C23A	64.43(17)
N11A-Nb1A-C24A-C23A	132.77(13)	C20A-Nb1A-C24A-C23A	112.87(19)
C22A-Nb1A-C24A-C23A	36.87(13)	C21A-Nb1A-C24A-C23A	76.44(14)
Nb2A-Nb1A-C24A-C23A	-91.31(13)	N1A-Nb1A-C24A-C29A	-7.8(2)
N2A-Nb1A-C24A-C29A	79.5(2)	N12A-Nb1A-C24A-C29A	-169.88(19)
N11A-Nb1A-C24A-C29A	-101.5(2)	C23A-Nb1A-C24A-C29A	125.7(3)
C20A-Nb1A-C24A-C29A	-121.4(3)	C22A-Nb1A-C24A-C29A	162.6(3)
C21A-Nb1A-C24A-C29A	-157.9(3)	Nb2A-Nb1A-C24A-C29A	34.4(2)
N2A-Nb2A-N31A-C30A	120.19(14)	N1A-Nb2A-N31A-C30A	41.99(17)
N32A-Nb2A-N31A-C30A	-5.91(12)	C44A-Nb2A-N31A-C30A	-135.12(13)
C40A-Nb2A-N31A-C30A	-129.28(14)	C43A-Nb2A-N31A-C30A	-98.09(15)
C41A-Nb2A-N31A-C30A	-97.76(14)	C42A-Nb2A-N31A-C30A	-79.71(14)
Nb1A-Nb2A-N31A-C30A	87.42(13)	N2A-Nb2A-N31A-C32A	-34.2(3)
N1A-Nb2A-N31A-C32A	-112.4(3)	N32A-Nb2A-N31A-C32A	-160.3(3)
C44A-Nb2A-N31A-C32A	70.5(3)	C40A-Nb2A-N31A-C32A	76.3(3)
C43A-Nb2A-N31A-C32A	107.5(3)	C41A-Nb2A-N31A-C32A	107.8(3)
C42A-Nb2A-N31A-C32A	125.9(3)	Nb1A-Nb2A-N31A-C32A	-67.0(3)
N2A-Nb2A-N32A-C30A	-59.32(15)	N1A-Nb2A-N32A-C30A	-144.25(14)
N31A-Nb2A-N32A-C30A	5.87(12)	C44A-Nb2A-N32A-C30A	103.52(16)
C40A-Nb2A-N32A-C30A	72.34(15)	C43A-Nb2A-N32A-C30A	131.45(14)
C41A-Nb2A-N32A-C30A	85.52(14)	C42A-Nb2A-N32A-C30A	116.91(14)
Nb1A-Nb2A-N32A-C30A	-103.98(13)	N2A-Nb2A-N32A-C35A	108.1(2)
N1A-Nb2A-N32A-C35A	23.1(2)	N31A-Nb2A-N32A-C35A	173.3(2)
C44A-Nb2A-N32A-C35A	-89.1(2)	C40A-Nb2A-N32A-C35A	-120.3(2)
C43A-Nb2A-N32A-C35A	-61.2(2)	C41A-Nb2A-N32A-C35A	-107.1(2)
C42A-Nb2A-N32A-C35A	-75.7(2)	Nb1A-Nb2A-N32A-C35A	63.4(2)
C32A-N31A-C30A-N32A	172.41(19)	Nb2A-N31A-C30A-N32A	8.69(18)
C32A-N31A-C30A-C31A	-6.8(3)	Nb2A-N31A-C30A-C31A	-170.5(2)
C35A-N32A-C30A-N31A	-178.2(2)	Nb2A-N32A-C30A-N31A	-9.8(2)
C35A-N32A-C30A-C31A	1.0(4)	Nb2A-N32A-C30A-C31A	169.4(2)
C30A-N31A-C32A-C33A	-145.0(2)	Nb2A-N31A-C32A-C33A	4.9(4)
C30A-N31A-C32A-C34A	90.1(3)	Nb2A-N31A-C32A-C34A	-119.9(3)
C30A-N32A-C35A-C36A	66.6(3)	Nb2A-N32A-C35A-C36A	-98.0(2)
C30A-N32A-C35A-C37A	-62.5(3)	Nb2A-N32A-C35A-C37A	133.0(2)
N2A-Nb2A-C40A-C41A	160.43(15)	N1A-Nb2A-C40A-C41A	-95.86(18)
N32A-Nb2A-C40A-C41A	25.43(18)	N31A-Nb2A-C40A-C41A	75.74(16)
C44A-Nb2A-C40A-C41A	-113.7(2)	C43A-Nb2A-C40A-C41A	-75.42(16)
C42A-Nb2A-C40A-C41A	-36.20(14)	Nb1A-Nb2A-C40A-C41A	-159.97(12)

N2A-Nb2A-C40A-C44A	-85.84(16)	N1A-Nb2A-C40A-C44A	17.9(2)
N32A-Nb2A-C40A-C44A	139.16(14)	N31A-Nb2A-C40A-C44A	-170.53(15)
C43A-Nb2A-C40A-C44A	38.30(14)	C41A-Nb2A-C40A-C44A	113.7(2)
C42A-Nb2A-C40A-C44A	77.53(16)	Nb1A-Nb2A-C40A-C44A	-46.24(18)
N2A-Nb2A-C40A-C45A	33.9(2)	N1A-Nb2A-C40A-C45A	137.6(2)
N32A-Nb2A-C40A-C45A	-101.1(2)	N31A-Nb2A-C40A-C45A	-50.8(2)
C44A-Nb2A-C40A-C45A	119.8(3)	C43A-Nb2A-C40A-C45A	158.1(3)
C41A-Nb2A-C40A-C45A	-126.5(3)	C42A-Nb2A-C40A-C45A	-162.7(3)
Nb1A-Nb2A-C40A-C45A	73.5(3)	C44A-C40A-C41A-C42A	1.0(3)
C45A-C40A-C41A-C42A	-173.9(2)	Nb2A-C40A-C41A-C42A	66.95(16)
C44A-C40A-C41A-C46A	176.7(2)	C45A-C40A-C41A-C46A	1.8(4)
Nb2A-C40A-C41A-C46A	-117.3(2)	C44A-C40A-C41A-Nb2A	-65.95(16)
C45A-C40A-C41A-Nb2A	119.2(3)	N2A-Nb2A-C41A-C40A	-29.0(2)
N1A-Nb2A-C41A-C40A	114.69(17)	N32A-Nb2A-C41A-C40A	-156.96(16)
N31A-Nb2A-C41A-C40A	-99.92(16)	C44A-Nb2A-C41A-C40A	38.39(15)
C43A-Nb2A-C41A-C40A	79.76(17)	C42A-Nb2A-C41A-C40A	115.4(2)
Nb1A-Nb2A-C41A-C40A	61.4(3)	N2A-Nb2A-C41A-C42A	-144.34(15)
N1A-Nb2A-C41A-C42A	-0.7(2)	N32A-Nb2A-C41A-C42A	87.66(15)
N31A-Nb2A-C41A-C42A	144.71(16)	C44A-Nb2A-C41A-C42A	-76.98(16)
C40A-Nb2A-C41A-C42A	-115.4(2)	C43A-Nb2A-C41A-C42A	-35.61(14)
Nb1A-Nb2A-C41A-C42A	-53.9(3)	N2A-Nb2A-C41A-C46A	93.7(3)
N1A-Nb2A-C41A-C46A	-122.7(2)	N32A-Nb2A-C41A-C46A	-34.3(2)
N31A-Nb2A-C41A-C46A	22.7(2)	C44A-Nb2A-C41A-C46A	161.0(3)
C40A-Nb2A-C41A-C46A	122.7(3)	C43A-Nb2A-C41A-C46A	-157.6(3)
C42A-Nb2A-C41A-C46A	-122.0(3)	Nb1A-Nb2A-C41A-C46A	-175.92(17)
C40A-C41A-C42A-C43A	-0.4(3)	C46A-C41A-C42A-C43A	-176.3(2)
Nb2A-C41A-C42A-C43A	62.95(17)	C40A-C41A-C42A-C47A	175.0(2)
C46A-C41A-C42A-C47A	-0.8(4)	Nb2A-C41A-C42A-C47A	-121.6(3)
C40A-C41A-C42A-Nb2A	-63.38(16)	C46A-C41A-C42A-Nb2A	120.7(2)
N2A-Nb2A-C42A-C43A	-35.4(3)	N1A-Nb2A-C42A-C43A	62.54(16)
N32A-Nb2A-C42A-C43A	153.43(16)	N31A-Nb2A-C42A-C43A	-152.78(15)
C44A-Nb2A-C42A-C43A	-38.09(15)	C40A-Nb2A-C42A-C43A	-79.93(17)
C41A-Nb2A-C42A-C43A	-116.9(2)	Nb1A-Nb2A-C42A-C43A	44.93(18)
N2A-Nb2A-C42A-C41A	81.6(3)	N1A-Nb2A-C42A-C41A	179.47(15)
N32A-Nb2A-C42A-C41A	-89.63(16)	N31A-Nb2A-C42A-C41A	-35.84(16)
C44A-Nb2A-C42A-C41A	78.84(17)	C40A-Nb2A-C42A-C41A	37.01(15)
C43A-Nb2A-C42A-C41A	116.9(2)	Nb1A-Nb2A-C42A-C41A	161.87(12)
N2A-Nb2A-C42A-C47A	-155.7(2)	N1A-Nb2A-C42A-C47A	-57.8(2)

N32A-Nb2A-C42A-C47A	33.1(2)	N31A-Nb2A-C42A-C47A	86.9(2)
C44A-Nb2A-C42A-C47A	-158.4(3)	C40A-Nb2A-C42A-C47A	159.7(3)
C43A-Nb2A-C42A-C47A	-120.3(3)	C41A-Nb2A-C42A-C47A	122.7(3)
Nb1A-Nb2A-C42A-C47A	-75.4(3)	C41A-C42A-C43A-C44A	-0.3(3)
C47A-C42A-C43A-C44A	-175.9(2)	Nb2A-C42A-C43A-C44A	63.71(16)
C41A-C42A-C43A-C48A	175.9(2)	C47A-C42A-C43A-C48A	0.3(4)
Nb2A-C42A-C43A-C48A	-120.1(2)	C41A-C42A-C43A-Nb2A	-64.03(17)
C47A-C42A-C43A-Nb2A	120.4(2)	N2A-Nb2A-C43A-C42A	163.46(14)
N1A-Nb2A-C43A-C42A	-118.22(16)	N32A-Nb2A-C43A-C42A	-28.87(17)
N31A-Nb2A-C43A-C42A	36.13(19)	C44A-Nb2A-C43A-C42A	114.6(2)
C40A-Nb2A-C43A-C42A	75.95(16)	C41A-Nb2A-C43A-C42A	35.72(15)
Nb1A-Nb2A-C43A-C42A	-149.31(13)	N2A-Nb2A-C43A-C44A	48.88(18)
N1A-Nb2A-C43A-C44A	127.21(15)	N32A-Nb2A-C43A-C44A	-143.44(14)
N31A-Nb2A-C43A-C44A	-78.44(17)	C40A-Nb2A-C43A-C44A	-38.62(14)
C41A-Nb2A-C43A-C44A	-78.86(16)	C42A-Nb2A-C43A-C44A	-114.6(2)
Nb1A-Nb2A-C43A-C44A	96.12(14)	N2A-Nb2A-C43A-C48A	-72.9(2)
N1A-Nb2A-C43A-C48A	5.4(2)	N32A-Nb2A-C43A-C48A	94.8(2)
N31A-Nb2A-C43A-C48A	159.8(2)	C44A-Nb2A-C43A-C48A	-121.8(3)
C40A-Nb2A-C43A-C48A	-160.4(3)	C41A-Nb2A-C43A-C48A	159.4(3)
C42A-Nb2A-C43A-C48A	123.7(3)	Nb1A-Nb2A-C43A-C48A	-25.6(2)
C41A-C40A-C44A-C43A	-1.2(3)	C45A-C40A-C44A-C43A	173.9(2)
Nb2A-C40A-C44A-C43A	-71.24(16)	C41A-C40A-C44A-C49A	-165.8(2)
C45A-C40A-C44A-C49A	9.3(4)	Nb2A-C40A-C44A-C49A	124.1(2)
C41A-C40A-C44A-Nb2A	70.04(16)	C45A-C40A-C44A-Nb2A	-114.9(2)
C42A-C43A-C44A-C40A	0.9(3)	C48A-C43A-C44A-C40A	-175.1(2)
Nb2A-C43A-C44A-C40A	69.77(16)	C42A-C43A-C44A-C49A	165.4(2)
C48A-C43A-C44A-C49A	-10.7(4)	Nb2A-C43A-C44A-C49A	-125.8(2)
C42A-C43A-C44A-Nb2A	-68.83(17)	C48A-C43A-C44A-Nb2A	115.1(2)
N2A-Nb2A-C44A-C40A	104.66(15)	N1A-Nb2A-C44A-C40A	-167.27(14)
N32A-Nb2A-C44A-C40A	-59.62(19)	N31A-Nb2A-C44A-C40A	10.73(17)
C43A-Nb2A-C44A-C40A	-112.6(2)	C41A-Nb2A-C44A-C40A	-37.08(14)
C42A-Nb2A-C44A-C40A	-76.42(16)	Nb1A-Nb2A-C44A-C40A	149.14(13)
N2A-Nb2A-C44A-C43A	-142.74(14)	N1A-Nb2A-C44A-C43A	-54.67(16)
N32A-Nb2A-C44A-C43A	52.97(19)	N31A-Nb2A-C44A-C43A	123.33(14)
C40A-Nb2A-C44A-C43A	112.6(2)	C41A-Nb2A-C44A-C43A	75.52(16)
C42A-Nb2A-C44A-C43A	36.17(14)	Nb1A-Nb2A-C44A-C43A	-98.26(14)
N2A-Nb2A-C44A-C49A	-17.8(3)	N1A-Nb2A-C44A-C49A	70.3(3)
N32A-Nb2A-C44A-C49A	178.0(2)	N31A-Nb2A-C44A-C49A	-111.7(2)

C40A-Nb2A-C44A-C49A	-122.4(3)	C43A-Nb2A-C44A-C49A	125.0(3)
C41A-Nb2A-C44A-C49A	-159.5(3)	C42A-Nb2A-C44A-C49A	161.2(3)
Nb1A-Nb2A-C44A-C49A	26.7(3)	N1B-Nb1B-Nb2B-N2B	173.15(12)
N12B-Nb1B-Nb2B-N2B	-71.22(11)	N11B-Nb1B-Nb2B-N2B	-131.91(10)
C24B-Nb1B-Nb2B-N2B	89.28(12)	C20B-Nb1B-Nb2B-N2B	111.29(13)
C23B-Nb1B-Nb2B-N2B	54.35(12)	C21B-Nb1B-Nb2B-N2B	59.1(2)
C22B-Nb1B-Nb2B-N2B	30.09(13)	N2B-Nb1B-Nb2B-N1B	-173.15(12)
N12B-Nb1B-Nb2B-N1B	115.63(10)	N11B-Nb1B-Nb2B-N1B	54.94(10)
C24B-Nb1B-Nb2B-N1B	-83.87(11)	C20B-Nb1B-Nb2B-N1B	-61.86(12)
C23B-Nb1B-Nb2B-N1B	-118.80(11)	C21B-Nb1B-Nb2B-N1B	-114.1(2)
C22B-Nb1B-Nb2B-N1B	-143.06(12)	N1B-Nb1B-Nb2B-N32B	-71.65(10)
N2B-Nb1B-Nb2B-N32B	115.20(11)	N12B-Nb1B-Nb2B-N32B	43.98(8)
N11B-Nb1B-Nb2B-N32B	-16.71(7)	C24B-Nb1B-Nb2B-N32B	-155.52(9)
C20B-Nb1B-Nb2B-N32B	-133.51(11)	C23B-Nb1B-Nb2B-N32B	169.55(9)
C21B-Nb1B-Nb2B-N32B	174.3(2)	C22B-Nb1B-Nb2B-N32B	145.29(11)
N1B-Nb1B-Nb2B-N31B	-132.96(10)	N2B-Nb1B-Nb2B-N31B	53.89(11)
N12B-Nb1B-Nb2B-N31B	-17.33(8)	N11B-Nb1B-Nb2B-N31B	-78.02(7)
C24B-Nb1B-Nb2B-N31B	143.17(9)	C20B-Nb1B-Nb2B-N31B	165.18(11)
C23B-Nb1B-Nb2B-N31B	108.24(9)	C21B-Nb1B-Nb2B-N31B	113.0(2)
C22B-Nb1B-Nb2B-N31B	83.98(11)	N1B-Nb1B-Nb2B-C44B	90.70(11)
N2B-Nb1B-Nb2B-C44B	-82.45(12)	N12B-Nb1B-Nb2B-C44B	-153.67(9)
N11B-Nb1B-Nb2B-C44B	145.65(9)	C24B-Nb1B-Nb2B-C44B	6.83(11)
C20B-Nb1B-Nb2B-C44B	28.85(12)	C23B-Nb1B-Nb2B-C44B	-28.10(11)
C21B-Nb1B-Nb2B-C44B	-23.4(2)	C22B-Nb1B-Nb2B-C44B	-52.36(12)
N1B-Nb1B-Nb2B-C43B	55.00(11)	N2B-Nb1B-Nb2B-C43B	-118.15(11)
N12B-Nb1B-Nb2B-C43B	170.63(9)	N11B-Nb1B-Nb2B-C43B	109.94(9)
C24B-Nb1B-Nb2B-C43B	-28.87(10)	C20B-Nb1B-Nb2B-C43B	-6.86(12)
C23B-Nb1B-Nb2B-C43B	-63.81(11)	C21B-Nb1B-Nb2B-C43B	-59.1(2)
C22B-Nb1B-Nb2B-C43B	-88.06(11)	N1B-Nb1B-Nb2B-C40B	112.62(13)
N2B-Nb1B-Nb2B-C40B	-60.54(13)	N12B-Nb1B-Nb2B-C40B	-131.75(11)
N11B-Nb1B-Nb2B-C40B	167.56(11)	C24B-Nb1B-Nb2B-C40B	28.75(12)
C20B-Nb1B-Nb2B-C40B	50.76(13)	C23B-Nb1B-Nb2B-C40B	-6.19(12)
C21B-Nb1B-Nb2B-C40B	-1.5(2)	C22B-Nb1B-Nb2B-C40B	-30.44(13)
N1B-Nb1B-Nb2B-C41B	52.2(2)	N2B-Nb1B-Nb2B-C41B	-120.9(2)
N12B-Nb1B-Nb2B-C41B	167.9(2)	N11B-Nb1B-Nb2B-C41B	107.2(2)
C24B-Nb1B-Nb2B-C41B	-31.6(2)	C20B-Nb1B-Nb2B-C41B	-9.6(2)
C23B-Nb1B-Nb2B-C41B	-66.6(2)	C21B-Nb1B-Nb2B-C41B	-61.8(3)
C22B-Nb1B-Nb2B-C41B	-90.8(2)	N1B-Nb1B-Nb2B-C42B	28.70(12)

N2B-Nb1B-Nb2B-C42B	-144.45(12)	N12B-Nb1B-Nb2B-C42B	144.33(10)
N11B-Nb1B-Nb2B-C42B	83.64(10)	C24B-Nb1B-Nb2B-C42B	-55.17(11)
C20B-Nb1B-Nb2B-C42B	-33.16(12)	C23B-Nb1B-Nb2B-C42B	-90.10(11)
C21B-Nb1B-Nb2B-C42B	-85.4(2)	C22B-Nb1B-Nb2B-C42B	-114.36(12)
N2B-Nb1B-N1B-Nb2B	4.58(8)	N12B-Nb1B-N1B-Nb2B	-83.06(9)
N11B-Nb1B-N1B-Nb2B	-132.71(8)	C24B-Nb1B-N1B-Nb2B	109.44(9)
C20B-Nb1B-N1B-Nb2B	142.69(8)	C23B-Nb1B-N1B-Nb2B	83.01(11)
C21B-Nb1B-N1B-Nb2B	154.12(10)	C22B-Nb1B-N1B-Nb2B	96.83(19)
N2B-Nb2B-N1B-Nb1B	-4.65(8)	N32B-Nb2B-N1B-Nb1B	114.42(8)
N31B-Nb2B-N1B-Nb1B	75.86(12)	C44B-Nb2B-N1B-Nb1B	-106.47(9)
C43B-Nb2B-N1B-Nb1B	-130.15(9)	C40B-Nb2B-N1B-Nb1B	-122.84(11)
C41B-Nb2B-N1B-Nb1B	-164.39(8)	C42B-Nb2B-N1B-Nb1B	-159.95(8)
N1B-Nb2B-N2B-Nb1B	4.58(8)	N32B-Nb2B-N2B-Nb1B	-82.82(10)
N31B-Nb2B-N2B-Nb1B	-133.34(8)	C44B-Nb2B-N2B-Nb1B	112.29(9)
C43B-Nb2B-N2B-Nb1B	84.83(11)	C40B-Nb2B-N2B-Nb1B	145.32(8)
C41B-Nb2B-N2B-Nb1B	157.11(10)	C42B-Nb2B-N2B-Nb1B	97.2(2)
N1B-Nb1B-N2B-Nb2B	-4.67(8)	N12B-Nb1B-N2B-Nb2B	115.14(8)
N11B-Nb1B-N2B-Nb2B	77.13(12)	C24B-Nb1B-N2B-Nb2B	-105.48(9)
C20B-Nb1B-N2B-Nb2B	-119.41(11)	C23B-Nb1B-N2B-Nb2B	-129.78(10)
C21B-Nb1B-N2B-Nb2B	-161.24(7)	C22B-Nb1B-N2B-Nb2B	-158.79(9)
N1B-Nb1B-N11B-C10B	120.95(13)	N2B-Nb1B-N11B-C10B	40.80(17)
N12B-Nb1B-N11B-C10B	-6.67(12)	C24B-Nb1B-N11B-C10B	-136.37(13)
C20B-Nb1B-N11B-C10B	-127.89(14)	C23B-Nb1B-N11B-C10B	-100.92(16)
C21B-Nb1B-N11B-C10B	-96.09(14)	C22B-Nb1B-N11B-C10B	-79.35(14)
Nb2B-Nb1B-N11B-C10B	87.19(12)	N1B-Nb1B-N11B-C12B	-33.7(3)
N2B-Nb1B-N11B-C12B	-113.9(3)	N12B-Nb1B-N11B-C12B	-161.3(3)
C24B-Nb1B-N11B-C12B	69.0(3)	C20B-Nb1B-N11B-C12B	77.4(3)
C23B-Nb1B-N11B-C12B	104.4(3)	C21B-Nb1B-N11B-C12B	109.2(3)
C22B-Nb1B-N11B-C12B	126.0(3)	Nb2B-Nb1B-N11B-C12B	-67.5(3)
N1B-Nb1B-N12B-C10B	-59.09(16)	N2B-Nb1B-N12B-C10B	-143.01(14)
N11B-Nb1B-N12B-C10B	6.67(12)	C24B-Nb1B-N12B-C10B	102.94(17)
C20B-Nb1B-N12B-C10B	74.37(15)	C23B-Nb1B-N12B-C10B	133.65(14)
C21B-Nb1B-N12B-C10B	89.27(14)	C22B-Nb1B-N12B-C10B	120.96(15)
Nb2B-Nb1B-N12B-C10B	-103.89(13)	N1B-Nb1B-N12B-C15B	104.0(2)
N2B-Nb1B-N12B-C15B	20.1(2)	N11B-Nb1B-N12B-C15B	169.7(2)
C24B-Nb1B-N12B-C15B	-94.0(2)	C20B-Nb1B-N12B-C15B	-122.6(2)
C23B-Nb1B-N12B-C15B	-63.3(2)	C21B-Nb1B-N12B-C15B	-107.7(2)
C22B-Nb1B-N12B-C15B	-76.0(2)	Nb2B-Nb1B-N12B-C15B	59.2(2)

C12B-N11B-C10B-N12B	173.32(19)	Nb1B-N11B-C10B-N12B	9.86(18)
C12B-N11B-C10B-C11B	-5.6(3)	Nb1B-N11B-C10B-C11B	-169.0(2)
C15B-N12B-C10B-N11B	-175.2(2)	Nb1B-N12B-C10B-N11B	-11.0(2)
C15B-N12B-C10B-C11B	3.7(4)	Nb1B-N12B-C10B-C11B	167.84(19)
C10B-N11B-C12B-C13B	-147.9(2)	Nb1B-N11B-C12B-C13B	2.2(4)
C10B-N11B-C12B-C14B	88.2(3)	Nb1B-N11B-C12B-C14B	-121.6(2)
C10B-N12B-C15B-C16B	64.0(3)	Nb1B-N12B-C15B-C16B	-95.1(3)
C10B-N12B-C15B-C17B	-65.3(3)	Nb1B-N12B-C15B-C17B	135.6(2)
N1B-Nb1B-C20B-C21B	166.53(15)	N2B-Nb1B-C20B-C21B	-88.88(18)
N12B-Nb1B-C20B-C21B	28.99(17)	N11B-Nb1B-C20B-C21B	79.84(15)
C24B-Nb1B-C20B-C21B	-114.0(2)	C23B-Nb1B-C20B-C21B	-76.07(17)
C22B-Nb1B-C20B-C21B	-36.50(15)	Nb2B-Nb1B-C20B-C21B	-153.62(12)
N1B-Nb1B-C20B-C24B	-79.45(17)	N2B-Nb1B-C20B-C24B	25.1(2)
N12B-Nb1B-C20B-C24B	143.01(16)	N11B-Nb1B-C20B-C24B	-166.14(16)
C23B-Nb1B-C20B-C24B	37.95(16)	C21B-Nb1B-C20B-C24B	114.0(2)
C22B-Nb1B-C20B-C24B	77.52(17)	Nb2B-Nb1B-C20B-C24B	-39.6(2)
N1B-Nb1B-C20B-C25B	40.1(2)	N2B-Nb1B-C20B-C25B	144.7(2)
N12B-Nb1B-C20B-C25B	-97.5(2)	N11B-Nb1B-C20B-C25B	-46.6(2)
C24B-Nb1B-C20B-C25B	119.5(3)	C23B-Nb1B-C20B-C25B	157.5(3)
C21B-Nb1B-C20B-C25B	-126.4(3)	C22B-Nb1B-C20B-C25B	-162.9(3)
Nb2B-Nb1B-C20B-C25B	79.9(2)	C24B-C20B-C21B-C22B	0.9(3)
C25B-C20B-C21B-C22B	-171.6(2)	Nb1B-C20B-C21B-C22B	66.13(17)
C24B-C20B-C21B-C26B	177.3(2)	C25B-C20B-C21B-C26B	4.8(4)
Nb1B-C20B-C21B-C26B	-117.5(2)	C24B-C20B-C21B-Nb1B	-65.20(15)
C25B-C20B-C21B-Nb1B	122.3(3)	N1B-Nb1B-C21B-C20B	-20.5(2)
N2B-Nb1B-C21B-C20B	119.95(16)	N12B-Nb1B-C21B-C20B	-153.35(16)
N11B-Nb1B-C21B-C20B	-96.26(15)	C24B-Nb1B-C21B-C20B	38.28(15)
C23B-Nb1B-C21B-C20B	79.34(17)	C22B-Nb1B-C21B-C20B	115.3(2)
Nb2B-Nb1B-C21B-C20B	73.8(3)	N1B-Nb1B-C21B-C22B	-135.80(17)
N2B-Nb1B-C21B-C22B	4.6(2)	N12B-Nb1B-C21B-C22B	91.35(16)
N11B-Nb1B-C21B-C22B	148.43(17)	C24B-Nb1B-C21B-C22B	-77.02(17)
C20B-Nb1B-C21B-C22B	-115.3(2)	C23B-Nb1B-C21B-C22B	-35.96(16)
Nb2B-Nb1B-C21B-C22B	-41.5(3)	N1B-Nb1B-C21B-C26B	101.0(3)
N2B-Nb1B-C21B-C26B	-118.6(2)	N12B-Nb1B-C21B-C26B	-31.9(2)
N11B-Nb1B-C21B-C26B	25.2(2)	C24B-Nb1B-C21B-C26B	159.8(3)
C20B-Nb1B-C21B-C26B	121.5(3)	C23B-Nb1B-C21B-C26B	-159.2(3)
C22B-Nb1B-C21B-C26B	-123.2(3)	Nb2B-Nb1B-C21B-C26B	-164.73(17)
C20B-C21B-C22B-C23B	-0.4(3)	C26B-C21B-C22B-C23B	-176.8(2)

Nb1B-C21B-C22B-C23B	63.25(17)	C20B-C21B-C22B-C27B	177.1(3)
C26B-C21B-C22B-C27B	0.7(4)	Nb1B-C21B-C22B-C27B	-119.2(3)
C20B-C21B-C22B-Nb1B	-63.67(16)	C26B-C21B-C22B-Nb1B	119.9(2)
N1B-Nb1B-C22B-C23B	-22.3(3)	N2B-Nb1B-C22B-C23B	67.28(18)
N12B-Nb1B-C22B-C23B	157.62(17)	N11B-Nb1B-C22B-C23B	-149.29(16)
C24B-Nb1B-C22B-C23B	-37.79(16)	C20B-Nb1B-C22B-C23B	-79.57(18)
C21B-Nb1B-C22B-C23B	-116.4(2)	Nb2B-Nb1B-C22B-C23B	47.6(2)
N1B-Nb1B-C22B-C21B	94.1(2)	N2B-Nb1B-C22B-C21B	-176.30(16)
N12B-Nb1B-C22B-C21B	-85.96(16)	N11B-Nb1B-C22B-C21B	-32.86(17)
C24B-Nb1B-C22B-C21B	78.64(17)	C20B-Nb1B-C22B-C21B	36.86(14)
C23B-Nb1B-C22B-C21B	116.4(2)	Nb2B-Nb1B-C22B-C21B	164.07(12)
N1B-Nb1B-C22B-C27B	-142.3(3)	N2B-Nb1B-C22B-C27B	-52.7(3)
N12B-Nb1B-C22B-C27B	37.6(3)	N11B-Nb1B-C22B-C27B	90.7(3)
C24B-Nb1B-C22B-C27B	-157.8(3)	C20B-Nb1B-C22B-C27B	160.5(3)
C23B-Nb1B-C22B-C27B	-120.0(3)	C21B-Nb1B-C22B-C27B	123.6(3)
Nb2B-Nb1B-C22B-C27B	-72.3(3)	C21B-C22B-C23B-C24B	-0.3(3)
C27B-C22B-C23B-C24B	-177.9(3)	Nb1B-C22B-C23B-C24B	64.68(17)
C21B-C22B-C23B-C28B	174.4(2)	C27B-C22B-C23B-C28B	-3.2(4)
Nb1B-C22B-C23B-C28B	-120.6(3)	C21B-C22B-C23B-Nb1B	-64.93(17)
C27B-C22B-C23B-Nb1B	117.5(3)	N1B-Nb1B-C23B-C22B	168.55(15)
N2B-Nb1B-C23B-C22B	-112.65(18)	N12B-Nb1B-C23B-C22B	-24.78(19)
N11B-Nb1B-C23B-C22B	42.1(2)	C24B-Nb1B-C23B-C22B	114.7(2)
C20B-Nb1B-C23B-C22B	76.17(17)	C21B-Nb1B-C23B-C22B	36.09(15)
Nb2B-Nb1B-C23B-C22B	-145.66(15)	N1B-Nb1B-C23B-C24B	53.89(17)
N2B-Nb1B-C23B-C24B	132.69(16)	N12B-Nb1B-C23B-C24B	-139.44(14)
N11B-Nb1B-C23B-C24B	-72.59(18)	C20B-Nb1B-C23B-C24B	-38.50(14)
C21B-Nb1B-C23B-C24B	-78.57(16)	C22B-Nb1B-C23B-C24B	-114.7(2)
Nb2B-Nb1B-C23B-C24B	99.67(14)	N1B-Nb1B-C23B-C28B	-68.8(3)
N2B-Nb1B-C23B-C28B	10.0(3)	N12B-Nb1B-C23B-C28B	97.9(3)
N11B-Nb1B-C23B-C28B	164.7(2)	C24B-Nb1B-C23B-C28B	-122.7(3)
C20B-Nb1B-C23B-C28B	-161.2(3)	C21B-Nb1B-C23B-C28B	158.8(3)
C22B-Nb1B-C23B-C28B	122.7(4)	Nb2B-Nb1B-C23B-C28B	-23.0(3)
C22B-C23B-C24B-C20B	0.8(3)	C28B-C23B-C24B-C20B	-173.6(2)
Nb1B-C23B-C24B-C20B	69.80(16)	C22B-C23B-C24B-C29B	168.1(2)
C28B-C23B-C24B-C29B	-6.4(4)	Nb1B-C23B-C24B-C29B	-123.0(3)
C22B-C23B-C24B-Nb1B	-68.97(18)	C28B-C23B-C24B-Nb1B	116.6(3)
C21B-C20B-C24B-C23B	-1.1(3)	C25B-C20B-C24B-C23B	171.7(2)
Nb1B-C20B-C24B-C23B	-70.34(17)	C21B-C20B-C24B-C29B	-169.1(2)

C25B-C20B-C24B-C29B	3.7(4)	Nb1B-C20B-C24B-C29B	121.7(2)
C21B-C20B-C24B-Nb1B	69.24(16)	C25B-C20B-C24B-Nb1B	-118.0(2)
N1B-Nb1B-C24B-C23B	-136.75(15)	N2B-Nb1B-C24B-C23B	-49.35(16)
N12B-Nb1B-C24B-C23B	59.14(19)	N11B-Nb1B-C24B-C23B	128.63(15)
C20B-Nb1B-C24B-C23B	113.0(2)	C21B-Nb1B-C24B-C23B	76.14(17)
C22B-Nb1B-C24B-C23B	36.44(15)	Nb2B-Nb1B-C24B-C23B	-93.15(15)
N1B-Nb1B-C24B-C20B	110.23(16)	N2B-Nb1B-C24B-C20B	-162.37(15)
N12B-Nb1B-C24B-C20B	-53.9(2)	N11B-Nb1B-C24B-C20B	15.62(18)
C23B-Nb1B-C24B-C20B	-113.0(2)	C21B-Nb1B-C24B-C20B	-36.88(15)
C22B-Nb1B-C24B-C20B	-76.58(17)	Nb2B-Nb1B-C24B-C20B	153.84(14)
N1B-Nb1B-C24B-C29B	-10.1(3)	N2B-Nb1B-C24B-C29B	77.3(3)
N12B-Nb1B-C24B-C29B	-174.2(2)	N11B-Nb1B-C24B-C29B	-104.7(2)
C20B-Nb1B-C24B-C29B	-120.4(3)	C23B-Nb1B-C24B-C29B	126.6(3)
C21B-Nb1B-C24B-C29B	-157.2(3)	C22B-Nb1B-C24B-C29B	163.1(3)
Nb2B-Nb1B-C24B-C29B	33.5(3)	N2B-Nb2B-N31B-C30B	121.25(14)
N1B-Nb2B-N31B-C30B	42.14(18)	N32B-Nb2B-N31B-C30B	-5.55(13)
C44B-Nb2B-N31B-C30B	-135.44(14)	C43B-Nb2B-N31B-C30B	-101.89(16)
C40B-Nb2B-N31B-C30B	-125.51(15)	C41B-Nb2B-N31B-C30B	-93.36(15)
C42B-Nb2B-N31B-C30B	-78.41(15)	Nb1B-Nb2B-N31B-C30B	88.07(13)
N2B-Nb2B-N31B-C32B	-33.5(3)	N1B-Nb2B-N31B-C32B	-112.6(3)
N32B-Nb2B-N31B-C32B	-160.3(3)	C44B-Nb2B-N31B-C32B	69.8(3)
C43B-Nb2B-N31B-C32B	103.3(3)	C40B-Nb2B-N31B-C32B	79.7(3)
C41B-Nb2B-N31B-C32B	111.9(3)	C42B-Nb2B-N31B-C32B	126.8(3)
Nb1B-Nb2B-N31B-C32B	-66.7(3)	N2B-Nb2B-N32B-C30B	-60.61(16)
N1B-Nb2B-N32B-C30B	-144.30(15)	N31B-Nb2B-N32B-C30B	5.56(13)
C44B-Nb2B-N32B-C30B	98.13(17)	C43B-Nb2B-N32B-C30B	130.63(14)
C40B-Nb2B-N32B-C30B	72.21(15)	C41B-Nb2B-N32B-C30B	88.03(15)
C42B-Nb2B-N32B-C30B	119.38(15)	Nb1B-Nb2B-N32B-C30B	-105.05(13)
N2B-Nb2B-N32B-C35B	107.6(2)	N1B-Nb2B-N32B-C35B	23.9(2)
N31B-Nb2B-N32B-C35B	173.8(2)	C44B-Nb2B-N32B-C35B	-93.6(2)
C43B-Nb2B-N32B-C35B	-61.1(2)	C40B-Nb2B-N32B-C35B	-119.6(2)
C41B-Nb2B-N32B-C35B	-103.7(2)	C42B-Nb2B-N32B-C35B	-72.4(2)
Nb1B-Nb2B-N32B-C35B	63.2(2)	C32B-N31B-C30B-N32B	171.0(2)
Nb2B-N31B-C30B-N32B	8.29(19)	C32B-N31B-C30B-C31B	-8.6(4)
Nb2B-N31B-C30B-C31B	-171.3(2)	C35B-N32B-C30B-N31B	-178.0(2)
Nb2B-N32B-C30B-N31B	-9.1(2)	C35B-N32B-C30B-C31B	1.5(4)
Nb2B-N32B-C30B-C31B	170.5(2)	C30B-N31B-C32B-C33B	-148.3(2)
Nb2B-N31B-C32B-C33B	1.6(4)	C30B-N31B-C32B-C34B	86.6(3)

Nb2B-N31B-C32B-C34B	-123.5(3)	C30B-N32B-C35B-C36B	68.0(3)
Nb2B-N32B-C35B-C36B	-97.2(3)	C30B-N32B-C35B-C37B	-61.8(3)
Nb2B-N32B-C35B-C37B	133.0(2)	N2B-Nb2B-C40B-C44B	-78.49(17)
N1B-Nb2B-C40B-C44B	29.5(2)	N32B-Nb2B-C40B-C44B	145.60(15)
N31B-Nb2B-C40B-C44B	-163.13(16)	C43B-Nb2B-C40B-C44B	38.61(15)
C41B-Nb2B-C40B-C44B	114.8(2)	C42B-Nb2B-C40B-C44B	78.57(17)
Nb1B-Nb2B-C40B-C44B	-38.8(2)	N2B-Nb2B-C40B-C41B	166.67(14)
N1B-Nb2B-C40B-C41B	-85.30(19)	N32B-Nb2B-C40B-C41B	30.76(17)
N31B-Nb2B-C40B-C41B	82.03(15)	C44B-Nb2B-C40B-C41B	-114.8(2)
C43B-Nb2B-C40B-C41B	-76.23(16)	C42B-Nb2B-C40B-C41B	-36.27(14)
Nb1B-Nb2B-C40B-C41B	-153.61(12)	N2B-Nb2B-C40B-C45B	40.3(3)
N1B-Nb2B-C40B-C45B	148.4(2)	N32B-Nb2B-C40B-C45B	-95.6(3)
N31B-Nb2B-C40B-C45B	-44.3(3)	C44B-Nb2B-C40B-C45B	118.8(3)
C43B-Nb2B-C40B-C45B	157.4(3)	C41B-Nb2B-C40B-C45B	-126.3(3)
C42B-Nb2B-C40B-C45B	-162.6(3)	Nb1B-Nb2B-C40B-C45B	80.0(3)
C44B-C40B-C41B-C42B	2.2(3)	C45B-C40B-C41B-C42B	-169.0(2)
Nb2B-C40B-C41B-C42B	66.37(16)	C44B-C40B-C41B-C46B	178.5(2)
C45B-C40B-C41B-C46B	7.3(4)	Nb2B-C40B-C41B-C46B	-117.4(2)
C44B-C40B-C41B-Nb2B	-64.14(15)	C45B-C40B-C41B-Nb2B	124.7(3)
N2B-Nb2B-C41B-C42B	-136.20(17)	N1B-Nb2B-C41B-C42B	8.52(19)
N32B-Nb2B-C41B-C42B	93.56(16)	N31B-Nb2B-C41B-C42B	151.71(16)
C44B-Nb2B-C41B-C42B	-77.66(17)	C43B-Nb2B-C41B-C42B	-36.26(15)
C40B-Nb2B-C41B-C42B	-115.3(2)	Nb1B-Nb2B-C41B-C42B	-33.0(3)
N2B-Nb2B-C41B-C40B	-20.9(2)	N1B-Nb2B-C41B-C40B	123.83(16)
N32B-Nb2B-C41B-C40B	-151.13(16)	N31B-Nb2B-C41B-C40B	-92.98(16)
C44B-Nb2B-C41B-C40B	37.65(15)	C43B-Nb2B-C41B-C40B	79.05(16)
C42B-Nb2B-C41B-C40B	115.3(2)	Nb1B-Nb2B-C41B-C40B	82.3(3)
N2B-Nb2B-C41B-C46B	101.3(3)	N1B-Nb2B-C41B-C46B	-114.0(2)
N32B-Nb2B-C41B-C46B	-29.0(2)	N31B-Nb2B-C41B-C46B	29.2(2)
C44B-Nb2B-C41B-C46B	159.8(3)	C43B-Nb2B-C41B-C46B	-158.8(3)
C40B-Nb2B-C41B-C46B	122.1(3)	C42B-Nb2B-C41B-C46B	-122.5(3)
Nb1B-Nb2B-C41B-C46B	-155.58(19)	C40B-C41B-C42B-C43B	-1.4(3)
C46B-C41B-C42B-C43B	-177.7(2)	Nb2B-C41B-C42B-C43B	62.93(16)
C40B-C41B-C42B-C47B	176.1(2)	C46B-C41B-C42B-C47B	-0.2(4)
Nb2B-C41B-C42B-C47B	-119.5(3)	C40B-C41B-C42B-Nb2B	-64.32(15)
C46B-C41B-C42B-Nb2B	119.4(2)	N2B-Nb2B-C42B-C43B	-19.6(3)
N1B-Nb2B-C42B-C43B	70.37(16)	N32B-Nb2B-C42B-C43B	160.42(16)
N31B-Nb2B-C42B-C43B	-145.68(15)	C44B-Nb2B-C42B-C43B	-38.01(15)

C40B-Nb2B-C42B-C43B	-79.43(17)	C41B-Nb2B-C42B-C43B	-116.4(2)
Nb1B-Nb2B-C42B-C43B	51.58(18)	N2B-Nb2B-C42B-C41B	96.8(2)
N1B-Nb2B-C42B-C41B	-173.20(16)	N32B-Nb2B-C42B-C41B	-83.15(16)
N31B-Nb2B-C42B-C41B	-29.24(17)	C44B-Nb2B-C42B-C41B	78.43(17)
C43B-Nb2B-C42B-C41B	116.4(2)	C40B-Nb2B-C42B-C41B	37.00(15)
Nb1B-Nb2B-C42B-C41B	168.01(12)	N2B-Nb2B-C42B-C47B	-138.8(3)
N1B-Nb2B-C42B-C47B	-48.8(3)	N32B-Nb2B-C42B-C47B	41.3(3)
N31B-Nb2B-C42B-C47B	95.2(3)	C44B-Nb2B-C42B-C47B	-157.2(3)
C43B-Nb2B-C42B-C47B	-119.2(3)	C40B-Nb2B-C42B-C47B	161.4(3)
C41B-Nb2B-C42B-C47B	124.4(3)	Nb1B-Nb2B-C42B-C47B	-67.6(3)
C41B-C42B-C43B-C44B	0.0(3)	C47B-C42B-C43B-C44B	-177.6(2)
Nb2B-C42B-C43B-C44B	65.06(15)	C41B-C42B-C43B-C48B	174.5(2)
C47B-C42B-C43B-C48B	-3.1(4)	Nb2B-C42B-C43B-C48B	-120.4(2)
C41B-C42B-C43B-Nb2B	-65.05(16)	C47B-C42B-C43B-Nb2B	117.3(2)
N2B-Nb2B-C43B-C42B	170.24(14)	N1B-Nb2B-C43B-C42B	-110.08(16)
N32B-Nb2B-C43B-C42B	-21.71(18)	N31B-Nb2B-C43B-C42B	46.3(2)
C44B-Nb2B-C43B-C42B	114.4(2)	C40B-Nb2B-C43B-C42B	75.93(16)
C41B-Nb2B-C43B-C42B	35.77(14)	Nb1B-Nb2B-C43B-C42B	-143.30(14)
N2B-Nb2B-C43B-C44B	55.79(18)	N1B-Nb2B-C43B-C44B	135.47(16)
N32B-Nb2B-C43B-C44B	-136.16(15)	N31B-Nb2B-C43B-C44B	-68.12(19)
C40B-Nb2B-C43B-C44B	-38.52(14)	C41B-Nb2B-C43B-C44B	-78.68(16)
C42B-Nb2B-C43B-C44B	-114.4(2)	Nb1B-Nb2B-C43B-C44B	102.25(14)
N2B-Nb2B-C43B-C48B	-67.7(3)	N1B-Nb2B-C43B-C48B	12.0(3)
N32B-Nb2B-C43B-C48B	100.3(3)	N31B-Nb2B-C43B-C48B	168.4(2)
C44B-Nb2B-C43B-C48B	-123.5(3)	C40B-Nb2B-C43B-C48B	-162.0(3)
C41B-Nb2B-C43B-C48B	157.8(3)	C42B-Nb2B-C43B-C48B	122.1(3)
Nb1B-Nb2B-C43B-C48B	-21.2(3)	C42B-C43B-C44B-C40B	1.4(3)
C48B-C43B-C44B-C40B	-172.9(2)	Nb2B-C43B-C44B-C40B	70.68(15)
C42B-C43B-C44B-C49B	168.1(2)	C48B-C43B-C44B-C49B	-6.2(4)
Nb2B-C43B-C44B-C49B	-122.6(2)	C42B-C43B-C44B-Nb2B	-69.32(16)
C48B-C43B-C44B-Nb2B	116.5(2)	C41B-C40B-C44B-C43B	-2.2(2)
C45B-C40B-C44B-C43B	169.3(2)	Nb2B-C40B-C44B-C43B	-70.27(15)
C41B-C40B-C44B-C49B	-169.3(2)	C45B-C40B-C44B-C49B	2.2(4)
Nb2B-C40B-C44B-C49B	122.6(2)	C41B-C40B-C44B-Nb2B	68.06(16)
C45B-C40B-C44B-Nb2B	-120.4(2)	N2B-Nb2B-C44B-C43B	-135.67(15)
N1B-Nb2B-C44B-C43B	-47.48(16)	N32B-Nb2B-C44B-C43B	63.33(19)
N31B-Nb2B-C44B-C43B	130.79(15)	C40B-Nb2B-C44B-C43B	112.4(2)
C41B-Nb2B-C44B-C43B	75.81(16)	C42B-Nb2B-C44B-C43B	36.59(14)

Nb1B-Nb2B-C44B-C43B	-92.14(15)	N2B-Nb2B-C44B-C40B	111.95(16)
N1B-Nb2B-C44B-C40B	-159.86(15)	N32B-Nb2B-C44B-C40B	-49.0(2)
N31B-Nb2B-C44B-C40B	18.41(18)	C43B-Nb2B-C44B-C40B	-112.4(2)
C41B-Nb2B-C44B-C40B	-36.57(15)	C42B-Nb2B-C44B-C40B	-75.79(16)
Nb1B-Nb2B-C44B-C40B	155.48(13)	N2B-Nb2B-C44B-C49B	-10.6(3)
N1B-Nb2B-C44B-C49B	77.6(3)	N32B-Nb2B-C44B-C49B	-171.6(2)
N31B-Nb2B-C44B-C49B	-104.1(3)	C43B-Nb2B-C44B-C49B	125.1(3)
C40B-Nb2B-C44B-C49B	-122.5(3)	C41B-Nb2B-C44B-C49B	-159.1(3)
C42B-Nb2B-C44B-C49B	161.7(3)	Nb1B-Nb2B-C44B-C49B	33.0(3)

Table 7. Anisotropic atomic displacement parameters (Å^2) for *cis*-4a.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1A	0.02780(9)	0.03635(11)	0.02805(10)	0.01489(8)	0.00243(7)	0.00703(7)
Nb2A	0.03305(10)	0.03822(11)	0.02823(10)	0.01281(9)	0.00629(7)	0.00511(8)
N1A	0.0461(11)	0.0331(10)	0.0412(11)	0.0132(9)	0.0139(9)	0.0060(8)
N2A	0.0407(10)	0.0349(10)	0.0477(12)	0.0182(9)	0.0127(9)	0.0107(8)
N11A	0.0427(10)	0.0384(11)	0.0303(10)	0.0110(8)	0.0016(8)	0.0078(8)
N12A	0.0448(10)	0.0448(11)	0.0331(10)	0.0180(9)	0.0032(8)	0.0165(9)
C10A	0.0350(11)	0.0552(15)	0.0295(12)	0.0168(11)	0.0051(9)	0.0101(10)
C11A	0.0734(18)	0.0702(19)	0.0342(14)	0.0215(13)	-0.0037(12)	0.0161(15)
C12A	0.0467(13)	0.0437(14)	0.0389(13)	0.0053(11)	0.0009(10)	0.0101(11)
C13A	0.0630(17)	0.0393(15)	0.0685(19)	0.0132(14)	0.0115(14)	0.0115(13)
C14A	0.0662(18)	0.0628(18)	0.0495(16)	0.0053(14)	0.0144(14)	0.0203(15)
C15A	0.0557(14)	0.0551(15)	0.0444(14)	0.0277(12)	0.0123(11)	0.0254(12)
C16A	0.0627(17)	0.091(2)	0.072(2)	0.0461(18)	0.0162(15)	0.0412(17)
C17A	0.079(2)	0.0679(19)	0.075(2)	0.0455(17)	0.0270(16)	0.0290(16)
C20A	0.0279(10)	0.0494(14)	0.0412(13)	0.0199(11)	0.0007(9)	0.0110(9)
C21A	0.0254(10)	0.0588(15)	0.0422(13)	0.0263(12)	0.0040(9)	0.0077(10)
C22A	0.0314(11)	0.0457(14)	0.0542(15)	0.0243(12)	0.0009(10)	-0.0005(10)
C23A	0.0358(12)	0.0488(15)	0.0403(13)	0.0123(11)	-0.0016(10)	0.0027(10)
C24A	0.0336(11)	0.0540(15)	0.0353(12)	0.0213(11)	-0.0030(9)	0.0059(10)
C25A	0.0503(15)	0.0653(18)	0.0663(18)	0.0241(15)	0.0031(13)	0.0266(13)
C26A	0.0385(13)	0.092(2)	0.0545(16)	0.0421(16)	0.0142(11)	0.0175(13)
C27A	0.0651(18)	0.0549(18)	0.099(2)	0.0406(18)	0.0009(17)	-0.0049(14)
C28A	0.0730(19)	0.0600(19)	0.0524(18)	0.0008(15)	0.0037(14)	0.0021(15)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C29A	0.0589(16)	0.093(2)	0.0527(17)	0.0442(17)	-0.0004(13)	0.0200(16)
N31A	0.0399(10)	0.0368(11)	0.0430(11)	0.0134(9)	0.0047(8)	0.0111(8)
N32A	0.0386(10)	0.0363(10)	0.0387(11)	0.0084(9)	0.0027(8)	0.0092(8)
C30A	0.0300(10)	0.0438(13)	0.0406(13)	0.0140(11)	0.0075(9)	0.0090(9)
C31A	0.0435(14)	0.0584(17)	0.0630(18)	0.0148(14)	-0.0108(12)	0.0130(12)
C32A	0.0612(16)	0.0436(14)	0.0518(16)	0.0158(12)	0.0065(12)	0.0205(12)
C33A	0.084(2)	0.0390(15)	0.072(2)	0.0177(14)	0.0045(16)	0.0132(14)
C34A	0.077(2)	0.0649(19)	0.077(2)	0.0212(17)	0.0183(17)	0.0394(16)
C35A	0.0379(12)	0.0394(13)	0.0496(15)	0.0062(11)	0.0035(10)	0.0088(10)
C36A	0.0548(16)	0.0692(19)	0.0497(16)	0.0025(14)	0.0075(13)	0.0185(14)
C37A	0.0431(14)	0.0475(16)	0.095(2)	0.0092(16)	0.0099(15)	-0.0005(12)
C40A	0.0652(16)	0.0492(15)	0.0336(13)	0.0161(12)	0.0203(12)	0.0130(13)
C41A	0.0499(14)	0.0658(17)	0.0419(14)	0.0288(13)	0.0208(11)	0.0143(13)
C42A	0.0526(14)	0.0508(15)	0.0430(14)	0.0239(12)	0.0152(11)	0.0042(12)
C43A	0.0552(15)	0.0554(16)	0.0409(14)	0.0273(12)	0.0132(11)	0.0124(12)
C44A	0.0536(14)	0.0574(16)	0.0323(13)	0.0196(12)	0.0080(11)	0.0044(12)
C45A	0.115(3)	0.0618(19)	0.0488(17)	0.0193(15)	0.0288(17)	0.0289(18)
C46A	0.0542(16)	0.103(3)	0.084(2)	0.054(2)	0.0356(16)	0.0270(17)
C47A	0.081(2)	0.0593(19)	0.079(2)	0.0309(17)	0.0099(17)	-0.0088(16)
C48A	0.077(2)	0.078(2)	0.081(2)	0.0485(19)	0.0219(17)	0.0281(17)
C49A	0.0682(19)	0.092(2)	0.0452(16)	0.0229(16)	-0.0012(14)	-0.0057(17)
Nb1B	0.03040(9)	0.04437(12)	0.03272(11)	0.02112(9)	0.00408(7)	0.01158(8)
Nb2B	0.02838(9)	0.04288(11)	0.03081(10)	0.01824(9)	0.00736(7)	0.01177(8)
N1B	0.0331(9)	0.0390(11)	0.0453(11)	0.0152(9)	0.0070(8)	0.0110(8)
N2B	0.0369(10)	0.0405(11)	0.0525(12)	0.0190(10)	-0.0031(9)	0.0101(8)
N11B	0.0353(9)	0.0437(11)	0.0412(11)	0.0191(9)	0.0093(8)	0.0113(8)
N12B	0.0470(11)	0.0437(11)	0.0459(12)	0.0252(10)	0.0132(9)	0.0170(9)
C10B	0.0307(10)	0.0538(15)	0.0396(13)	0.0249(12)	0.0092(9)	0.0144(10)
C11B	0.0545(15)	0.0661(18)	0.0526(16)	0.0313(14)	0.0223(12)	0.0176(13)
C12B	0.0481(14)	0.0469(15)	0.0499(15)	0.0184(12)	0.0098(11)	0.0136(11)
C13B	0.0600(17)	0.0473(16)	0.080(2)	0.0195(15)	0.0084(15)	0.0041(13)
C14B	0.0645(18)	0.0575(18)	0.082(2)	0.0198(16)	0.0166(16)	0.0272(15)
C15B	0.0503(14)	0.0486(15)	0.0769(19)	0.0342(14)	0.0228(13)	0.0192(12)
C16B	0.078(2)	0.091(2)	0.111(3)	0.078(2)	0.0396(19)	0.0391(18)
C17B	0.0577(18)	0.0559(19)	0.133(3)	0.036(2)	0.0296(19)	0.0114(15)
C20B	0.0483(13)	0.0640(17)	0.0401(13)	0.0293(13)	0.0023(10)	0.0249(12)
C21B	0.0371(12)	0.0792(19)	0.0442(14)	0.0314(14)	-0.0001(10)	0.0204(12)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C22B	0.0537(15)	0.0626(18)	0.0514(16)	0.0210(14)	-0.0171(12)	0.0107(13)
C23B	0.0604(16)	0.072(2)	0.0376(14)	0.0124(14)	-0.0058(12)	0.0313(15)
C24B	0.0484(14)	0.082(2)	0.0355(13)	0.0298(14)	0.0063(11)	0.0278(14)
C25B	0.089(2)	0.077(2)	0.075(2)	0.0430(18)	0.0039(17)	0.0362(18)
C26B	0.0402(14)	0.121(3)	0.072(2)	0.048(2)	0.0077(13)	0.0293(16)
C27B	0.092(3)	0.080(2)	0.105(3)	0.037(2)	-0.038(2)	-0.011(2)
C28B	0.100(3)	0.103(3)	0.057(2)	-0.0022(19)	-0.0075(18)	0.056(2)
C29B	0.0670(19)	0.145(3)	0.065(2)	0.069(2)	0.0218(16)	0.036(2)
N31B	0.0454(11)	0.0502(12)	0.0441(12)	0.0278(10)	0.0076(9)	0.0159(9)
N32B	0.0484(11)	0.0512(12)	0.0335(10)	0.0169(9)	0.0035(8)	0.0178(9)
C30B	0.0423(13)	0.0682(17)	0.0399(14)	0.0313(13)	0.0055(10)	0.0210(12)
C31B	0.098(2)	0.092(2)	0.0477(17)	0.0434(17)	0.0086(16)	0.0327(19)
C32B	0.0685(17)	0.0550(17)	0.0667(19)	0.0388(15)	0.0196(14)	0.0219(14)
C33B	0.080(2)	0.0477(17)	0.080(2)	0.0262(16)	0.0157(17)	0.0100(15)
C34B	0.104(3)	0.084(2)	0.112(3)	0.063(2)	0.022(2)	0.050(2)
C35B	0.0595(16)	0.0602(17)	0.0378(14)	0.0135(13)	-0.0022(12)	0.0158(13)
C36B	0.086(2)	0.090(2)	0.0542(18)	0.0191(17)	0.0138(16)	0.0429(19)
C37B	0.080(2)	0.093(3)	0.058(2)	0.0126(18)	-0.0194(16)	0.0148(19)
C40B	0.0389(12)	0.0544(16)	0.0614(17)	0.0248(14)	0.0247(12)	0.0200(11)
C41B	0.0299(11)	0.0717(18)	0.0562(16)	0.0317(14)	0.0137(11)	0.0187(11)
C42B	0.0307(11)	0.0569(16)	0.0605(17)	0.0201(14)	0.0145(11)	0.0078(11)
C43B	0.0401(13)	0.0645(18)	0.0675(18)	0.0391(15)	0.0258(12)	0.0197(12)
C44B	0.0384(12)	0.0720(18)	0.0429(14)	0.0261(13)	0.0193(11)	0.0178(12)
C45B	0.079(2)	0.069(2)	0.107(3)	0.034(2)	0.047(2)	0.0362(17)
C46B	0.0432(15)	0.122(3)	0.084(2)	0.053(2)	0.0070(15)	0.0360(17)
C47B	0.0566(18)	0.073(2)	0.098(3)	0.010(2)	0.0148(17)	-0.0058(16)
C48B	0.071(2)	0.091(2)	0.125(3)	0.078(2)	0.037(2)	0.0268(18)
C49B	0.071(2)	0.138(3)	0.0455(17)	0.0300(19)	0.0242(15)	0.040(2)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for *cis*-4a.

	x/a	y/b	z/c	U(eq)
H11A	0.9794	0.2379	0.5454	0.089
H11B	0.9560	0.1486	0.5294	0.089
H11C	1.0766	0.1932	0.5179	0.089
H12A	0.9971	0.0708	0.5693	0.056

	x/a	y/b	z/c	U(eq)
H13A	1.1036	0.0453	0.6870	0.089
H13B	1.0185	-0.0199	0.6182	0.089
H13C	0.9731	0.0465	0.6796	0.089
H14A	1.1798	0.0988	0.5301	0.096
H14B	1.1487	0.0129	0.5260	0.096
H14C	1.2345	0.0794	0.5935	0.096
H15A	1.0623	0.3991	0.7325	0.057
H16A	0.8869	0.3102	0.6121	0.101
H16B	0.8956	0.3957	0.6714	0.101
H16C	0.8704	0.3256	0.6974	0.101
H17A	1.1916	0.3945	0.6401	0.1
H17B	1.0982	0.4395	0.6357	0.1
H17C	1.0865	0.3537	0.5764	0.1
H25A	1.4039	0.1530	0.7757	0.089
H25B	1.3429	0.1387	0.6965	0.089
H25C	1.2715	0.1128	0.7544	0.089
H26A	1.2858	0.2832	0.6457	0.086
H26B	1.3670	0.2296	0.6484	0.086
H26C	1.4161	0.3205	0.6783	0.086
H27A	1.3798	0.4719	0.8366	0.11
H27B	1.2450	0.4535	0.8210	0.11
H27C	1.3193	0.4290	0.7528	0.11
H28A	1.3324	0.4497	0.9621	0.106
H28B	1.2710	0.3849	0.9898	0.106
H28C	1.1974	0.4195	0.9486	0.106
H29A	1.2290	0.1717	0.8905	0.095
H29B	1.2476	0.2531	0.9591	0.095
H29C	1.3545	0.2218	0.9259	0.095
H31A	0.5678	0.2630	0.7333	0.087
H31B	0.6000	0.1880	0.6754	0.087
H31C	0.6639	0.2711	0.6800	0.087
H32A	0.7273	0.3833	0.7797	0.062
H33A	0.8677	0.4636	0.9200	0.1
H33B	0.8392	0.5013	0.8641	0.1
H33C	0.9168	0.4412	0.8408	0.1
H34A	0.5735	0.3635	0.8488	0.107
H34B	0.6280	0.4536	0.8763	0.107

	x/a	y/b	z/c	U(eq)
H34C	0.6549	0.4086	0.9255	0.107
H35A	0.7731	0.0782	0.7284	0.055
H36A	0.7204	0.1230	0.6108	0.096
H36B	0.7567	0.0458	0.6010	0.096
H36C	0.8465	0.1270	0.6392	0.096
H37A	0.5741	0.0836	0.7541	0.104
H37B	0.5931	0.0101	0.6861	0.104
H37C	0.5563	0.0771	0.6702	0.104
H45A	0.7758	0.3955	1.0181	0.112
H45B	0.9088	0.4190	1.0126	0.112
H45C	0.8649	0.4042	1.0838	0.112
H46A	0.6103	0.2277	0.8855	0.11
H46B	0.6230	0.2944	0.9669	0.11
H46C	0.5812	0.2065	0.9558	0.11
H47A	0.7032	0.0654	0.9306	0.115
H47B	0.7565	0.0559	0.8541	0.115
H47C	0.6456	0.0884	0.8709	0.115
H48A	1.0000	0.1095	0.8967	0.107
H48B	0.9387	0.0900	0.9612	0.107
H48C	1.0518	0.1573	0.9820	0.107
H49A	1.0478	0.3249	1.0935	0.111
H49B	1.0829	0.3675	1.0385	0.111
H49C	1.1170	0.2888	1.0252	0.111
H11D	0.7597	0.1852	0.0997	0.082
H11E	0.8738	0.1757	0.1327	0.082
H11F	0.8596	0.2593	0.1450	0.082
H12B	0.6993	0.0742	0.1242	0.058
H13D	0.6146	0.0179	0.2348	0.098
H13E	0.5949	-0.0321	0.1468	0.098
H13F	0.5378	0.0386	0.1818	0.098
H14D	0.8846	0.0788	0.1712	0.102
H14E	0.8083	-0.0074	0.1392	0.102
H14F	0.8308	0.0419	0.2273	0.102
H15B	0.7762	0.3964	0.3166	0.065
H16D	0.7384	0.3357	0.1574	0.117
H16E	0.7396	0.4217	0.2122	0.117
H16F	0.6412	0.3516	0.2115	0.117

	x/a	y/b	z/c	U(eq)
H17D	0.9669	0.3832	0.3045	0.124
H17E	0.9408	0.4445	0.2746	0.124
H17F	0.9449	0.3608	0.2167	0.124
H25D	0.7845	0.0797	0.3506	0.11
H25E	0.6563	0.0659	0.3697	0.11
H25F	0.7577	0.0846	0.4321	0.11
H26D	0.9404	0.2386	0.3270	0.11
H26E	0.9393	0.1698	0.3529	0.11
H26F	1.0072	0.2553	0.4052	0.11
H27D	0.9241	0.4166	0.5137	0.148
H27E	0.8416	0.4236	0.4533	0.148
H27F	0.9453	0.3850	0.4276	0.148
H28D	0.6199	0.3870	0.5047	0.138
H28E	0.7190	0.4059	0.5687	0.138
H28F	0.6025	0.3451	0.5615	0.138
H29D	0.5939	0.1614	0.5247	0.123
H29E	0.5164	0.1344	0.4477	0.123
H29F	0.5173	0.2145	0.5143	0.123
H31D	0.3545	0.3198	0.0974	0.109
H31E	0.4303	0.2590	0.0680	0.109
H31F	0.4893	0.3476	0.1160	0.109
H32B	0.5109	0.4351	0.2250	0.069
H33D	0.4746	0.4741	0.3789	0.104
H33E	0.5465	0.5330	0.3477	0.104
H33F	0.5907	0.4606	0.3453	0.104
H34D	0.3143	0.4307	0.2007	0.132
H34E	0.3840	0.5156	0.2532	0.132
H34F	0.3048	0.4635	0.2885	0.132
H35B	0.3699	0.1063	0.1438	0.065
H36D	0.5149	0.1706	0.0585	0.114
H36E	0.4898	0.0835	0.0508	0.114
H36F	0.5597	0.1512	0.1250	0.114
H37D	0.2153	0.1307	0.0844	0.125
H37E	0.2703	0.0660	0.0286	0.125
H37F	0.3002	0.1506	0.0292	0.125
H45D	0.2362	0.4100	0.3656	0.122
H45E	0.3269	0.4252	0.4332	0.122

	x/a	y/b	z/c	U(eq)
H45F	0.1944	0.3999	0.4392	0.122
H46D	0.1853	0.2524	0.1930	0.115
H46E	0.1447	0.3206	0.2554	0.115
H46F	0.0671	0.2348	0.2252	0.115
H47D	0.0989	0.0717	0.2486	0.13
H47E	0.2211	0.0709	0.2199	0.13
H47F	0.1367	0.1073	0.1886	0.13
H48D	0.2156	0.0837	0.3722	0.124
H48E	0.3096	0.1426	0.4392	0.124
H48F	0.3459	0.1008	0.3580	0.124
H49D	0.2810	0.3118	0.5242	0.127
H49E	0.3935	0.3592	0.5062	0.127
H49F	0.3891	0.2764	0.5062	0.127

Table 9. Data collection details for *cis*-4a.

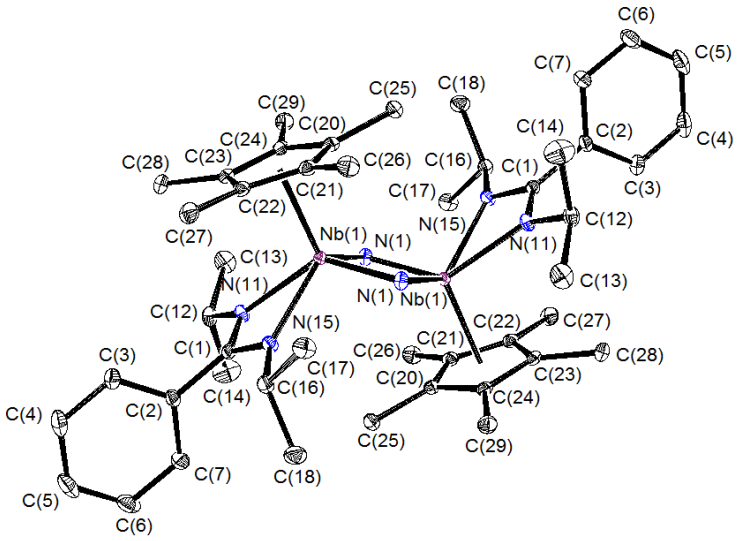
Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s
Omega	50.075	-31.50	-31.50	0.00	54.71	0.50	366	25.00
Omega	50.075	-31.50	-31.50	120.00	54.71	0.50	366	25.00
Omega	50.075	-31.50	-31.50	240.00	54.71	0.50	366	25.00
Phi	50.075	-31.50	-211.50	0.00	54.71	0.50	720	25.00
Phi	50.075	-31.50	-30.00	0.00	54.71	0.50	1	10.00

Table 10. CheckCIF output for *cis*-4a.

```
#===============================================================================
==
# PLATON/CHECK-(201107) versus check.def version of 141107  for entry: 2195
# Data From: 2195.cif - Data Type: CIF          Bond Precision   C-C = 0.0041
A
# Refl Data: 2195.fcf - Data Type: SHELXL                          Temp = 295
K
#
# UCL 11.9347(14)   19.054(2)   19.120(2) 112.5059(17)
90.9022(17)102.7028(17)
# WaveLength 0.71073    Volume Reported    3894.3(8)  Calculated    3894.4(7)
# SpaceGroup from Symmetry P -1          Hall: -P 1
#                 Reported P-1                -P 1
# MoietyFormula C36 H64 N6 Nb2
#      Reported C36 H64 N6 Nb2
#    SumFormula C36 H64 N6 Nb2
#      Reported C36 H64 N6 Nb2
# Mr        =    766.75[Calc],    766.75[Rep]
# Dx,gcm-3  =     1.308[Calc],     1.308[Rep]
# Z         =         4[Calc],         4[Rep]
# Mu (mm-1) =     0.620[Calc],     0.620[Rep]
```

```
# F000      =    1616.0[Calc],    1616.0[Rep]  or F000' =   1599.47[Calc]
# Reported   T Limits: Tmin=0.822              Tmax=0.917  AbsCorr=MULTI-SCAN
# Calculated T Limits: Tmin=0.875 Tmin'=0.856  Tmax=0.917
# Reported   Hmax= 15, Kmax= 24, Lmax= 24, Nref=17869       , Th(max)= 27.500
# Obs in FCF Hmax= 15, Kmax= 24, Lmax= 24, Nref=17869       , Th(max)= 27.498
# Calculated Hmax= 15, Kmax= 24, Lmax= 24, Nref=17893       , Ratio  =  0.999
# Rho(min) = -0.29, Rho(max) =  0.40 e/Ang^3
# R= 0.0300(14751), wR2= 0.0603(17869), S = 1.000, Npar= 833
#===============================================================================
==
152_ALERT_1_C Supplied and Calc Volume s.u. Inconsistent .....          ?
154_ALERT_1_C The su's on the Cell Angles are Equal  (x 10000)        170
Deg.
220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       2.54
Ratio
601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .      53.00
A**3
910_ALERT_3_C # Missing FCF Reflections Below Th(Min) ........          4
912_ALERT_3_C # Missing FCF Reflections Above    STh/L=  0.600         19
#===============================================================================
==
```

trans-{Cp*Nb[N(iPr)C(Ph)N(iPr](μ-N)}$_2$ (*trans*-4b)



A dark orange-red prism-like specimen of $C_{46}H_{68}N_6Nb_2$, approximate dimensions 0.21 mm × 0.26 mm × 0.28 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 1.52 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using an orthorhombic unit cell yielded a total of 48682 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 6351 were independent (average redundancy 7.665, completeness = 100.0%, R_{int} = 4.10%) and 5334 (83.99%) were greater than $2\sigma(F^2)$. The final cell constants of *a* = 16.5274(18) Å, *b* = 15.3353(17) Å, *c* = 17.1720(19) Å, *V* = 4352.3(8) Å^3, are based upon the

refinement of the XYZ-centroids of 9954 reflections above 20 σ(I) with 4.330° < 2θ < 63.70°. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8090 and 0.8880.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group Pbca, with Z = 4 for the formula unit, $C_{46}H_{68}N_6Nb_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 269 variables converged at R_1 = 2.34%, for the observed data and wR_2 = 5.33% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.365 $e^-/Å^3$ and the largest hole was -0.370 $e^-/Å^3$ with an RMS deviation of 0.059 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.360 g/cm^3 and F(000), 1872 e^-.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for *trans*-4b.

Identification code	***trans*-4b**	
Chemical formula	$C_{46}H_{68}N_6Nb_2$	
Formula weight	890.88	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.21 × 0.26 × 0.28 mm	
Crystal habit	dark orange-red prism	
Crystal system	orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 16.5274(18) Å	α = 90°
	b = 15.3353(17) Å	β = 90°
	c = 17.1720(19) Å	γ = 90°
Volume	4352.3(8) $Å^3$	
Z	4	
Density (calculated)	1.360 Mg/cm^3	
Absorption coefficient	0.565 mm^{-1}	
F(000)	1872	

Table 2. Data collection and structure refinement for *trans*-4b.

Diffractometer	Bruker APEX-II CCD
Radiation source	sealed tube, MoKα

Theta range for data collection	2.17 to 30.00°	
Index ranges	$-23 \leq h \leq 23$, $-21 \leq k \leq 21$, $-24 \leq l \leq 24$	
Reflections collected	48682	
Independent reflections	6351 [R(int) = 0.0410]	
Coverage of independent reflections	100.0%	
Absorption correction	multi-scan	
Max. and min. transmission	0.8880 and 0.8090	
Structure solution technique	direct methods	
Structure solution program	ShelXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	ShelXL-2012 (Sheldrick, 2012)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6351 / 0 / 269	
Goodness-of-fit on F^2	1.000	
Δ/σ_{max}	0.001	
Final R indices	5334 data; $I>2\sigma(I)$	$R_1 = 0.0234$, $wR_2 = 0.0496$
	all data	$R_1 = 0.0311$, $wR_2 = 0.0533$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0100P)^2+3.8300P]$, $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.365 and -0.370 eÅ^{-3}	
R.M.S. deviation from mean	0.059 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for *trans*-4b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Nb1	0.53898(2)	0.43429(2)	0.45768(2)	0.01413(3)
N1	0.43197(7)	0.46061(8)	0.48848(7)	0.0187(2)
C1	0.55863(8)	0.43926(9)	0.29996(8)	0.0173(3)
C2	0.57730(9)	0.43305(10)	0.21439(8)	0.0200(3)
C3	0.62541(9)	0.36509(10)	0.18721(9)	0.0249(3)
C4	0.64595(11)	0.36051(12)	0.10857(10)	0.0336(4)
C5	0.61852(12)	0.42349(13)	0.05734(10)	0.0387(5)
C6	0.57098(13)	0.49097(13)	0.08376(10)	0.0374(4)
C7	0.55021(11)	0.49619(11)	0.16219(9)	0.0283(3)
N11	0.49487(7)	0.40336(8)	0.33417(7)	0.0191(2)
C12	0.42893(9)	0.36058(10)	0.29114(9)	0.0235(3)
C13	0.37592(10)	0.30926(12)	0.34726(10)	0.0345(4)
C14	0.37504(12)	0.42537(13)	0.24829(13)	0.0452(5)
N15	0.60659(7)	0.48016(8)	0.35018(7)	0.0188(2)
C16	0.68100(9)	0.52520(10)	0.32588(8)	0.0209(3)
C17	0.73739(10)	0.53579(11)	0.39515(9)	0.0282(3)
C18	0.66496(11)	0.61532(11)	0.29076(10)	0.0300(3)
C20	0.57431(9)	0.34254(9)	0.56732(8)	0.0192(3)
C21	0.65169(9)	0.35904(9)	0.53294(8)	0.0198(3)
C22	0.65382(9)	0.31613(9)	0.46038(8)	0.0199(3)
C23	0.57876(9)	0.27099(9)	0.44995(8)	0.0194(3)
C24	0.53028(9)	0.28583(9)	0.51673(8)	0.0192(3)
C25	0.55132(10)	0.36565(10)	0.64958(9)	0.0261(3)
C26	0.71844(10)	0.40931(11)	0.57192(10)	0.0288(3)
C27	0.72452(10)	0.30648(11)	0.40590(10)	0.0282(3)
C28	0.56258(10)	0.20971(10)	0.38344(9)	0.0264(3)
C29	0.45062(9)	0.24437(10)	0.53687(9)	0.0267(3)

Table 4. Bond lengths (Å) for *trans*-4b.

Nb1-N1	1.8895(12)	Nb1-N1	1.9192(12)
Nb1-N15	2.2696(12)	Nb1-N11	2.2922(12)
Nb1-C20	2.4220(14)	Nb1-C24	2.4965(14)
Nb1-C21	2.5440(14)	Nb1-C23	2.5926(14)
Nb1-C22	2.6246(14)	Nb1-Nb1	2.7990(3)
N1-Nb1	1.9192(12)	C1-N11	1.3262(18)
C1-N15	1.3286(17)	C1-C2	1.5045(19)

C2-C3	1.391(2)	C2-C7	1.393(2)
C3-C4	1.394(2)	C3-H3	0.95
C4-C5	1.383(3)	C4-H4	0.95
C5-C6	1.376(3)	C5-H5	0.95
C6-C7	1.392(2)	C6-H6	0.95
C7-H7	0.95	N11-C12	1.4712(18)
C12-C13	1.522(2)	C12-C14	1.524(2)
C12-H12	1.0	C13-H13A	0.98
C13-H13B	0.98	C13-H13C	0.98
C14-H14A	0.98	C14-H14B	0.98
C14-H14C	0.98	N15-C16	1.4710(18)
C16-C17	1.520(2)	C16-C18	1.531(2)
C16-H16	1.0	C17-H17A	0.98
C17-H17B	0.98	C17-H17C	0.98
C18-H18A	0.98	C18-H18B	0.98
C18-H18C	0.98	C20-C24	1.428(2)
C20-C21	1.431(2)	C20-C25	1.505(2)
C21-C22	1.410(2)	C21-C26	1.503(2)
C22-C23	1.432(2)	C22-C27	1.504(2)
C23-C24	1.417(2)	C23-C28	1.503(2)
C24-C29	1.502(2)	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C26-H26A	0.98	C26-H26B	0.98
C26-H26C	0.98	C27-H27A	0.98
C27-H27B	0.98	C27-H27C	0.98
C28-H28A	0.98	C28-H28B	0.98
C28-H28C	0.98	C29-H29A	0.98
C29-H29B	0.98	C29-H29C	0.98

Table 5. Bond angles (°) for *trans*-4b.

N1-Nb1-N1	85.41(5)	N1-Nb1-N15	128.49(5)
N1-Nb1-N15	90.48(5)	N1-Nb1-N11	90.32(5)
N1-Nb1-N11	134.36(5)	N15-Nb1-N11	57.87(4)
N1-Nb1-C20	97.59(5)	N1-Nb1-C20	93.04(5)
N15-Nb1-C20	133.92(5)	N11-Nb1-C20	132.51(5)
N1-Nb1-C24	91.56(5)	N1-Nb1-C24	125.77(5)
N15-Nb1-C24	129.89(4)	N11-Nb1-C24	99.72(5)

C20-Nb1-C24	33.72(5)	N1-Nb1-C21	129.80(5)
N1-Nb1-C21	87.30(5)	N15-Nb1-C21	101.14(5)
N11-Nb1-C21	127.52(5)	C20-Nb1-C21	33.39(5)
C24-Nb1-C21	54.70(5)	N1-Nb1-C23	117.26(5)
N1-Nb1-C23	140.57(5)	N15-Nb1-C23	97.63(4)
N11-Nb1-C23	80.41(4)	C20-Nb1-C23	54.37(5)
C24-Nb1-C23	32.27(4)	C21-Nb1-C23	53.28(5)
N1-Nb1-C22	145.03(5)	N1-Nb1-C22	112.97(5)
N15-Nb1-C22	82.66(4)	N11-Nb1-C22	95.94(4)
C20-Nb1-C22	53.90(5)	C24-Nb1-C22	53.48(5)
C21-Nb1-C22	31.60(4)	C23-Nb1-C22	31.85(5)
N1-Nb1-Nb1	43.12(4)	N1-Nb1-Nb1	42.29(4)
N15-Nb1-Nb1	115.20(3)	N11-Nb1-Nb1	118.89(3)
C20-Nb1-Nb1	97.21(3)	C24-Nb1-Nb1	114.79(3)
C21-Nb1-Nb1	113.57(3)	C23-Nb1-Nb1	147.02(3)
C22-Nb1-Nb1	145.17(3)	Nb1-N1-Nb1	94.59(5)
N11-C1-N15	112.49(12)	N11-C1-C2	124.70(12)
N15-C1-C2	122.78(13)	C3-C2-C7	119.23(14)
C3-C2-C1	119.49(13)	C7-C2-C1	121.22(13)
C2-C3-C4	120.12(16)	C2-C3-H3	119.9
C4-C3-H3	119.9	C5-C4-C3	120.07(16)
C5-C4-H4	120.0	C3-C4-H4	120.0
C6-C5-C4	120.18(15)	C6-C5-H5	119.9
C4-C5-H5	119.9	C5-C6-C7	120.19(17)
C5-C6-H6	119.9	C7-C6-H6	119.9
C6-C7-C2	120.20(16)	C6-C7-H7	119.9
C2-C7-H7	119.9	C1-N11-C12	123.45(12)
C1-N11-Nb1	94.09(8)	C12-N11-Nb1	142.43(10)
N11-C12-C13	109.81(12)	N11-C12-C14	112.63(13)
C13-C12-C14	107.85(14)	N11-C12-H12	108.8
C13-C12-H12	108.8	C14-C12-H12	108.8
C12-C13-H13A	109.5	C12-C13-H13B	109.5
H13A-C13-H13B	109.5	C12-C13-H13C	109.5
H13A-C13-H13C	109.5	H13B-C13-H13C	109.5
C12-C14-H14A	109.5	C12-C14-H14B	109.5
H14A-C14-H14B	109.5	C12-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
C1-N15-C16	122.43(12)	C1-N15-Nb1	95.04(9)

C16-N15-Nb1	141.99(9)	N15-C16-C17	109.92(12)
N15-C16-C18	113.00(13)	C17-C16-C18	108.55(13)
N15-C16-H16	108.4	C17-C16-H16	108.4
C18-C16-H16	108.4	C16-C17-H17A	109.5
C16-C17-H17B	109.5	H17A-C17-H17B	109.5
C16-C17-H17C	109.5	H17A-C17-H17C	109.5
H17B-C17-H17C	109.5	C16-C18-H18A	109.5
C16-C18-H18B	109.5	H18A-C18-H18B	109.5
C16-C18-H18C	109.5	H18A-C18-H18C	109.5
H18B-C18-H18C	109.5	C24-C20-C21	108.18(12)
C24-C20-C25	125.85(13)	C21-C20-C25	124.83(13)
C24-C20-Nb1	76.00(8)	C21-C20-Nb1	77.99(8)
C25-C20-Nb1	122.13(10)	C22-C21-C20	107.73(13)
C22-C21-C26	127.93(14)	C20-C21-C26	124.25(13)
C22-C21-Nb1	77.35(8)	C20-C21-Nb1	68.62(8)
C26-C21-Nb1	122.08(10)	C21-C22-C23	108.33(12)
C21-C22-C27	127.96(14)	C23-C22-C27	123.21(13)
C21-C22-Nb1	71.05(8)	C23-C22-Nb1	72.84(8)
C27-C22-Nb1	128.23(10)	C24-C23-C22	108.12(12)
C24-C23-C28	127.92(14)	C22-C23-C28	123.47(13)
C24-C23-Nb1	70.13(8)	C22-C23-Nb1	75.31(8)
C28-C23-Nb1	126.70(10)	C23-C24-C20	107.57(13)
C23-C24-C29	127.86(14)	C20-C24-C29	124.33(13)
C23-C24-Nb1	77.60(8)	C20-C24-Nb1	70.28(8)
C29-C24-Nb1	122.00(10)	C20-C25-H25A	109.5
C20-C25-H25B	109.5	H25A-C25-H25B	109.5
C20-C25-H25C	109.5	H25A-C25-H25C	109.5
H25B-C25-H25C	109.5	C21-C26-H26A	109.5
C21-C26-H26B	109.5	H26A-C26-H26B	109.5
C21-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C22-C27-H27A	109.5
C22-C27-H27B	109.5	H27A-C27-H27B	109.5
C22-C27-H27C	109.5	H27A-C27-H27C	109.5
H27B-C27-H27C	109.5	C23-C28-H28A	109.5
C23-C28-H28B	109.5	H28A-C28-H28B	109.5
C23-C28-H28C	109.5	H28A-C28-H28C	109.5
H28B-C28-H28C	109.5	C24-C29-H29A	109.5
C24-C29-H29B	109.5	H29A-C29-H29B	109.5

C24-C29-H29C	109.5	H29A-C29-H29C	109.5
H29B-C29-H29C	109.5		

Table 6. Torsion angles (°) for *trans*-4b.

N1-Nb1-N1-Nb1	0.002	N15-Nb1-N1-Nb1	-86.95(6)
N11-Nb1-N1-Nb1	-134.50(5)	C20-Nb1-N1-Nb1	92.47(5)
C24-Nb1-N1-Nb1	125.77(5)	C21-Nb1-N1-Nb1	82.63(7)
C23-Nb1-N1-Nb1	146.13(5)	C22-Nb1-N1-Nb1	124.64(7)
N11-C1-C2-C3	-90.92(18)	N15-C1-C2-C3	87.17(18)
N11-C1-C2-C7	91.87(19)	N15-C1-C2-C7	-90.04(18)
C7-C2-C3-C4	-0.1(2)	C1-C2-C3-C4	-177.37(14)
C2-C3-C4-C5	0.0(2)	C3-C4-C5-C6	0.1(3)
C4-C5-C6-C7	0.0(3)	C5-C6-C7-C2	-0.1(3)
C3-C2-C7-C6	0.2(2)	C1-C2-C7-C6	177.39(15)
N15-C1-N11-C12	174.74(13)	C2-C1-N11-C12	-7.0(2)
N15-C1-N11-Nb1	-6.77(12)	C2-C1-N11-Nb1	171.49(12)
C1-N11-C12-C13	167.34(14)	Nb1-N11-C12-C13	-10.2(2)
C1-N11-C12-C14	-72.44(19)	Nb1-N11-C12-C14	110.02(18)
N11-C1-N15-C16	-179.83(12)	C2-C1-N15-C16	1.9(2)
N11-C1-N15-Nb1	6.85(12)	C2-C1-N15-Nb1	-171.45(12)
C1-N15-C16-C17	-159.14(13)	Nb1-N15-C16-C17	10.0(2)
C1-N15-C16-C18	79.43(17)	Nb1-N15-C16-C18	-111.41(15)
C24-C20-C21-C22	2.56(15)	C25-C20-C21-C22	170.88(13)
Nb1-C20-C21-C22	-68.16(10)	C24-C20-C21-C26	-174.23(13)
C25-C20-C21-C26	-5.9(2)	Nb1-C20-C21-C26	115.05(14)
C24-C20-C21-Nb1	70.72(10)	C25-C20-C21-Nb1	-120.96(14)
C20-C21-C22-C23	-1.38(15)	C26-C21-C22-C23	175.25(14)
Nb1-C21-C22-C23	-63.74(10)	C20-C21-C22-C27	-173.46(14)
C26-C21-C22-C27	3.2(2)	Nb1-C21-C22-C27	124.19(15)
C20-C21-C22-Nb1	62.36(9)	C26-C21-C22-Nb1	-121.00(15)
C21-C22-C23-C24	-0.32(16)	C27-C22-C23-C24	172.22(13)
Nb1-C22-C23-C24	-62.90(9)	C21-C22-C23-C28	-172.85(13)
C27-C22-C23-C28	-0.3(2)	Nb1-C22-C23-C28	124.56(13)
C21-C22-C23-Nb1	62.59(10)	C27-C22-C23-Nb1	-124.88(13)
C22-C23-C24-C20	1.89(15)	C28-C23-C24-C20	173.99(14)
Nb1-C23-C24-C20	-64.40(9)	C22-C23-C24-C29	-172.62(14)
C28-C23-C24-C29	-0.5(2)	Nb1-C23-C24-C29	121.08(15)

C22-C23-C24-Nb1	66.29(10)	C28-C23-C24-Nb1	-121.60(14)
C21-C20-C24-C23	-2.75(16)	C25-C20-C24-C23	-170.92(13)
Nb1-C20-C24-C23	69.34(10)	C21-C20-C24-C29	172.01(13)
C25-C20-C24-C29	3.8(2)	Nb1-C20-C24-C29	-115.90(14)
C21-C20-C24-Nb1	-72.09(10)	C25-C20-C24-Nb1	119.74(14)

Table 7. Anisotropic atomic displacement parameters (Å^2) for *trans*-4b.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Nb1	0.01546(6)	0.01345(6)	0.01349(6)	-0.00089(4)	0.00039(4)	0.00190(4)
N1	0.0163(5)	0.0191(6)	0.0206(6)	-0.0045(5)	0.0010(4)	-0.0009(4)
C1	0.0196(6)	0.0164(6)	0.0159(6)	-0.0010(5)	-0.0013(5)	0.0041(5)
C2	0.0219(7)	0.0223(7)	0.0157(6)	-0.0033(5)	0.0001(5)	-0.0033(6)
C3	0.0241(7)	0.0242(7)	0.0263(7)	-0.0073(6)	0.0028(6)	-0.0022(6)
C4	0.0306(9)	0.0371(9)	0.0330(9)	-0.0178(7)	0.0122(7)	-0.0113(7)
C5	0.0479(11)	0.0488(11)	0.0193(7)	-0.0096(7)	0.0090(7)	-0.0255(9)
C6	0.0547(11)	0.0390(10)	0.0186(7)	0.0038(7)	-0.0058(7)	-0.0136(9)
C7	0.0388(9)	0.0273(8)	0.0186(7)	0.0005(6)	-0.0043(6)	0.0001(7)
N11	0.0170(6)	0.0240(6)	0.0164(5)	-0.0030(5)	-0.0019(4)	-0.0011(5)
C12	0.0202(7)	0.0271(7)	0.0232(7)	-0.0072(6)	-0.0036(6)	-0.0005(6)
C13	0.0248(8)	0.0426(10)	0.0362(9)	-0.0037(8)	-0.0018(7)	-0.0112(7)
C14	0.0307(9)	0.0468(11)	0.0582(12)	0.0091(10)	-0.0232(9)	-0.0054(8)
N15	0.0201(6)	0.0210(6)	0.0152(5)	-0.0004(4)	0.0003(4)	-0.0031(5)
C16	0.0211(7)	0.0217(7)	0.0199(7)	-0.0018(5)	0.0018(5)	-0.0035(6)
C17	0.0239(8)	0.0310(8)	0.0297(8)	0.0021(6)	-0.0049(6)	-0.0086(6)
C18	0.0342(9)	0.0270(8)	0.0290(8)	0.0048(6)	-0.0014(7)	-0.0080(7)
C20	0.0228(7)	0.0172(6)	0.0177(6)	0.0023(5)	0.0002(5)	0.0038(5)
C21	0.0198(6)	0.0184(6)	0.0211(7)	0.0028(5)	-0.0020(5)	0.0037(5)
C22	0.0209(6)	0.0180(6)	0.0210(6)	0.0034(5)	0.0023(5)	0.0055(5)
C23	0.0239(7)	0.0134(6)	0.0211(7)	0.0012(5)	0.0015(6)	0.0040(5)
C24	0.0222(7)	0.0148(6)	0.0207(6)	0.0023(5)	0.0021(5)	0.0022(5)
C25	0.0340(9)	0.0260(8)	0.0182(7)	-0.0001(6)	0.0019(6)	0.0054(6)
C26	0.0252(8)	0.0332(9)	0.0279(8)	0.0017(7)	-0.0058(6)	-0.0002(6)
C27	0.0246(7)	0.0276(8)	0.0325(8)	0.0007(7)	0.0083(6)	0.0069(6)
C28	0.0344(8)	0.0186(7)	0.0262(8)	-0.0053(6)	0.0017(6)	0.0039(6)

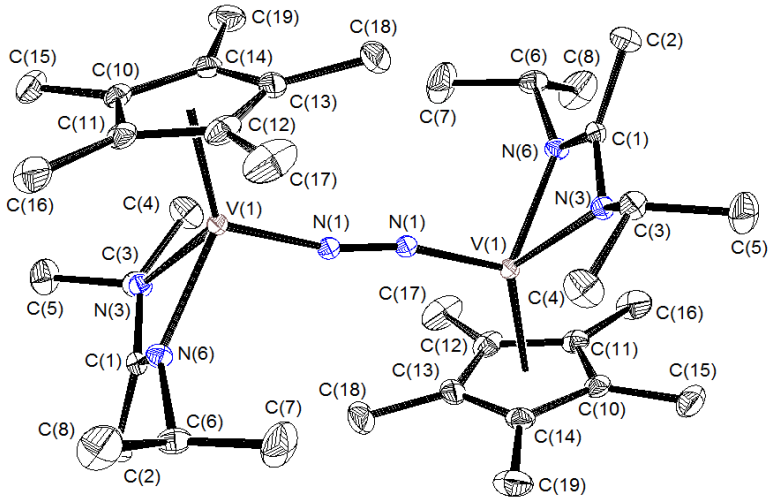
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C29	0.0287(8)	0.0234(7)	0.0281(8)	0.0012(6)	0.0055(6)	-0.0055(6)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for *trans*-4b.

	x/a	y/b	z/c	U(eq)
H3	0.6443	0.3217	0.2223	0.025(5)
H4	0.6788	0.3141	0.0902	0.042(6)
H5	0.6325	0.4202	0.0038	0.044(6)
H6	0.5523	0.5341	0.0484	0.044(6)
H7	0.5175	0.5430	0.1802	0.028(5)
H12	0.4529	0.3193	0.2524	0.025(5)
H13A	0.4082	0.2636	0.3723	0.050(4)
H13B	0.3311	0.2825	0.3186	0.050(4)
H13C	0.3543	0.3486	0.3871	0.050(4)
H14A	0.3486	0.4639	0.2861	0.063(4)
H14B	0.3338	0.3936	0.2187	0.063(4)
H14C	0.4080	0.4603	0.2126	0.063(4)
H16	0.7088	0.4886	0.2858	0.021(4)
H17A	0.7107	0.5709	0.4353	0.038(3)
H17B	0.7871	0.5651	0.3784	0.038(3)
H17C	0.7507	0.4783	0.4164	0.038(3)
H18A	0.6288	0.6095	0.2458	0.038(3)
H18B	0.7162	0.6413	0.2740	0.038(3)
H18C	0.6395	0.6528	0.3300	0.038(3)
H25A	0.5777	0.4204	0.6644	0.079(5)
H25B	0.5688	0.3191	0.6848	0.079(5)
H25C	0.4925	0.3725	0.6531	0.079(5)
H26A	0.7027	0.4707	0.5764	0.048(4)
H26B	0.7680	0.4047	0.5408	0.048(4)
H26C	0.7281	0.3853	0.6240	0.048(4)
H27A	0.7355	0.2444	0.3973	0.043(3)
H27B	0.7723	0.3343	0.4288	0.043(3)
H27C	0.7118	0.3344	0.3561	0.043(3)
H28A	0.5116	0.1787	0.3927	0.050(4)
H28B	0.6069	0.1675	0.3794	0.050(4)
H28C	0.5586	0.2430	0.3349	0.050(4)

	x/a	y/b	z/c	U(eq)
H29A	0.4354	0.2030	0.4959	0.047(4)
H29B	0.4090	0.2896	0.5412	0.047(4)
H29C	0.4555	0.2135	0.5866	0.047(4)

{Cp*V[N(iPr)C(Me)N(iPr]}$_2$(μ-η^1:η^1-N$_2$) (5)



A specimen of $C_{36}H_{64}N_6V_2$, approximate dimensions 0.20 mm × 0.20 mm × 0.24 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 7.63 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 18413 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 5579 were independent (average redundancy 3.300, completeness = 98.9%, R_{int} = 1.88%) and 4836 (86.68%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.5699(5) Å, b = 10.2174(4) Å, c = 15.4022(7) Å, β = 101.5360(10)°, V = 1938.17(14) Å^3, are based upon the refinement of the XYZ-centroids of 8899 reflections above 20 σ(I) with 4.814° < 2θ < 61.68°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8370 and 0.9020.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/c$, with Z = 2 for the formula unit, $C_{36}H_{64}N_6V_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 209 variables converged at R_1 = 3.69%, for the observed data and wR_2 = 8.20% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.587 e$^-$/Å^3 and the largest hole was -0.340 e$^-$/Å^3 with an RMS deviation of 0.054 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.170 g/cm^3 and F(000), 736 e$^-$.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 5.

Identification code	**5**	
Chemical formula	$C_{36}H_{64}N_6V_2$	
Formula weight	682.81	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.20 × 0.20 × 0.24 mm	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.5699(5) Å	α = 90°
	b = 10.2174(4) Å	β = 101.5360(10)°
	c = 15.4022(7) Å	γ = 90°
Volume	1938.17(14) $Å^3$	
Z	2	
Density (calculated)	1.170 Mg/cm^3	
Absorption coefficient	0.513 mm^{-1}	
F(000)	736	

Table 2. Data collection and structure refinement for 5.

Diffractometer	Bruker APEX-II CCD
Radiation source	sealed tube, MoKα
Theta range for data collection	2.41 to 30.00°
Index ranges	$-17 \le h \le 17$, $-14 \le k \le 14$, $-18 \le l \le 21$
Reflections collected	18413
Independent reflections	5579 [R(int) = 0.0188]
Coverage of independent reflections	98.9%
Absorption correction	multi-scan
Max. and min. transmission	0.9020 and 0.8370
Structure solution	direct methods

technique		
Structure solution program	ShelXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	ShelXL-2012 (Sheldrick, 2012)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5579 / 0 / 209	
Goodness-of-fit on F^2	1.000	
Final R indices	4836 data; $I>2\sigma(I)$	$R_1 = 0.0369$, $wR_2 = 0.0784$
	all data	$R_1 = 0.0437$, $wR_2 = 0.0820$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0150P)^2+1.9400P]$, $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.587 and -0.340 eÅ^{-3}	
R.M.S. deviation from mean	0.054 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
V1	0.18504(2)	0.53708(2)	0.06736(2)	0.01862(6)
N1	0.04932(9)	0.50294(12)	0.01268(8)	0.0217(2)
C1	0.28608(10)	0.36714(13)	0.99989(9)	0.0202(2)
C2	0.31536(13)	0.25498(15)	0.94502(11)	0.0303(3)
N3	0.25557(9)	0.35138(11)	0.07736(8)	0.0209(2)
C3	0.23602(12)	0.22104(14)	0.11023(10)	0.0262(3)
C4	0.14727(15)	0.22836(19)	0.16437(13)	0.0428(4)
C5	0.33920(15)	0.16273(19)	0.16575(13)	0.0433(4)
N6	0.28190(9)	0.49181(12)	0.97446(8)	0.0221(2)
C6	0.29671(13)	0.53137(16)	0.88641(10)	0.0295(3)

	x/a	y/b	z/c	U(eq)
C7	0.19543(18)	0.5964(3)	0.83624(14)	0.0601(6)
C8	0.39437(18)	0.6193(3)	0.89133(14)	0.0612(7)
C10	0.27908(12)	0.60862(15)	0.20567(10)	0.0271(3)
C11	0.30363(12)	0.69527(15)	0.14137(10)	0.0281(3)
C12	0.20442(15)	0.75586(15)	0.09835(11)	0.0349(4)
C13	0.12024(13)	0.70552(17)	0.13880(12)	0.0344(4)
C14	0.16626(13)	0.61390(17)	0.20405(10)	0.0305(3)
C15	0.36158(15)	0.5271(2)	0.26725(12)	0.0410(4)
C16	0.41530(15)	0.7234(2)	0.12498(13)	0.0471(5)
C17	0.1902(2)	0.86080(19)	0.02895(15)	0.0604(6)
C18	0.00302(15)	0.7487(2)	0.12035(15)	0.0528(6)
C19	0.10770(16)	0.5455(2)	0.26789(12)	0.0450(5)

Table 4. Bond lengths (Å) for 5.

V1-N1	1.7795(11)	V1-N3	2.0868(12)
V1-N6	2.1071(12)	V1-C13	2.2792(15)
V1-C12	2.2886(15)	V1-C14	2.3029(15)
V1-C11	2.3355(14)	V1-C10	2.3372(14)
V1-C1	2.4971(13)	N1-N1	1.225(2)
C1-N6	1.3306(17)	C1-N3	1.3341(17)
C1-C2	1.5124(19)	C2-H2A	0.98
C2-H2B	0.98	C2-H2C	0.98
N3-C3	1.4629(18)	C3-C4	1.522(2)
C3-C5	1.525(2)	C3-H3	1.0
C4-H4A	0.98	C4-H4B	0.98
C4-H4C	0.98	C5-H5A	0.98
C5-H5B	0.98	C5-H5C	0.98
N6-C6	1.4623(18)	C6-C7	1.505(3)
C6-C8	1.511(3)	C6-H6	1.0
C7-H7A	0.98	C7-H7B	0.98
C7-H7C	0.98	C8-H8A	0.98
C8-H8B	0.98	C8-H8C	0.98
C10-C11	1.408(2)	C10-C14	1.414(2)
C10-C15	1.509(2)	C11-C12	1.431(2)
C11-C16	1.503(2)	C12-C13	1.427(3)
C12-C17	1.499(3)	C13-C14	1.410(3)

C13-C18	1.510(2)	C14-C19	1.512(2)
C15-H15A	0.98	C15-H15B	0.98
C15-H15C	0.98	C16-H16A	0.98
C16-H16B	0.98	C16-H16C	0.98
C17-H17A	0.98	C17-H17B	0.98
C17-H17C	0.98	C18-H18A	0.98
C18-H18B	0.98	C18-H18C	0.98
C19-H19A	0.98	C19-H19B	0.98
C19-H19C	0.98		

Table 5. Bond angles (°) for 5.

N1-V1-N3	102.10(5)	N1-V1-N6	105.37(5)
N3-V1-N6	63.64(4)	N1-V1-C13	88.57(5)
N3-V1-C13	146.98(6)	N6-V1-C13	143.55(6)
N1-V1-C12	110.01(6)	N3-V1-C12	147.86(6)
N6-V1-C12	107.71(6)	C13-V1-C12	36.41(7)
N1-V1-C14	103.63(5)	N3-V1-C14	111.23(6)
N6-V1-C14	150.97(5)	C13-V1-C14	35.84(6)
C12-V1-C14	60.17(6)	N1-V1-C11	145.54(6)
N3-V1-C11	111.90(5)	N6-V1-C11	94.84(5)
C13-V1-C11	59.78(6)	C12-V1-C11	36.03(6)
C14-V1-C11	59.33(5)	N1-V1-C10	139.01(5)
N3-V1-C10	95.00(5)	N6-V1-C10	115.59(5)
C13-V1-C10	59.22(6)	C12-V1-C10	59.41(6)
C14-V1-C10	35.48(5)	C11-V1-C10	35.07(5)
N1-V1-C1	100.72(5)	N3-V1-C1	32.29(4)
N6-V1-C1	32.20(4)	C13-V1-C1	170.60(5)
C12-V1-C1	136.40(6)	C14-V1-C1	140.46(5)
C11-V1-C1	110.87(5)	C10-V1-C1	112.97(5)
N1-N1-V1	166.96(14)	N6-C1-N3	112.17(12)
N6-C1-C2	124.10(13)	N3-C1-C2	123.64(13)
N6-C1-V1	57.55(7)	N3-C1-V1	56.67(7)
C2-C1-V1	163.79(10)	C1-C2-H2A	109.5
C1-C2-H2B	109.5	H2A-C2-H2B	109.5
C1-C2-H2C	109.5	H2A-C2-H2C	109.5
H2B-C2-H2C	109.5	C1-N3-C3	121.17(12)
C1-N3-V1	91.04(8)	C3-N3-V1	139.02(9)

N3-C3-C4	109.70(13)	N3-C3-C5	111.53(13)
C4-C3-C5	110.26(14)	N3-C3-H3	108.4
C4-C3-H3	108.4	C5-C3-H3	108.4
C3-C4-H4A	109.5	C3-C4-H4B	109.5
H4A-C4-H4B	109.5	C3-C4-H4C	109.5
H4A-C4-H4C	109.5	H4B-C4-H4C	109.5
C3-C5-H5A	109.5	C3-C5-H5B	109.5
H5A-C5-H5B	109.5	C3-C5-H5C	109.5
H5A-C5-H5C	109.5	H5B-C5-H5C	109.5
C1-N6-C6	122.19(12)	C1-N6-V1	90.25(8)
C6-N6-V1	140.10(10)	N6-C6-C7	110.28(14)
N6-C6-C8	111.76(14)	C7-C6-C8	111.03(17)
N6-C6-H6	107.9	C7-C6-H6	107.9
C8-C6-H6	107.9	C6-C7-H7A	109.5
C6-C7-H7B	109.5	H7A-C7-H7B	109.5
C6-C7-H7C	109.5	H7A-C7-H7C	109.5
H7B-C7-H7C	109.5	C6-C8-H8A	109.5
C6-C8-H8B	109.5	H8A-C8-H8B	109.5
C6-C8-H8C	109.5	H8A-C8-H8C	109.5
H8B-C8-H8C	109.5	C11-C10-C14	108.89(14)
C11-C10-C15	124.73(15)	C14-C10-C15	126.36(15)
C11-C10-V1	72.40(8)	C14-C10-V1	70.94(8)
C15-C10-V1	123.99(11)	C10-C11-C12	107.73(14)
C10-C11-C16	125.60(16)	C12-C11-C16	126.59(16)
C10-C11-V1	72.53(8)	C12-C11-V1	70.20(8)
C16-C11-V1	125.24(11)	C13-C12-C11	107.19(15)
C13-C12-C17	125.18(18)	C11-C12-C17	127.45(19)
C13-C12-V1	71.44(9)	C11-C12-V1	73.77(9)
C17-C12-V1	123.87(12)	C14-C13-C12	108.43(14)
C14-C13-C18	125.04(18)	C12-C13-C18	126.40(18)
C14-C13-V1	72.99(9)	C12-C13-V1	72.15(9)
C18-C13-V1	124.02(11)	C13-C14-C10	107.75(14)
C13-C14-C19	125.92(16)	C10-C14-C19	125.99(16)
C13-C14-V1	71.16(9)	C10-C14-V1	73.58(8)
C19-C14-V1	126.08(11)	C10-C15-H15A	109.5
C10-C15-H15B	109.5	H15A-C15-H15B	109.5
C10-C15-H15C	109.5	H15A-C15-H15C	109.5
H15B-C15-H15C	109.5	C11-C16-H16A	109.5

C11-C16-H16B	109.5	H16A-C16-H16B	109.5
C11-C16-H16C	109.5	H16A-C16-H16C	109.5
H16B-C16-H16C	109.5	C12-C17-H17A	109.5
C12-C17-H17B	109.5	H17A-C17-H17B	109.5
C12-C17-H17C	109.5	H17A-C17-H17C	109.5
H17B-C17-H17C	109.5	C13-C18-H18A	109.5
C13-C18-H18B	109.5	H18A-C18-H18B	109.5
C13-C18-H18C	109.5	H18A-C18-H18C	109.5
H18B-C18-H18C	109.5	C14-C19-H19A	109.5
C14-C19-H19B	109.5	H19A-C19-H19B	109.5
C14-C19-H19C	109.5	H19A-C19-H19C	109.5
H19B-C19-H19C	109.5		

Table 6. Torsion angles (°) for 5.

N3-V1-N1-N1	137.5(7)	N6-V1-N1-N1	-156.8(7)
C13-V1-N1-N1	-11.0(7)	C12-V1-N1-N1	-41.0(7)
C14-V1-N1-N1	21.8(7)	C11-V1-N1-N1	-33.1(7)
C10-V1-N1-N1	25.0(7)	C1-V1-N1-N1	170.4(7)
N6-C1-N3-C3	169.30(12)	C2-C1-N3-C3	-7.2(2)
V1-C1-N3-C3	153.31(14)	N6-C1-N3-V1	15.98(11)
C2-C1-N3-V1	-160.54(12)	C1-N3-C3-C4	-147.95(14)
V1-N3-C3-C4	-11.2(2)	C1-N3-C3-C5	89.60(17)
V1-N3-C3-C5	-133.62(14)	N3-C1-N6-C6	-171.23(12)
C2-C1-N6-C6	5.3(2)	V1-C1-N6-C6	-155.40(14)
N3-C1-N6-V1	-15.82(11)	C2-C1-N6-V1	160.68(12)
C1-N6-C6-C7	117.66(18)	V1-N6-C6-C7	-21.9(2)
C1-N6-C6-C8	-118.33(18)	V1-N6-C6-C8	102.12(19)
C14-C10-C11-C12	-0.18(17)	C15-C10-C11-C12	-178.66(14)
V1-C10-C11-C12	61.74(10)	C14-C10-C11-C16	176.84(15)
C15-C10-C11-C16	-1.6(3)	V1-C10-C11-C16	-121.24(16)
C14-C10-C11-V1	-61.92(10)	C15-C10-C11-V1	119.59(15)
C10-C11-C12-C13	0.83(17)	C16-C11-C12-C13	-176.15(15)
V1-C11-C12-C13	64.08(10)	C10-C11-C12-C17	176.21(16)
C16-C11-C12-C17	-0.8(3)	V1-C11-C12-C17	-120.54(18)
C10-C11-C12-V1	-63.25(10)	C16-C11-C12-V1	119.77(16)
C11-C12-C13-C14	-1.18(17)	C17-C12-C13-C14	-176.69(16)
V1-C12-C13-C14	64.46(11)	C11-C12-C13-C18	174.83(15)

C17-C12-C13-C18	-0.7(3)	V1-C12-C13-C18	-119.53(16)
C11-C12-C13-V1	-65.64(10)	C17-C12-C13-V1	118.85(16)
C12-C13-C14-C10	1.07(17)	C18-C13-C14-C10	-175.00(15)
V1-C13-C14-C10	64.99(10)	C12-C13-C14-C19	174.66(15)
C18-C13-C14-C19	-1.4(3)	V1-C13-C14-C19	-121.42(16)
C12-C13-C14-V1	-63.92(11)	C18-C13-C14-V1	120.01(16)
C11-C10-C14-C13	-0.56(17)	C15-C10-C14-C13	177.90(15)
V1-C10-C14-C13	-63.40(10)	C11-C10-C14-C19	-174.14(15)
C15-C10-C14-C19	4.3(3)	V1-C10-C14-C19	123.01(16)
C11-C10-C14-V1	62.85(11)	C15-C10-C14-V1	-118.70(16)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 5.

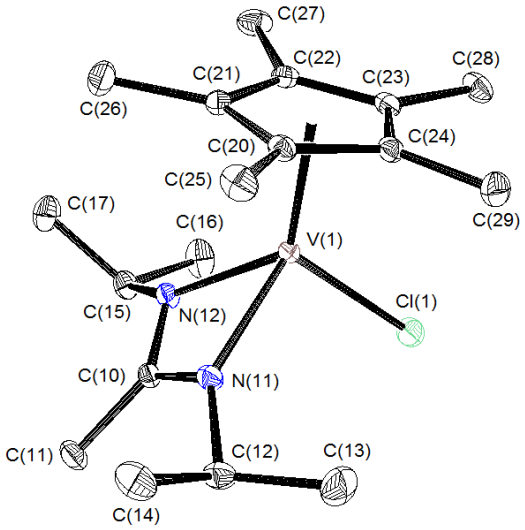
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.01582(10)	0.02040(11)	0.01894(11)	-0.00418(9)	0.00184(8)	-0.00044(8)
N1	0.0198(5)	0.0235(5)	0.0210(5)	-0.0054(4)	0.0023(4)	0.0003(4)
C1	0.0161(5)	0.0236(6)	0.0208(6)	-0.0005(5)	0.0036(5)	0.0011(5)
C2	0.0364(8)	0.0265(7)	0.0315(8)	-0.0026(6)	0.0151(6)	0.0039(6)
N3	0.0209(5)	0.0216(5)	0.0205(5)	0.0017(4)	0.0050(4)	0.0008(4)
C3	0.0297(7)	0.0238(7)	0.0254(7)	0.0044(5)	0.0060(6)	-0.0009(5)
C4	0.0445(10)	0.0401(10)	0.0502(11)	0.0115(8)	0.0249(9)	-0.0037(8)
C5	0.0431(10)	0.0416(10)	0.0429(10)	0.0194(8)	0.0026(8)	0.0081(8)
N6	0.0244(5)	0.0230(5)	0.0202(5)	0.0012(4)	0.0074(4)	0.0001(4)
C6	0.0408(8)	0.0279(7)	0.0218(7)	0.0026(6)	0.0108(6)	-0.0017(6)
C7	0.0519(12)	0.0864(17)	0.0384(11)	0.0301(11)	0.0003(9)	0.0047(12)
C8	0.0551(12)	0.0891(18)	0.0424(11)	0.0178(12)	0.0168(10)	-0.0278(12)
C10	0.0271(7)	0.0308(7)	0.0221(7)	-0.0083(6)	0.0018(5)	-0.0049(6)
C11	0.0275(7)	0.0299(7)	0.0261(7)	-0.0093(6)	0.0041(6)	-0.0102(6)
C12	0.0507(10)	0.0207(7)	0.0288(8)	-0.0069(6)	-0.0030(7)	-0.0015(6)
C13	0.0279(7)	0.0344(8)	0.0385(9)	-0.0202(7)	0.0007(6)	0.0040(6)
C14	0.0286(7)	0.0373(8)	0.0266(7)	-0.0139(6)	0.0080(6)	-0.0061(6)
C15	0.0395(9)	0.0473(10)	0.0307(8)	-0.0022(8)	-0.0065(7)	-0.0011(8)
C16	0.0369(9)	0.0633(13)	0.0427(10)	-0.0128(9)	0.0123(8)	-0.0251(9)
C17	0.1036(19)	0.0252(9)	0.0444(11)	0.0018(8)	-0.0041(12)	-0.0045(10)
C18	0.0377(9)	0.0552(12)	0.0603(13)	-0.0279(10)	-0.0027(9)	0.0181(9)
C19	0.0449(10)	0.0579(12)	0.0371(9)	-0.0138(9)	0.0203(8)	-0.0127(9)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 5.

	x/a	y/b	z/c	U(eq)
H2A	0.2527	0.2331	-0.1017	0.046
H2B	0.3358	0.1785	-0.0169	0.046
H2C	0.3765	0.2806	-0.0820	0.046
H3	0.2105	0.1625	0.0582	0.031
H4A	0.1718	0.2834	0.2167	0.064
H4B	0.1313	0.1402	0.1832	0.064
H4C	0.0815	0.2663	0.1281	0.064
H5A	0.3960	0.1599	0.1305	0.065
H5B	0.3243	0.0738	0.1840	0.065
H5C	0.3636	0.2170	0.2184	0.065
H6	0.3093	0.4505	-0.1467	0.035
H7A	0.1336	0.5369	-0.1670	0.09
H7B	0.2048	0.6177	-0.2238	0.09
H7C	0.1819	0.6769	-0.1331	0.09
H8A	0.3829	0.7007	-0.0782	0.092
H8B	0.4044	0.6393	-0.1687	0.092
H8C	0.4592	0.5748	-0.0759	0.092
H15A	0.4181	0.4981	0.2361	0.062
H15B	0.3257	0.4505	0.2868	0.062
H15C	0.3945	0.5796	0.3189	0.062
H16A	0.4566	0.7731	0.1750	0.071
H16B	0.4094	0.7748	0.0705	0.071
H16C	0.4527	0.6408	0.1188	0.071
H17A	0.1250	0.8427	-0.0161	0.091
H17B	0.2538	0.8624	0.0011	0.091
H17C	0.1827	0.9458	0.0565	0.091
H18A	-0.0440	0.6723	0.1203	0.079
H18B	-0.0143	0.7918	0.0624	0.079
H18C	-0.0087	0.8102	0.1664	0.079
H19A	0.0841	0.6103	0.3070	0.067
H19B	0.1568	0.4826	0.3036	0.067
H19C	0.0442	0.4992	0.2345	0.067

Cp*V[N(iPr)C(Me)N(iPr]Cl (8)



A dark red needle-like specimen of $C_{18}H_{32}ClN_2V$, approximate dimensions 0.15 mm × 0.17 mm × 0.41 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 15.15 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 27990 reflections to a maximum θ angle of 30.00° (0.71 Å resolution), of which 5708 were independent (average redundancy 4.904, completeness = 100.0%, R_{int} = 1.95%) and 5179 (90.73%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.9672(9) Å, b = 9.1331(6) Å, c = 16.5204(11) Å, β = 91.1382(10)°, V = 1956.1(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 9950 reflections above 20 σ(I) with 4.932° < 2θ < 61.29°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8010 and 0.9080.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/n$, with Z = 4 for the formula unit, $C_{18}H_{32}ClN_2V$. The final anisotropic full-matrix least-squares refinement on F^2 with 245 variables converged at R_1 = 2.59%, for the observed data and wR_2 = 5.70% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.387 $e^-/Å^3$ and the largest hole was -0.294 $e^-/Å^3$ with an RMS deviation of 0.044 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.232 g/cm^3 and F(000), 776 e^-.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)

XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 8.

Identification code	**8**	
Chemical formula	$C_{18}H_{32}ClN_2V$	
Formula weight	362.84	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.15 × 0.17 × 0.41 mm	
Crystal habit	dark red needle	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.9672(9) Å	α = 90°
	b = 9.1331(6) Å	β = 91.1382(10)°
	c = 16.5204(11) Å	γ = 90°
Volume	1956.1(2) $Å^3$	
Z	4	
Density (calculated)	1.232 Mg/cm^3	
Absorption coefficient	0.643 mm^{-1}	
F(000)	776	

Table 2. Data collection and structure refinement for 8.

Diffractometer	Bruker APEX-II CCD
Radiation source	sealed tube, MoKα
Theta range for data collection	1.98 to 30.00°
Index ranges	$-18 \le h \le 18$, $-12 \le k \le 12$, $-23 \le l \le 23$
Reflections collected	27990
Independent reflections	5708 [R(int) = 0.0195]
Coverage of independent reflections	100.0%
Absorption correction	multi-scan
Max. and min. transmission	0.9080 and 0.8010
Structure solution technique	direct methods
Structure solution	ShelXS-97 (Sheldrick, 2008)

program		
Refinement method	Full-matrix least-squares on F^2	
Refinement program	ShelXL-2012 (Sheldrick, 2012)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5708 / 0 / 245	
Goodness-of-fit on F^2	1.000	
Δ/σ_{max}	0.001	
Final R indices	5179 data; $I>2\sigma(I)$	$R_1 = 0.0259$, $wR_2 = 0.0551$
	all data	$R_1 = 0.0295$, $wR_2 = 0.0570$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0100P)^2+1.2610P]$, $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.387 and -0.294 eÅ^{-3}	
R.M.S. deviation from mean	0.044 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 8.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
V1	0.26274(2)	0.21680(2)	0.04856(2)	0.01552(4)
Cl1	0.27635(2)	0.97830(3)	0.09366(2)	0.03132(7)
C10	0.08394(8)	0.21310(11)	0.99142(6)	0.01906(19)
C11	0.97496(8)	0.19392(14)	0.95921(8)	0.0281(2)
N11	0.10904(7)	0.25407(10)	0.06677(5)	0.02037(17)
N12	0.16815(7)	0.18844(10)	0.94852(5)	0.01967(17)
C12	0.03178(9)	0.26290(14)	0.13026(7)	0.0263(2)
C13	0.08212(12)	0.21945(19)	0.21072(8)	0.0417(3)
C14	0.98250(10)	0.41414(16)	0.13640(9)	0.0381(3)
C15	0.16357(9)	0.12558(13)	0.86708(6)	0.0238(2)

	x/a	y/b	z/c	U(eq)
C16	0.24281(11)	0.00347(16)	0.86160(8)	0.0382(3)
C17	0.18085(11)	0.24128(16)	0.80236(7)	0.0353(3)
C20	0.31558(8)	0.44396(11)	0.09743(6)	0.01943(19)
C21	0.33386(8)	0.43796(12)	0.01292(6)	0.0205(2)
C22	0.40888(8)	0.32697(12)	0.99909(6)	0.0206(2)
C23	0.43562(7)	0.26340(11)	0.07526(6)	0.01950(19)
C24	0.37768(8)	0.33530(11)	0.13588(6)	0.01879(19)
C25	0.24892(9)	0.55524(13)	0.13771(8)	0.0287(2)
C26	0.28983(11)	0.54205(14)	0.95090(8)	0.0335(3)
C27	0.45955(10)	0.29689(15)	0.91968(7)	0.0311(3)
C28	0.51524(8)	0.14726(13)	0.09171(8)	0.0279(2)
C29	0.38688(9)	0.30350(14)	0.22496(7)	0.0281(2)

Table 4. Bond lengths (Å) for 8.

V1-N11	2.0500(9)	V1-N12	2.0548(9)
V1-C21	2.3019(10)	V1-Cl1	2.3078(3)
V1-C22	2.3093(10)	V1-C23	2.3156(10)
V1-C24	2.3213(10)	V1-C20	2.3246(10)
C10-N12	1.3327(13)	C10-N11	1.3340(13)
C10-C11	1.5102(14)	C11-H11A	0.98
C11-H11B	0.98	C11-H11C	0.98
N11-C12	1.4669(13)	N12-C15	1.4630(13)
C12-C13	1.5219(18)	C12-C14	1.5261(18)
C12-H12	1.0	C13-H13A	0.98
C13-H13B	0.98	C13-H13C	0.98
C14-H14A	0.98	C14-H14B	0.98
C14-H14C	0.98	C15-C16	1.5203(17)
C15-C17	1.5229(17)	C15-H15	1.0
C16-H16A	0.98	C16-H16B	0.98
C16-H16C	0.98	C17-H17A	0.98
C17-H17B	0.98	C17-H17C	0.98
C20-C24	1.4200(14)	C20-C21	1.4219(15)
C20-C25	1.4986(15)	C21-C22	1.4265(15)
C21-C26	1.5020(15)	C22-C23	1.4224(15)
C22-C27	1.5042(15)	C23-C24	1.4243(14)
C23-C28	1.5013(15)	C24-C29	1.5025(15)

C25-H25A	0.98	C25-H25B	0.98
C25-H25C	0.98	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C26-H26D	0.98	C26-H26E	0.98
C26-H26F	0.98	C27-H27A	0.98
C27-H27B	0.98	C27-H27C	0.98
C28-H28A	0.98	C28-H28B	0.98
C28-H28C	0.98	C29-H29A	0.98
C29-H29B	0.98	C29-H29C	0.98

Table 5. Bond angles (°) for 8.

N11-V1-N12	64.69(4)	N11-V1-C21	106.70(4)
N12-V1-C21	98.08(4)	N11-V1-Cl1	100.24(3)
N12-V1-Cl1	100.45(3)	C21-V1-Cl1	151.93(3)
N11-V1-C22	141.87(4)	N12-V1-C22	104.55(4)
C21-V1-C22	36.04(4)	Cl1-V1-C22	117.87(3)
N11-V1-C23	151.87(4)	N12-V1-C23	137.44(4)
C21-V1-C23	59.75(4)	Cl1-V1-C23	92.55(3)
C22-V1-C23	35.82(4)	N11-V1-C24	116.45(4)
N12-V1-C24	157.55(4)	C21-V1-C24	59.62(4)
Cl1-V1-C24	101.27(3)	C22-V1-C24	59.70(4)
C23-V1-C24	35.78(4)	N11-V1-C20	94.68(4)
N12-V1-C20	123.98(4)	C21-V1-C20	35.79(4)
Cl1-V1-C20	135.25(3)	C22-V1-C20	59.72(4)
C23-V1-C20	59.48(4)	C24-V1-C20	35.59(4)
N12-C10-N11	110.87(9)	N12-C10-C11	124.32(10)
N11-C10-C11	124.79(10)	C10-C11-H11A	109.5
C10-C11-H11B	109.5	H11A-C11-H11B	109.5
C10-C11-H11C	109.5	H11A-C11-H11C	109.5
H11B-C11-H11C	109.5	C10-N11-C12	121.68(9)
C10-N11-V1	92.08(6)	C12-N11-V1	142.55(7)
C10-N12-C15	122.46(9)	C10-N12-V1	91.91(6)
C15-N12-V1	143.30(7)	N11-C12-C13	108.84(9)
N11-C12-C14	112.96(10)	C13-C12-C14	110.54(11)
N11-C12-H12	108.1	C13-C12-H12	108.1
C14-C12-H12	108.1	C12-C13-H13A	109.5
C12-C13-H13B	109.5	H13A-C13-H13B	109.5

C12-C13-H13C	109.5	H13A-C13-H13C	109.5
H13B-C13-H13C	109.5	C12-C14-H14A	109.5
C12-C14-H14B	109.5	H14A-C14-H14B	109.5
C12-C14-H14C	109.5	H14A-C14-H14C	109.5
H14B-C14-H14C	109.5	N12-C15-C16	109.12(9)
N12-C15-C17	111.68(10)	C16-C15-C17	110.99(11)
N12-C15-H15	108.3	C16-C15-H15	108.3
C17-C15-H15	108.3	C15-C16-H16A	109.5
C15-C16-H16B	109.5	H16A-C16-H16B	109.5
C15-C16-H16C	109.5	H16A-C16-H16C	109.5
H16B-C16-H16C	109.5	C15-C17-H17A	109.5
C15-C17-H17B	109.5	H17A-C17-H17B	109.5
C15-C17-H17C	109.5	H17A-C17-H17C	109.5
H17B-C17-H17C	109.5	C24-C20-C21	107.95(9)
C24-C20-C25	127.04(10)	C21-C20-C25	124.82(10)
C24-C20-V1	72.08(6)	C21-C20-V1	71.23(6)
C25-C20-V1	126.22(7)	C20-C21-C22	108.18(9)
C20-C21-C26	125.23(10)	C22-C21-C26	126.28(10)
C20-C21-V1	72.98(6)	C22-C21-V1	72.26(6)
C26-C21-V1	125.53(8)	C23-C22-C21	107.67(9)
C23-C22-C27	126.44(10)	C21-C22-C27	125.49(10)
C23-C22-V1	72.33(6)	C21-C22-V1	71.70(6)
C27-C22-V1	127.22(8)	C22-C23-C24	108.12(9)
C22-C23-C28	127.11(10)	C24-C23-C28	124.67(10)
C22-C23-V1	71.85(6)	C24-C23-V1	72.33(6)
C28-C23-V1	124.36(7)	C20-C24-C23	108.06(9)
C20-C24-C29	127.34(10)	C23-C24-C29	124.53(10)
C20-C24-V1	72.33(6)	C23-C24-V1	71.89(6)
C29-C24-V1	123.79(7)	C20-C25-H25A	109.5
C20-C25-H25B	109.5	H25A-C25-H25B	109.5
C20-C25-H25C	109.5	H25A-C25-H25C	109.5
H25B-C25-H25C	109.5	C21-C26-H26A	109.5
C21-C26-H26B	109.5	H26A-C26-H26B	109.5
C21-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C21-C26-H26D	109.5
H26A-C26-H26D	141.1	H26B-C26-H26D	56.3
H26C-C26-H26D	56.3	C21-C26-H26E	109.5
H26A-C26-H26E	56.3	H26B-C26-H26E	141.1

H26C-C26-H26E	56.3	H26D-C26-H26E	109.5
C21-C26-H26F	109.5	H26A-C26-H26F	56.3
H26B-C26-H26F	56.3	H26C-C26-H26F	141.1
H26D-C26-H26F	109.5	H26E-C26-H26F	109.5
C22-C27-H27A	109.5	C22-C27-H27B	109.5
H27A-C27-H27B	109.5	C22-C27-H27C	109.5
H27A-C27-H27C	109.5	H27B-C27-H27C	109.5
C23-C28-H28A	109.5	C23-C28-H28B	109.5
H28A-C28-H28B	109.5	C23-C28-H28C	109.5
H28A-C28-H28C	109.5	H28B-C28-H28C	109.5
C24-C29-H29A	109.5	C24-C29-H29B	109.5
H29A-C29-H29B	109.5	C24-C29-H29C	109.5
H29A-C29-H29C	109.5	H29B-C29-H29C	109.5

Table 6. Torsion angles (°) for 8.

N12-C10-N11-C12	-169.10(10)	C11-C10-N11-C12	9.70(16)
N12-C10-N11-V1	-6.17(9)	C11-C10-N11-V1	172.62(10)
N11-C10-N12-C15	172.56(9)	C11-C10-N12-C15	-6.23(16)
N11-C10-N12-V1	6.16(9)	C11-C10-N12-V1	-172.64(10)
C10-N11-C12-C13	145.63(11)	V1-N11-C12-C13	-5.51(18)
C10-N11-C12-C14	-91.20(13)	V1-N11-C12-C14	117.66(13)
C10-N12-C15-C16	-132.80(11)	V1-N12-C15-C16	24.05(17)
C10-N12-C15-C17	104.12(12)	V1-N12-C15-C17	-99.03(13)
C24-C20-C21-C22	-1.01(11)	C25-C20-C21-C22	174.26(10)
V1-C20-C21-C22	-64.15(7)	C24-C20-C21-C26	-175.01(10)
C25-C20-C21-C26	0.27(17)	V1-C20-C21-C26	121.85(11)
C24-C20-C21-V1	63.14(7)	C25-C20-C21-V1	-121.58(10)
C20-C21-C22-C23	0.78(11)	C26-C21-C22-C23	174.69(10)
V1-C21-C22-C23	-63.84(7)	C20-C21-C22-C27	-172.25(10)
C26-C21-C22-C27	1.66(17)	V1-C21-C22-C27	123.13(11)
C20-C21-C22-V1	64.62(7)	C26-C21-C22-V1	-121.47(11)
C21-C22-C23-C24	-0.25(11)	C27-C22-C23-C24	172.69(10)
V1-C22-C23-C24	-63.67(7)	C21-C22-C23-C28	-176.80(10)
C27-C22-C23-C28	-3.85(17)	V1-C22-C23-C28	119.78(11)
C21-C22-C23-V1	63.42(7)	C27-C22-C23-V1	-123.63(11)
C21-C20-C24-C23	0.86(11)	C25-C20-C24-C23	-174.28(10)
V1-C20-C24-C23	63.45(7)	C21-C20-C24-C29	177.99(10)

C25-C20-C24-C29	2.85(17)	V1-C20-C24-C29	-119.41(11)
C21-C20-C24-V1	-62.60(7)	C25-C20-C24-V1	122.26(11)
C22-C23-C24-C20	-0.37(11)	C28-C23-C24-C20	176.28(10)
V1-C23-C24-C20	-63.74(7)	C22-C23-C24-C29	-177.61(10)
C28-C23-C24-C29	-0.96(16)	V1-C23-C24-C29	119.03(10)
C22-C23-C24-V1	63.36(7)	C28-C23-C24-V1	-119.99(10)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 8.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

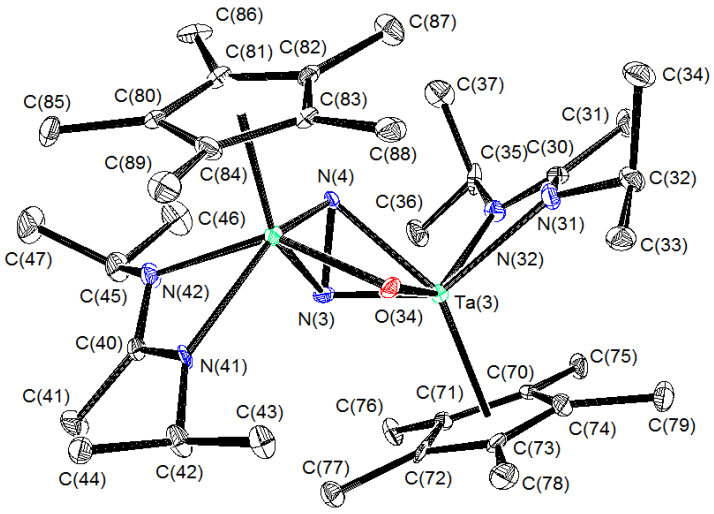
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.01376(7)	0.01593(8)	0.01682(8)	0.00082(6)	-0.00074(5)	-0.00044(6)
Cl1	0.02641(13)	0.02027(12)	0.04699(18)	0.01058(12)	-0.00648(12)	-0.00219(10)
C10	0.0158(4)	0.0179(4)	0.0233(5)	0.0031(4)	-0.0024(4)	0.0010(3)
C11	0.0174(5)	0.0333(6)	0.0334(6)	0.0007(5)	-0.0059(4)	0.0009(4)
N11	0.0161(4)	0.0243(4)	0.0207(4)	0.0002(3)	0.0014(3)	0.0012(3)
N12	0.0175(4)	0.0230(4)	0.0184(4)	-0.0009(3)	-0.0021(3)	0.0012(3)
C12	0.0207(5)	0.0317(6)	0.0267(5)	0.0001(5)	0.0066(4)	0.0003(4)
C13	0.0430(8)	0.0572(9)	0.0252(6)	0.0081(6)	0.0100(5)	0.0084(7)
C14	0.0273(6)	0.0416(7)	0.0456(8)	-0.0058(6)	0.0081(5)	0.0102(5)
C15	0.0238(5)	0.0271(5)	0.0204(5)	-0.0038(4)	-0.0039(4)	0.0024(4)
C16	0.0456(8)	0.0356(7)	0.0331(7)	-0.0095(6)	-0.0035(6)	0.0156(6)
C17	0.0445(7)	0.0402(7)	0.0211(6)	0.0028(5)	-0.0025(5)	0.0042(6)
C20	0.0169(4)	0.0163(4)	0.0251(5)	-0.0016(4)	-0.0014(4)	-0.0013(3)
C21	0.0195(4)	0.0187(5)	0.0233(5)	0.0030(4)	-0.0027(4)	-0.0036(4)
C22	0.0171(4)	0.0229(5)	0.0219(5)	-0.0005(4)	0.0020(4)	-0.0049(4)
C23	0.0136(4)	0.0197(5)	0.0251(5)	-0.0011(4)	-0.0015(3)	-0.0008(3)
C24	0.0168(4)	0.0191(5)	0.0203(5)	-0.0009(4)	-0.0023(3)	-0.0019(4)
C25	0.0264(5)	0.0214(5)	0.0385(7)	-0.0063(5)	0.0008(5)	0.0040(4)
C26	0.0379(7)	0.0278(6)	0.0345(7)	0.0109(5)	-0.0098(5)	-0.0037(5)
C27	0.0276(6)	0.0403(7)	0.0255(6)	-0.0044(5)	0.0077(4)	-0.0078(5)
C28	0.0187(5)	0.0258(5)	0.0391(7)	-0.0032(5)	-0.0041(4)	0.0043(4)
C29	0.0308(6)	0.0323(6)	0.0209(5)	0.0013(4)	-0.0037(4)	-0.0014(5)

Table 8. Hydrogen atomic coordinates and isotropic

atomic displacement parameters (Å^2) for 8.

	x/a	y/b	z/c	U(eq)
H11A	-0.0302	0.2325	-0.0961	0.045(5)
H11B	-0.0727	0.2472	-0.0061	0.056(5)
H11C	-0.0429	0.0896	-0.0411	0.065(6)
H12	-0.0240	0.1905	0.1172	0.027(4)
H13A	0.1132	0.1221	0.2057	0.054(5)
H13B	0.0299	0.2174	0.2528	0.053(5)
H13C	0.1357	0.2908	0.2255	0.054(5)
H14A	0.0333	0.4839	0.1582	0.053(5)
H14B	-0.0765	0.4094	0.1724	0.050(5)
H14C	-0.0409	0.4463	0.0825	0.052(5)
H15	0.0935	0.0823	-0.1421	0.028(4)
H16A	0.3122	0.0441	-0.1300	0.045(5)
H16B	0.2378	-0.0422	-0.1920	0.053(5)
H16C	0.2295	-0.0702	-0.0967	0.052(5)
H17A	0.1279	0.3174	-0.1938	0.051(5)
H17B	0.1766	0.1956	-0.2513	0.046(5)
H17C	0.2492	0.2853	-0.1895	0.043(4)
H25A	0.2851	0.6494	0.1402	0.042(4)
H25B	0.2338	0.5226	0.1927	0.040(4)
H25C	0.1843	0.5665	0.1066	0.043(4)
H26A	0.2148	0.5302	-0.0526	0.047(10)
H26B	0.3195	0.5211	-0.1019	0.040(9)
H26C	0.3065	0.6428	-0.0332	0.030(8)
H26D	0.3457	0.5992	-0.0726	0.049(13)
H26E	0.2410	0.6083	-0.0232	0.038(12)
H26F	0.2540	0.4865	-0.0919	0.031(11)
H27A	0.4069	0.2932	-0.1236	0.070(6)
H27B	0.4958	0.2028	-0.0773	0.066(6)
H27C	0.5090	0.3751	-0.0917	0.056(5)
H28A	0.5722	0.1888	0.1241	0.047(5)
H28B	0.5416	0.1108	0.0403	0.052(5)
H28C	0.4839	0.0664	0.1215	0.056(5)
H29A	0.3915	0.1975	0.2334	0.047(5)
H29B	0.3261	0.3417	0.2523	0.044(4)
H29C	0.4491	0.3506	0.2473	0.045(4)

{Cp*Ta[N(iPr)C(Me)N(iPr]}$_2$(μ-η^2:η^2-N$_2$)(μ-O) (9a)



A purple needle of $C_{36}H_{64}N_6OTa_2$, approximate dimensions 0.050×0.075×0.130 mm^3, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 100(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoKα fine-focus sealed tube (λ= 0.71073 Å) . The detector was placed at a distance of 5.000 cm from the crystal.

A total of 1035 frames were collected with a scan width of -0.30° an exposure time of 90 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 27.6 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of the data using a Monoclinic unit cell yielded a total of 21445 reflections to a maximum θ angle of 28.43°, of which 13935 were independent (completeness = 97.2%, R_{int} = 2.89%, R_{sig} = 5.80%) and 12749 were greater than 2σ(I). The final cell dimensions of a = 12.3334(16) Å, b = 18.228(2) Å, c = 16.578(2) Å, α = 90°, β = 90.162(2)°, γ = 90°, V = 3726.9(8) Å^3, are based upon the refinement of the XYZ-centroids of 9565 reflections with 2.4 < θ < 28.3° using Apex2 software. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.580 and 0.744.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group $P2_1$ with Z = 4 for the formula unit $C_{36}H_{64}N_6OTa_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 788 variables converged at R_1 = 3.84 % for the observed data and wR_2 = 8.34 % for all data. The goodness-of-fit was 1.001. The largest peak on the final difference map was 2.373 e$^-$/Å^3 and the largest hole was -2.681 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.709 g/cm^3 and F(000), 1904 e$^-$.

Comments:

Data quality: 50 microns thick needle were measured with 90 sec/frame exposure (3 x 30 sec) still yielding quality.

Twinning:

1) Non-merohedral twinning (components 1 & 2, refined as merohedral twinning by reflection in **ab** plane). It is actually pseudo-merohedral because of monoclinic angle β being close to 90°.
2) Merohedral twinning/racemic mixture possible because of non-centrosymmetric group and refined as components 3 & 4 that inversion of components 1 & 2 respectively.
3) Scale factors refined for components 1 - 4 are: 0.30(1), 0.22(1), 0.28(1) and 0.20(1)

Restraints and Constraints:

1) H-atoms were constrained geometry as riding on attached atom (A) with isotropic atomic displacement parameters set as

Uiso(H)=1.5Uiso(A) for CH3 and 1.2Uiso(A) for other groups

2) Two independent Ta_2_ -complexes which are related to each other by pseudo-symmetry element - 2_1 screw axis parallel to **c** axis. This quite accurately transform complexes into each other with the exception of iso-propyl groups with have different orientation in two independent complexes. The presence of this pseudo-symmetry makes this structure pseudo-orthorhombic causing pseudo-merohedral symmetry described above.
   Because of the pseudo-symmetry the correlation between two independent molecules especially between anisotropic displacement parameters is quite high. On the other hand pseudo-symmetry is almost exact with the exception of flexible iso-proplyl group which orientations also slightly affects Me_5_ Cp ligands as well, the following constraints and restraints were used:
   a) anisotropic parameters of Ta and coordinating N and O atoms were constrained to be the same taking into account 2 fold rotation around c-axis (all Uij are the same but U13 and U23 change signs);
   b) anisotropic parameters of atoms in rigid group (e.g. iso-propyl, Me_5_ Cp) were restrained using rigid body restrains (DELU)

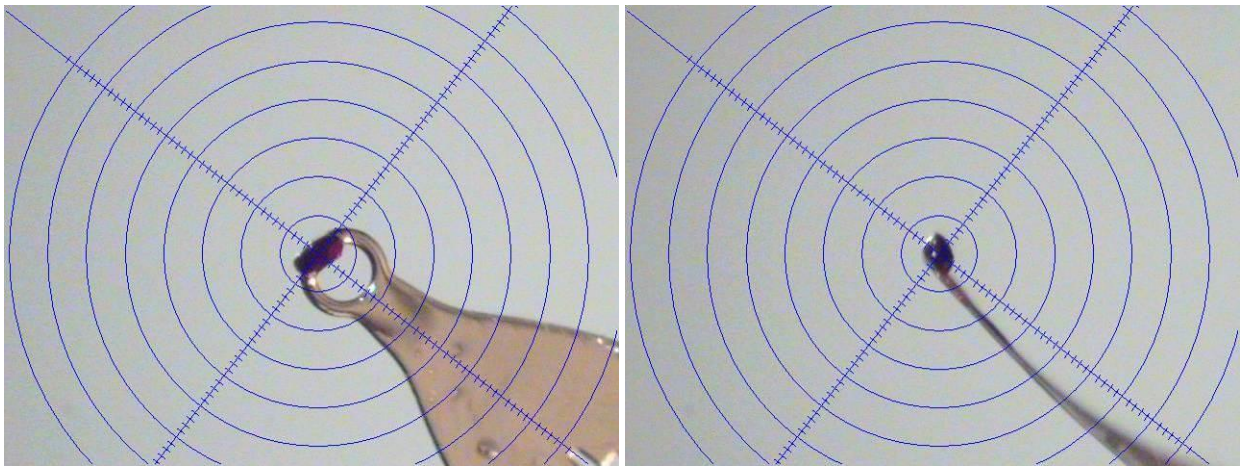


Table 1. Crystal data and structure refinement for **9a**.

X-ray lab book No.		**9a**
Crystal ID		**9a**
Empirical formula		$C_{36}H_{64}N_6OTa_2$
Formula weight		958.83
Temperature		100(2) K
Wavelength		0.71073 Å
Crystal size		0.130×0.075×0.050 mm^3
Crystal habit		purple needle
Crystal system		Monoclinic
Space group		$P2_1$
Unit cell dimensions		a = 12.3334(16) Å α = 90°
		b = 18.228(2) Å β = 90.162(2)°
		c = 16.578(2) Å γ = 90°
Volume		3726.9(8) $Å^3$
Z		4
Density, ρ_{calc}		1.709 g/cm^3
Absorption coefficient, μ		5.904 mm^{-1}
F(000)		1904 $\bar{e}$
Diffractometer		Bruker Smart Apex II CCD area detector
Radiation source		fine-focus sealed tube, MoKα
Detector distance		5.000 cm
Data collection method		ω omega scans
Total frames		1035
Frame size		512 pixels
Frame width		-0.30°
Exposure per frame		90 sec
Total measurement time		27.6 hours
θ range for data collection		1.99 to 28.43°
Index ranges		$-15 \le h \le 16$, $-24 \le k \le 16$, $-15 \le l \le 22$
Reflections collected		21445
Independent reflections		13935
Observed reflection, I>2σ(I)		12749
Coverage of independent reflections		97.2 %
Variation in check reflections		0 %
Absorption correction		Semi-empirical from equivalents
		SADABS (Sheldrick, 1996)
Max. and min. transmission		0.744 and 0.580
Structure solution technique		direct
Structure solution program		SHELXS-97 (Sheldrick, 1990)
Refinement technique		Full-matrix least-squares on F^2
Refinement program		SHELXL-97 (Sheldrick, 1997)
Function minimized		$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters		13935 / 174 / 788
Goodness-of-fit on F^2		0.994
Δ/σ_{max}		0.001
Final R indices:	R_1, I>2σ(I)	0.0384
	wR_2, all data	0.0834
	R_{int}	0.0289
	R_{sig}	0.0580
Weighting scheme		$w = 1/[\sigma^2(F_o^2)+ (0.044P)^2 + 4.95P]$, $P = [max(F_o^2 ,0) + 2F_o^2]/3$
Absolute structure parameter		0.51(1)
Largest diff. peak and hole		2.373 and -2.681 $\bar{e}/Å^3$

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table 2. Atomic coordinates and equivalent* isotropic atomic displacement parameters (Å^2) for **9a**.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Ta1	0.83946(4)	0.30297(2)	0.51884(3)	0.01533(6)
Ta2	0.64910(4)	0.22698(2)	0.46129(3)	0.01476(6)
O12	0.6825(7)	0.3240(4)	0.5073(5)	0.0157(11)
N1	0.8115(10)	0.1998(7)	0.5212(6)	0.0196(13)
N2	0.7985(8)	0.2098(6)	0.4324(6)	0.0147(13)
N11	0.8810(10)	0.3946(6)	0.4292(7)	0.0227(13)
N12	0.9838(8)	0.2959(7)	0.4436(6)	0.0199(12)
C10	0.9729(11)	0.3616(8)	0.4085(7)	0.0222(15)
C11	1.0559(13)	0.3980(10)	0.3546(10)	0.036(3)
C12	0.8579(13)	0.4727(7)	0.4115(7)	0.028(2)
C13	0.7701(14)	0.4988(7)	0.4621(9)	0.035(3)
C14	0.8336(15)	0.4868(9)	0.3208(8)	0.036(4)
C15	1.0617(10)	0.2422(9)	0.4131(8)	0.027(2)
C16	1.0727(13)	0.1761(9)	0.4701(10)	0.038(4)
C17	1.0300(15)	0.2155(11)	0.3286(9)	0.044(4)
N21	0.5445(10)	0.1922(6)	0.5668(7)	0.0187(12)
N22	0.6377(9)	0.1101(6)	0.4963(7)	0.0235(13)
C20	0.5803(11)	0.1213(7)	0.5612(7)	0.0182(14)
C21	0.5522(12)	0.0673(7)	0.6263(8)	0.022(2)
C22	0.4763(11)	0.2196(8)	0.6295(8)	0.023(2)
C23	0.4718(13)	0.3054(8)	0.6239(8)	0.027(3)
C24	0.3630(11)	0.1872(8)	0.6285(8)	0.026(3)
C25	0.7024(10)	0.0441(7)	0.4776(8)	0.026(2)
C26	0.7869(13)	0.0241(7)	0.5399(10)	0.039(4)
C27	0.6324(12)	-0.0216(7)	0.4532(9)	0.026(3)
C50	0.5101(12)	0.1838(7)	0.3586(8)	0.023(2)
C51	0.6105(11)	0.1882(8)	0.3220(8)	0.022(2)
C52	0.6416(11)	0.2630(7)	0.3196(7)	0.018(2)
C53	0.5570(10)	0.3045(8)	0.3576(7)	0.0182(19)
C54	0.4786(11)	0.2541(7)	0.3836(7)	0.0180(19)
C55	0.4402(12)	0.1165(8)	0.3677(8)	0.029(3)
C56	0.6750(12)	0.1277(7)	0.2819(7)	0.025(2)
C57	0.7408(11)	0.2913(8)	0.2795(7)	0.020(2)
C58	0.5520(12)	0.3839(8)	0.3673(9)	0.026(3)
C59	0.3682(11)	0.2749(9)	0.4137(8)	0.028(3)
C60	0.9922(12)	0.3296(8)	0.6185(9)	0.025(2)
C61	0.9327(11)	0.2698(8)	0.6470(9)	0.023(2)
C62	0.8289(11)	0.2928(7)	0.6644(7)	0.022(2)
C63	0.8199(11)	0.3695(7)	0.6497(7)	0.0219(19)
C64	0.9217(12)	0.3922(8)	0.6213(8)	0.024(2)
C65	1.1097(11)	0.3356(9)	0.5980(9)	0.032(3)
C66	0.9745(12)	0.1922(8)	0.6667(8)	0.026(3)
C67	0.7437(11)	0.2442(8)	0.7017(7)	0.021(2)
C68	0.7203(12)	0.4173(8)	0.6629(9)	0.028(3)
C69	0.9604(13)	0.4693(8)	0.6100(9)	0.031(3)
Ta3	0.33272(4)	0.36041(2)	0.96299(3)	0.01533(6)
Ta4	0.15680(4)	0.44776(2)	1.02433(3)	0.01476(6)
O34	0.1771(7)	0.3474(4)	0.9798(5)	0.0157(11)
N3	0.3139(9)	0.4664(7)	0.9594(6)	0.0196(13)
N4	0.3103(8)	0.4550(6)	1.0494(6)	0.0147(13)
N31	0.3697(9)	0.2678(6)	1.0523(7)	0.0227(13)
N32	0.4844(8)	0.3584(6)	1.0328(6)	0.0199(12)

C30	0.4688(11)	0.2926(8)	1.0682(7)	0.0222(15)
C31	0.5576(13)	0.2534(8)	1.1158(9)	0.032(3)
C32	0.3441(15)	0.1887(7)	1.0691(7)	0.027(2)
C33	0.2415(11)	0.1689(8)	1.0233(8)	0.026(3)
C34	0.3270(16)	0.1768(8)	1.1602(8)	0.035(4)
C35	0.5728(10)	0.4091(7)	1.0607(9)	0.025(2)
C36	0.5824(14)	0.4737(8)	1.0040(10)	0.034(3)
C37	0.5519(14)	0.4363(9)	1.1471(10)	0.036(4)
N41	0.0449(10)	0.4846(6)	0.9240(7)	0.0187(13)
N42	0.1447(9)	0.5664(5)	0.9855(6)	0.0235(13)
C40	0.0824(11)	0.5513(7)	0.9237(8)	0.0182(14)
C41	0.0590(14)	0.6059(8)	0.8546(8)	0.031(3)
C42	-0.0316(11)	0.4551(8)	0.8612(9)	0.026(2)
C43	-0.0433(12)	0.3740(7)	0.8682(9)	0.024(3)
C44	-0.1409(13)	0.4915(9)	0.8637(8)	0.033(3)
C45	0.2120(12)	0.6358(7)	0.9873(9)	0.031(3)
C46	0.3208(12)	0.6239(8)	1.0296(10)	0.040(3)
C47	0.1530(17)	0.6986(8)	1.0296(10)	0.047(4)
C70	0.4695(12)	0.3232(7)	0.8595(7)	0.020(2)
C71	0.4188(11)	0.3898(7)	0.8321(7)	0.019(2)
C72	0.3060(10)	0.3707(7)	0.8176(7)	0.019(2)
C73	0.2906(11)	0.2941(7)	0.8339(7)	0.0213(19)
C74	0.3906(12)	0.2663(8)	0.8593(8)	0.025(2)
C75	0.5913(11)	0.3122(8)	0.8735(8)	0.028(3)
C76	0.4686(11)	0.4607(8)	0.8103(9)	0.026(3)
C77	0.2264(12)	0.4261(8)	0.7832(8)	0.024(3)
C78	0.1862(13)	0.2527(8)	0.8210(9)	0.032(3)
C79	0.4209(12)	0.1841(7)	0.8696(9)	0.030(3)
C80	0.0298(12)	0.4998(8)	1.1300(7)	0.021(2)
C81	0.1344(11)	0.4870(8)	1.1655(7)	0.021(2)
C82	0.1585(12)	0.4113(7)	1.1655(7)	0.0202(19)
C83	0.0656(12)	0.3747(7)	1.1293(7)	0.020(2)
C84	-0.0127(12)	0.4297(8)	1.1058(8)	0.024(2)
C85	-0.0332(14)	0.5704(8)	1.1217(9)	0.034(3)
C86	0.2065(12)	0.5438(9)	1.2073(8)	0.029(3)
C87	0.2535(12)	0.3732(10)	1.2049(10)	0.034(3)
C88	0.0439(14)	0.2933(8)	1.1191(8)	0.030(3)
C89	-0.1264(11)	0.4149(9)	1.0780(9)	0.029(3)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic atomic displacement parameters* ($Å^2$) for **9a**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.01768(12)	0.01440(13)	0.01391(13)	0.00056(13)	-0.00002(18)	-0.00255(11)
Ta2	0.01595(12)	0.01316(12)	0.01516(14)	-0.00106(12)	0.00063(17)	-0.00064(11)
O12	0.018(2)	0.013(2)	0.016(3)	-0.005(2)	0.001(2)	0.0006(18)
N1	0.020(3)	0.027(3)	0.011(2)	-0.004(3)	0.002(3)	-0.005(2)
N2	0.015(3)	0.015(3)	0.014(3)	0.004(3)	0.000(2)	-0.006(2)
N11	0.026(2)	0.017(2)	0.025(4)	0.005(2)	-0.004(2)	-0.0062(19)
N12	0.013(2)	0.026(3)	0.020(4)	0.001(2)	0.000(2)	-0.0038(19)
C10	0.027(3)	0.026(3)	0.013(4)	0.000(3)	0.000(3)	-0.007(2)
C11	0.030(6)	0.043(8)	0.036(8)	0.012(6)	0.003(5)	-0.014(5)

C12	0.041(7)	0.018(3)	0.025(5)	0.009(5)	-0.013(5)	-0.009(5)
C13	0.062(10)	0.012(5)	0.032(6)	0.004(6)	-0.008(6)	0.004(5)
C14	0.051(10)	0.032(7)	0.025(4)	0.016(4)	-0.012(6)	-0.024(7)
C15	0.009(5)	0.041(7)	0.030(6)	-0.007(4)	0.003(5)	-0.003(4)
C16	0.035(8)	0.044(7)	0.036(6)	-0.004(6)	0.017(7)	0.026(6)
C17	0.040(9)	0.063(13)	0.029(5)	-0.016(5)	0.006(6)	0.004(8)
N21	0.026(3)	0.009(2)	0.021(3)	0.003(2)	0.008(2)	-0.008(2)
N22	0.029(3)	0.014(2)	0.027(3)	0.000(2)	0.007(2)	-0.003(2)
C20	0.022(3)	0.013(2)	0.020(3)	0.002(2)	0.000(3)	-0.003(2)
C21	0.025(7)	0.012(4)	0.031(6)	0.007(4)	0.005(5)	-0.002(5)
C22	0.017(5)	0.028(5)	0.023(6)	-0.002(5)	0.000(4)	0.004(5)
C23	0.035(8)	0.027(4)	0.020(6)	-0.008(5)	0.008(6)	0.004(4)
C24	0.015(4)	0.033(6)	0.030(7)	0.004(6)	-0.002(4)	0.006(4)
C25	0.030(6)	0.021(4)	0.026(6)	-0.001(5)	0.003(4)	0.003(2)
C26	0.054(8)	0.011(6)	0.054(9)	0.010(6)	-0.021(6)	-0.005(4)
C27	0.029(6)	0.015(3)	0.034(7)	-0.004(5)	0.000(5)	0.009(4)
C50	0.032(6)	0.019(3)	0.020(6)	-0.002(5)	0.004(5)	-0.004(3)
C51	0.024(5)	0.016(3)	0.025(7)	-0.003(5)	-0.001(4)	0.002(3)
C52	0.016(5)	0.016(3)	0.023(6)	-0.001(4)	-0.005(4)	0.003(3)
C53	0.019(4)	0.018(3)	0.017(5)	-0.009(5)	-0.005(4)	-0.001(3)
C54	0.023(4)	0.020(3)	0.011(5)	0.003(4)	-0.002(4)	0.003(3)
C55	0.035(6)	0.026(4)	0.025(7)	0.000(5)	-0.003(5)	-0.010(4)
C56	0.038(6)	0.019(4)	0.019(5)	-0.005(4)	0.000(5)	0.005(5)
C57	0.018(5)	0.023(5)	0.018(6)	0.000(5)	-0.005(4)	0.000(4)
C58	0.025(7)	0.018(3)	0.036(8)	-0.002(5)	0.004(5)	0.004(4)
C59	0.024(4)	0.038(7)	0.023(7)	0.002(5)	0.003(5)	0.004(4)
C60	0.028(4)	0.019(3)	0.030(7)	-0.001(5)	0.001(5)	-0.008(3)
C61	0.021(4)	0.018(3)	0.031(7)	0.002(5)	-0.009(5)	-0.008(3)
C62	0.024(4)	0.020(3)	0.022(6)	0.001(4)	-0.005(5)	-0.006(3)
C63	0.034(4)	0.020(3)	0.012(5)	-0.001(4)	0.001(5)	-0.002(3)
C64	0.036(5)	0.018(3)	0.018(6)	0.001(5)	0.001(5)	-0.005(3)
C65	0.028(4)	0.034(7)	0.033(8)	0.005(6)	0.001(6)	-0.010(4)
C66	0.031(6)	0.023(4)	0.025(7)	0.007(5)	-0.009(6)	-0.002(4)
C67	0.033(5)	0.023(5)	0.007(5)	-0.002(5)	0.003(5)	-0.005(4)
C68	0.035(5)	0.022(5)	0.027(7)	-0.018(5)	-0.005(5)	-0.001(4)
C69	0.039(7)	0.018(3)	0.036(8)	-0.005(6)	-0.006(6)	-0.009(4)
Ta3	0.01768(12)	0.01440(13)	0.01391(13)	0.00056(13)	0.00002(18)	0.00255(11)
Ta4	0.01595(12)	0.01316(12)	0.01516(14)	-0.00106(12)	-0.00063(17)	0.00064(11)
O34	0.018(2)	0.013(2)	0.016(3)	-0.005(2)	-0.001(2)	-0.0006(18)
N3	0.020(3)	0.027(3)	0.011(2)	-0.004(3)	-0.002(3)	0.005(2)
N4	0.015(3)	0.015(3)	0.014(3)	0.004(3)	0.000(2)	0.006(2)
N31	0.026(2)	0.017(2)	0.025(4)	0.005(2)	0.004(2)	0.0062(19)
N32	0.013(2)	0.026(3)	0.020(4)	0.001(2)	0.000(2)	0.0038(19)
C30	0.027(3)	0.026(3)	0.013(4)	0.000(3)	0.000(3)	0.007(2)
C31	0.037(5)	0.026(6)	0.035(8)	-0.001(5)	-0.010(5)	0.012(5)
C32	0.039(7)	0.020(4)	0.023(4)	0.006(5)	-0.003(5)	-0.001(6)
C33	0.032(7)	0.027(6)	0.019(5)	0.003(5)	0.005(5)	-0.003(4)
C34	0.055(11)	0.027(7)	0.023(4)	0.007(4)	-0.004(6)	-0.008(7)
C35	0.015(5)	0.011(5)	0.048(6)	0.001(4)	0.009(5)	0.002(3)
C36	0.046(9)	0.017(5)	0.039(6)	0.003(5)	-0.015(7)	-0.001(4)
C37	0.037(9)	0.034(9)	0.037(5)	-0.002(5)	-0.014(6)	-0.010(7)
N41	0.026(3)	0.009(2)	0.021(3)	0.003(2)	-0.008(2)	0.008(2)
N42	0.029(3)	0.014(2)	0.027(3)	0.000(2)	-0.007(2)	0.003(2)
C40	0.022(3)	0.013(2)	0.020(3)	0.002(2)	0.000(3)	0.003(2)
C41	0.048(10)	0.016(5)	0.028(6)	0.009(4)	-0.007(5)	-0.001(6)
C42	0.019(5)	0.019(4)	0.039(7)	0.005(5)	-0.012(5)	-0.003(5)

C43	0.017(7)	0.019(4)	0.037(8)	0.003(5)	-0.007(5)	-0.004(4)
C44	0.033(5)	0.035(7)	0.031(7)	-0.016(6)	-0.018(6)	0.016(6)
C45	0.039(6)	0.016(5)	0.039(8)	0.005(5)	0.000(5)	-0.002(3)
C46	0.039(6)	0.023(7)	0.058(10)	0.010(7)	-0.009(7)	-0.015(4)
C47	0.063(10)	0.017(4)	0.062(10)	-0.011(6)	-0.004(10)	0.002(6)
C70	0.033(3)	0.018(3)	0.008(5)	0.002(4)	0.002(4)	0.007(3)
C71	0.026(4)	0.018(3)	0.012(6)	0.004(4)	0.006(4)	0.005(2)
C72	0.026(3)	0.012(3)	0.020(6)	-0.008(4)	0.006(4)	0.006(2)
C73	0.037(4)	0.014(3)	0.014(5)	-0.006(4)	0.002(4)	0.002(2)
C74	0.039(4)	0.018(3)	0.018(6)	0.006(5)	0.005(5)	0.005(3)
C75	0.031(3)	0.025(7)	0.027(7)	0.007(6)	0.012(5)	0.014(3)
C76	0.023(5)	0.022(4)	0.034(7)	0.012(6)	0.002(5)	0.004(4)
C77	0.026(5)	0.020(4)	0.027(7)	0.005(5)	-0.003(5)	-0.001(4)
C78	0.049(5)	0.018(5)	0.029(7)	-0.005(5)	-0.011(6)	-0.007(4)
C79	0.038(7)	0.018(3)	0.033(8)	0.002(6)	0.012(6)	0.007(3)
C80	0.031(5)	0.021(3)	0.012(6)	-0.005(5)	-0.001(4)	0.008(3)
C81	0.022(5)	0.023(3)	0.018(6)	-0.007(4)	0.004(4)	0.000(3)
C82	0.020(5)	0.026(3)	0.015(5)	-0.005(4)	0.003(4)	0.006(3)
C83	0.026(5)	0.019(3)	0.015(6)	-0.005(4)	0.003(4)	0.004(3)
C84	0.029(5)	0.024(3)	0.019(6)	0.002(5)	-0.009(5)	0.001(3)
C85	0.042(7)	0.028(4)	0.032(8)	0.000(6)	0.011(6)	0.018(5)
C86	0.040(6)	0.035(5)	0.014(6)	-0.004(5)	0.004(5)	-0.015(5)
C87	0.017(5)	0.047(7)	0.038(8)	0.015(6)	0.005(5)	0.008(5)
C88	0.051(8)	0.019(3)	0.019(7)	0.004(5)	0.005(6)	-0.005(4)
C89	0.019(4)	0.039(7)	0.029(8)	0.004(6)	0.006(5)	-0.001(4)

* The anisotropic atomic displacement factor exponent takes the form:$-2\pi^2$ [$h^2a^{*2}U_{11}$ +... + 2hka*b*U_{12}]

Table 4. H atom coordinates and isotropic atomic displacement parameters ($Å^2$) for **9a**.

Atom	*x/a*	*y/b*	*z/c*	U_{iso}
H11A	1.0359	0.3902	0.2980	0.055
H11B	1.1275	0.3765	0.3649	0.055
H11C	1.0581	0.4507	0.3660	0.055
H12	0.9242	0.5015	0.4259	0.033
H13A	0.7049	0.4696	0.4517	0.053
H13B	0.7553	0.5505	0.4499	0.053
H13C	0.7909	0.4940	0.5190	0.053
H14A	0.7689	0.4592	0.3047	0.054
H14B	0.8955	0.4709	0.2883	0.054
H14C	0.8210	0.5393	0.3121	0.054
H15	1.1340	0.2666	0.4094	0.032
H16A	1.0973	0.1930	0.5232	0.058
H16B	1.1256	0.1415	0.4480	0.058
H16C	1.0022	0.1518	0.4755	0.058
H17A	0.9601	0.1901	0.3311	0.066
H17B	1.0856	0.1818	0.3085	0.066
H17C	1.0241	0.2577	0.2921	0.066
H21A	0.4820	0.0446	0.6141	0.034
H21B	0.5482	0.0927	0.6782	0.034
H21C	0.6082	0.0292	0.6290	0.034
H22	0.5106	0.2065	0.6823	0.027
H23A	0.5411	0.3260	0.6420	0.041

H23B	0.4133	0.3239	0.6584	0.041
H23C	0.4581	0.3201	0.5679	0.041
H24A	0.3223	0.2070	0.5825	0.039
H24B	0.3257	0.1998	0.6787	0.039
H24C	0.3677	0.1337	0.6235	0.039
H25	0.7444	0.0571	0.4281	0.031
H26A	0.8285	0.0679	0.5547	0.059
H26B	0.8359	-0.0130	0.5176	0.059
H26C	0.7511	0.0043	0.5880	0.059
H27A	0.5874	-0.0365	0.4990	0.039
H27B	0.6793	-0.0625	0.4373	0.039
H27C	0.5857	-0.0078	0.4078	0.039
H55A	0.3808	0.1183	0.3284	0.043
H55B	0.4103	0.1150	0.4224	0.043
H55C	0.4841	0.0726	0.3583	0.043
H56A	0.6606	0.0810	0.3091	0.038
H56B	0.7526	0.1390	0.2855	0.038
H56C	0.6537	0.1239	0.2250	0.038
H57A	0.8031	0.2853	0.3157	0.030
H57B	0.7312	0.3434	0.2668	0.030
H57C	0.7534	0.2638	0.2296	0.030
H58A	0.4765	0.4002	0.3631	0.039
H58B	0.5952	0.4074	0.3251	0.039
H58C	0.5811	0.3974	0.4204	0.039
H59A	0.3741	0.3179	0.4489	0.042
H59B	0.3372	0.2338	0.4441	0.042
H59C	0.3210	0.2864	0.3677	0.042
H65A	1.1479	0.2917	0.6171	0.047
H65B	1.1405	0.3792	0.6241	0.047
H65C	1.1178	0.3398	0.5394	0.047
H66A	0.9637	0.1820	0.7241	0.039
H66B	1.0520	0.1891	0.6539	0.039
H66C	0.9345	0.1561	0.6344	0.039
H67A	0.7423	0.1969	0.6737	0.032
H67B	0.6725	0.2678	0.6969	0.032
H67C	0.7608	0.2364	0.7589	0.032
H68A	0.7430	0.4682	0.6720	0.042
H68B	0.6803	0.3996	0.7100	0.042
H68C	0.6734	0.4149	0.6151	0.042
H69A	0.9028	0.5035	0.6253	0.046
H69B	0.9796	0.4770	0.5534	0.046
H69C	1.0243	0.4777	0.6441	0.046
H31A	0.5457	0.2606	1.1737	0.049
H31B	0.6285	0.2735	1.1008	0.049
H31C	0.5557	0.2008	1.1034	0.049
H32	0.4052	0.1571	1.0501	0.033
H33A	0.1804	0.1969	1.0451	0.039
H33B	0.2271	0.1163	1.0293	0.039
H33C	0.2507	0.1807	0.9661	0.039
H34A	0.2558	0.1958	1.1758	0.052
H34B	0.3837	0.2027	1.1904	0.052
H34C	0.3307	0.1242	1.1724	0.052
H35	0.6429	0.3815	1.0602	0.030
H36A	0.6117	0.4571	0.9522	0.051
H36B	0.6311	0.5105	1.0276	0.051
H36C	0.5106	0.4955	0.9954	0.051

H37A	0.6143	0.4650	1.1658	0.054
H37B	0.5414	0.3941	1.1829	0.054
H37C	0.4868	0.4671	1.1477	0.054
H41A	0.0175	0.6476	0.8755	0.046
H41B	0.0169	0.5813	0.8123	0.046
H41C	0.1276	0.6235	0.8321	0.046
H42	0.0008	0.4657	0.8072	0.031
H43A	-0.0838	0.3621	0.9173	0.037
H43B	0.0287	0.3514	0.8708	0.037
H43C	-0.0825	0.3551	0.8210	0.037
H44A	-0.1897	0.4675	0.8251	0.050
H44B	-0.1333	0.5435	0.8494	0.050
H44C	-0.1710	0.4874	0.9181	0.050
H45	0.2265	0.6509	0.9304	0.037
H46A	0.3083	0.6044	1.0839	0.060
H46B	0.3595	0.6707	1.0334	0.060
H46C	0.3643	0.5889	0.9986	0.060
H47A	0.0759	0.6974	1.0150	0.071
H47B	0.1844	0.7455	1.0126	0.071
H47C	0.1607	0.6932	1.0881	0.071
H75A	0.6076	0.3171	0.9311	0.041
H75B	0.6319	0.3493	0.8432	0.041
H75C	0.6124	0.2632	0.8550	0.041
H76A	0.5431	0.4624	0.8309	0.039
H76B	0.4265	0.5008	0.8340	0.039
H76C	0.4693	0.4659	0.7514	0.039
H77A	0.1536	0.4045	0.7820	0.037
H77B	0.2481	0.4393	0.7283	0.037
H77C	0.2259	0.4701	0.8171	0.037
H78A	0.2022	0.2039	0.7994	0.048
H78B	0.1404	0.2796	0.7827	0.048
H78C	0.1480	0.2478	0.8725	0.048
H79A	0.3554	0.1539	0.8646	0.045
H79B	0.4535	0.1765	0.9230	0.045
H79C	0.4729	0.1699	0.8278	0.045
H85A	0.0124	0.6116	1.1388	0.051
H85B	-0.0980	0.5681	1.1556	0.051
H85C	-0.0547	0.5772	1.0652	0.051
H86A	0.1984	0.5394	1.2659	0.044
H86B	0.1850	0.5932	1.1903	0.044
H86C	0.2824	0.5352	1.1927	0.044
H87A	0.3154	0.4068	1.2072	0.051
H87B	0.2730	0.3297	1.1734	0.051
H87C	0.2336	0.3583	1.2598	0.051
H88A	0.1095	0.2656	1.1328	0.045
H88B	0.0236	0.2833	1.0630	0.045
H88C	-0.0153	0.2785	1.1548	0.045
H89A	-0.1285	0.3686	1.0480	0.044
H89B	-0.1507	0.4550	1.0429	0.044
H89C	-0.1744	0.4116	1.1249	0.044

Table 5. Bond lengths (Å) and angles (°) for **9a**.

Ta1-N1	1.913(12)	Ta1-O12	1.982(9)	Ta1-N12	2.180(10)
Ta1-N2	2.279(10)	Ta1-N11	2.295(11)	Ta1-C62	2.424(12)
Ta1-C61	2.487(14)	Ta1-C63	2.498(11)	Ta1-C60	2.550(14)
Ta1-C64	2.559(14)	Ta1-C10	2.686(13)	Ta1-Ta2	2.8859(7)
Ta2-N2	1.932(11)	Ta2-O12	1.969(8)	Ta2-N22	2.212(10)
Ta2-N21	2.267(10)	Ta2-N1	2.288(12)	Ta2-C52	2.440(12)
Ta2-C51	2.461(14)	Ta2-C53	2.496(13)	Ta2-C54	2.512(13)
Ta2-C50	2.538(14)	Ta2-C20	2.680(12)	N1-N2	1.493(14)
N11-C10	1.330(18)	N11-C12	1.481(17)	N12-C10	1.337(17)
N12-C15	1.463(17)	C10-C11	1.514(19)	C12-C13	1.45(2)
C12-C14	1.554(17)	C15-C17	1.53(2)	C15-C16	1.54(2)
N21-C20	1.369(16)	N21-C22	1.429(17)	N22-C20	1.305(16)
N22-C25	1.478(16)	C20-C21	1.501(17)	C22-C24	1.518(19)
C22-C23	1.57(2)	C25-C26	1.510(19)	C25-C27	1.529(19)
C50-C51	1.384(19)	C50-C54	1.401(18)	C50-C55	1.507(19)
C51-C52	1.418(18)	C51-C56	1.514(18)	C52-C53	1.435(18)
C52-C57	1.486(18)	C53-C54	1.402(19)	C53-C58	1.458(19)
C54-C59	1.500(19)	C60-C61	1.397(19)	C60-C64	1.44(2)
C60-C65	1.493(19)	C61-C62	1.379(19)	C61-C66	1.541(19)
C62-C63	1.423(17)	C62-C67	1.508(18)	C63-C64	1.404(19)
C63-C68	1.523(19)	C64-C69	1.495(19)	Ta3-N3	1.948(12)
Ta3-O34	1.955(9)	Ta3-N32	2.197(10)	Ta3-N4	2.258(10)
Ta3-N31	2.290(11)	Ta3-C72	2.440(12)	Ta3-C71	2.478(12)
Ta3-C70	2.502(13)	Ta3-C73	2.511(12)	Ta3-C74	2.533(14)
Ta3-Ta4	2.8791(7)	Ta4-N4	1.941(10)	Ta4-O34	1.988(8)
Ta4-N3	2.246(11)	Ta4-N41	2.259(11)	Ta4-N42	2.261(10)
Ta4-C82	2.433(11)	Ta4-C81	2.463(12)	Ta4-C83	2.466(14)
Ta4-C84	2.514(16)	Ta4-C80	2.536(13)	Ta4-C40	2.680(13)
N3-N4	1.507(13)	N31-C30	1.330(17)	N31-C32	1.502(15)
N32-C30	1.349(18)	N32-C35	1.501(16)	C30-C31	1.526(18)
C32-C33	1.52(2)	C32-C34	1.541(18)	C35-C36	1.51(2)
C35-C37	1.54(2)	N41-C40	1.301(17)	N41-C42	1.504(17)
N42-C40	1.308(17)	N42-C45	1.512(16)	C40-C41	1.544(18)
C42-C43	1.490(19)	C42-C44	1.50(2)	C45-C46	1.528(19)
C45-C47	1.53(2)	C70-C74	1.42(2)	C70-C71	1.439(18)
C70-C75	1.534(19)	C71-C72	1.454(18)	C71-C76	1.475(19)
C72-C73	1.436(18)	C72-C77	1.517(17)	C73-C74	1.397(19)
C73-C78	1.507(19)	C74-C79	1.554(18)	C80-C81	1.436(19)
C80-C84	1.437(19)	C80-C85	1.509(19)	C81-C82	1.412(18)
C81-C86	1.529(18)	C82-C83	1.454(19)	C82-C87	1.509(19)
C83-C84	1.444(19)	C83-C88	1.52(2)	C84-C89	1.50(2)
N1-Ta1-O12	90.9(4)	N1-Ta1-N12	95.8(4)	O12-Ta1-N12	139.0(4)
N1-Ta1-N2	40.6(4)	O12-Ta1-N2	82.5(3)	N12-Ta1-N2	77.0(4)
N1-Ta1-N11	140.4(4)	O12-Ta1-N11	90.9(4)	N12-Ta1-N11	59.2(4)
N2-Ta1-N11	100.7(4)	N1-Ta1-C62	83.9(4)	O12-Ta1-C62	93.2(4)
N12-Ta1-C62	127.7(4)	N2-Ta1-C62	123.8(4)	N11-Ta1-C62	135.5(4)
N1-Ta1-C61	80.0(4)	O12-Ta1-C61	125.4(4)	N12-Ta1-C61	95.6(4)
N2-Ta1-C61	117.2(4)	N11-Ta1-C61	128.8(4)	C62-Ta1-C61	32.6(5)
N1-Ta1-C63	116.2(4)	O12-Ta1-C63	83.9(4)	N12-Ta1-C63	127.3(4)
N2-Ta1-C63	152.5(4)	N11-Ta1-C63	103.4(4)	C62-Ta1-C63	33.6(4)
C61-Ta1-C63	54.7(4)	N1-Ta1-C60	107.9(5)	O12-Ta1-C60	138.2(4)
N12-Ta1-C60	77.2(4)	N2-Ta1-C60	135.4(4)	N11-Ta1-C60	96.6(4)
C62-Ta1-C60	53.9(4)	C61-Ta1-C60	32.2(4)	C63-Ta1-C60	54.4(4)
N1-Ta1-C64	133.0(4)	O12-Ta1-C64	109.0(4)	N12-Ta1-C64	95.4(4)
N2-Ta1-C64	168.0(4)	N11-Ta1-C64	83.0(4)	C62-Ta1-C64	53.9(4)
C61-Ta1-C64	53.6(4)	C63-Ta1-C64	32.2(4)	C60-Ta1-C64	32.6(4)
N1-Ta1-C10	121.1(4)	O12-Ta1-C10	117.2(4)	N12-Ta1-C10	29.6(4)
N2-Ta1-C10	90.2(4)	N11-Ta1-C10	29.7(4)	C62-Ta1-C10	138.0(4)
C61-Ta1-C10	113.3(4)	C63-Ta1-C10	117.3(4)	C60-Ta1-C10	85.0(4)

C64-Ta1-C10	87.5(4)	N1-Ta1-Ta2	52.3(4)	O12-Ta1-Ta2	42.9(2)
N12-Ta1-Ta2	116.6(3)	N2-Ta1-Ta2	41.9(3)	N11-Ta1-Ta2	108.6(3)
C62-Ta1-Ta2	104.3(3)	C61-Ta1-Ta2	122.7(3)	C63-Ta1-Ta2	116.1(3)
C60-Ta1-Ta2	154.8(3)	C64-Ta1-Ta2	147.7(3)	C10-Ta1-Ta2	117.7(3)
N2-Ta2-O12	92.5(4)	N2-Ta2-N22	88.3(4)	O12-Ta2-N22	140.9(4)
N2-Ta2-N21	133.8(4)	O12-Ta2-N21	94.1(4)	N22-Ta2-N21	59.4(4)
N2-Ta2-N1	40.3(4)	O12-Ta2-N1	81.1(4)	N22-Ta2-N1	74.5(4)
N21-Ta2-N1	96.0(4)	N2-Ta2-C52	80.7(4)	O12-Ta2-C52	97.9(4)
N22-Ta2-C52	120.7(4)	N21-Ta2-C52	142.9(4)	N1-Ta2-C52	120.5(4)
N2-Ta2-C51	84.4(4)	O12-Ta2-C51	131.4(4)	N22-Ta2-C51	87.6(4)
N21-Ta2-C51	122.3(4)	N1-Ta2-C51	120.8(4)	C52-Ta2-C51	33.6(4)
N2-Ta2-C53	110.7(4)	O12-Ta2-C53	81.5(4)	N22-Ta2-C53	134.2(4)
N21-Ta2-C53	115.5(4)	N1-Ta2-C53	144.9(4)	C52-Ta2-C53	33.8(4)
C51-Ta2-C53	55.2(4)	N2-Ta2-C54	134.6(4)	O12-Ta2-C54	101.3(4)
N22-Ta2-C54	105.7(4)	N21-Ta2-C54	88.5(4)	N1-Ta2-C54	174.9(4)
C52-Ta2-C54	54.9(4)	C51-Ta2-C54	54.3(4)	C53-Ta2-C54	32.5(4)
N2-Ta2-C50	115.2(4)	O12-Ta2-C50	132.7(4)	N22-Ta2-C50	80.5(4)
N21-Ta2-C50	92.6(4)	N1-Ta2-C50	144.4(4)	C52-Ta2-C50	54.2(4)
C51-Ta2-C50	32.1(4)	C53-Ta2-C50	53.7(4)	C54-Ta2-C50	32.2(4)
N2-Ta2-C20	109.9(4)	O12-Ta2-C20	118.2(4)	N22-Ta2-C20	29.0(4)
N21-Ta2-C20	30.7(4)	N1-Ta2-C20	81.6(4)	C52-Ta2-C20	141.0(4)
C51-Ta2-C20	108.2(4)	C53-Ta2-C20	133.5(4)	C54-Ta2-C20	101.1(4)
C50-Ta2-C20	88.7(4)	N2-Ta2-Ta1	52.0(3)	O12-Ta2-Ta1	43.3(3)
N22-Ta2-Ta1	115.3(3)	N21-Ta2-Ta1	110.1(3)	N1-Ta2-Ta1	41.4(3)
C52-Ta2-Ta1	102.6(3)	C51-Ta2-Ta1	127.1(3)	C53-Ta2-Ta1	108.9(3)
C54-Ta2-Ta1	139.0(3)	C50-Ta2-Ta1	156.6(3)	C20-Ta2-Ta1	113.5(3)
Ta2-O12-Ta1	93.8(3)	N2-N1-Ta1	83.0(7)	N2-N1-Ta2	56.9(6)
Ta1-N1-Ta2	86.3(5)	N1-N2-Ta2	82.8(7)	N1-N2-Ta1	56.4(6)
Ta2-N2-Ta1	86.1(4)	C10-N11-C12	123.2(12)	C10-N11-Ta1	91.7(8)
C12-N11-Ta1	141.8(9)	C10-N12-C15	121.0(11)	C10-N12-Ta1	96.6(8)
C15-N12-Ta1	140.8(9)	N11-C10-N12	112.2(12)	N11-C10-C11	122.2(13)
N12-C10-C11	125.6(13)	N11-C10-Ta1	58.6(7)	N12-C10-Ta1	53.8(6)
C11-C10-Ta1	173.3(10)	C13-C12-N11	110.0(11)	C13-C12-C14	111.3(13)
N11-C12-C14	112.8(11)	N12-C15-C17	111.2(12)	N12-C15-C16	111.7(11)
C17-C15-C16	109.6(14)	C20-N21-C22	124.8(11)	C20-N21-Ta2	91.5(8)
C22-N21-Ta2	143.2(9)	C20-N22-C25	126.5(11)	C20-N22-Ta2	95.8(8)
C25-N22-Ta2	134.0(8)	N22-C20-N21	112.3(11)	N22-C20-C21	128.1(12)
N21-C20-C21	119.7(11)	N22-C20-Ta2	55.2(6)	N21-C20-Ta2	57.7(6)
C21-C20-Ta2	171.6(9)	N21-C22-C24	113.5(11)	N21-C22-C23	109.1(11)
C24-C22-C23	110.8(12)	N22-C25-C26	115.1(12)	N22-C25-C27	112.9(11)
C26-C25-C27	112.3(11)	C51-C50-C54	109.1(12)	C51-C50-C55	127.1(13)
C54-C50-C55	123.7(13)	C51-C50-Ta2	70.9(8)	C54-C50-Ta2	72.9(8)
C55-C50-Ta2	124.8(9)	C50-C51-C52	108.0(12)	C50-C51-C56	128.6(13)
C52-C51-C56	123.1(12)	C50-C51-Ta2	77.0(8)	C52-C51-Ta2	72.4(7)
C56-C51-Ta2	121.4(9)	C51-C52-C53	107.3(12)	C51-C52-C57	124.7(12)
C53-C52-C57	127.9(12)	C51-C52-Ta2	74.0(8)	C53-C52-Ta2	75.2(7)
C57-C52-Ta2	119.7(8)	C54-C53-C52	107.1(12)	C54-C53-C58	125.9(12)
C52-C53-C58	127.0(13)	C54-C53-Ta2	74.4(7)	C52-C53-Ta2	71.0(7)
C58-C53-Ta2	120.3(9)	C50-C54-C53	108.4(12)	C50-C54-C59	125.5(13)
C53-C54-C59	124.3(12)	C50-C54-Ta2	74.9(8)	C53-C54-Ta2	73.1(7)
C59-C54-Ta2	129.7(8)	C61-C60-C64	106.9(12)	C61-C60-C65	130.2(14)
C64-C60-C65	122.6(13)	C61-C60-Ta1	71.5(8)	C64-C60-Ta1	74.0(8)
C65-C60-Ta1	125.6(10)	C62-C61-C60	108.8(12)	C62-C61-C66	123.0(13)
C60-C61-C66	127.8(13)	C62-C61-Ta1	71.2(8)	C60-C61-Ta1	76.4(8)
C66-C61-Ta1	123.9(9)	C61-C62-C63	109.5(12)	C61-C62-C67	123.8(12)
C63-C62-C67	126.4(12)	C61-C62-Ta1	76.2(8)	C63-C62-Ta1	76.0(7)
C67-C62-Ta1	119.5(8)	C64-C63-C62	106.2(12)	C64-C63-C68	127.0(12)
C62-C63-C68	126.9(12)	C64-C63-Ta1	76.3(8)	C62-C63-Ta1	70.4(6)
C68-C63-Ta1	118.8(8)	C63-C64-C60	108.6(12)	C63-C64-C69	127.3(13)
C60-C64-C69	123.2(13)	C63-C64-Ta1	71.5(7)	C60-C64-Ta1	73.3(8)
C69-C64-Ta1	129.8(10)	N3-Ta3-O34	90.4(4)	N3-Ta3-N32	97.7(4)
O34-Ta3-N32	139.2(4)	N3-Ta3-N4	41.2(4)	O34-Ta3-N4	83.1(3)

N32-Ta3-N4	77.6(4)	N3-Ta3-N31	140.8(4)	O34-Ta3-N31	90.7(4)
N32-Ta3-N31	58.6(4)	N4-Ta3-N31	100.2(4)	N3-Ta3-C72	82.9(4)
O34-Ta3-C72	91.2(4)	N32-Ta3-C72	129.4(4)	N4-Ta3-C72	123.4(4)
N31-Ta3-C72	136.2(4)	N3-Ta3-C71	79.0(4)	O34-Ta3-C71	125.1(4)
N32-Ta3-C71	95.7(4)	N4-Ta3-C71	116.3(4)	N31-Ta3-C71	129.8(4)
C72-Ta3-C71	34.4(4)	N3-Ta3-C70	109.2(4)	O34-Ta3-C70	136.8(4)
N32-Ta3-C70	77.4(4)	N4-Ta3-C70	136.5(4)	N31-Ta3-C70	96.3(4)
C72-Ta3-C70	55.5(4)	C71-Ta3-C70	33.6(4)	N3-Ta3-C73	115.3(4)
O34-Ta3-C73	82.1(4)	N32-Ta3-C73	127.9(4)	N4-Ta3-C73	151.9(4)
N31-Ta3-C73	103.6(4)	C72-Ta3-C73	33.7(4)	C71-Ta3-C73	56.4(4)
C70-Ta3-C73	54.8(4)	N3-Ta3-C74	133.3(4)	O34-Ta3-C74	107.1(4)
N32-Ta3-C74	96.0(4)	N4-Ta3-C74	169.3(4)	N31-Ta3-C74	83.3(4)
C72-Ta3-C74	54.5(4)	C71-Ta3-C74	55.3(4)	C70-Ta3-C74	32.8(4)
C73-Ta3-C74	32.2(4)	N3-Ta3-Ta4	51.1(3)	O34-Ta3-Ta4	43.6(2)
N32-Ta3-Ta4	117.7(3)	N4-Ta3-Ta4	42.3(3)	N31-Ta3-Ta4	109.2(3)
C72-Ta3-Ta4	101.9(3)	C71-Ta3-Ta4	121.0(3)	C70-Ta3-Ta4	154.4(3)
C73-Ta3-Ta4	114.4(3)	C74-Ta3-Ta4	145.9(3)	N4-Ta4-O34	91.0(4)
N4-Ta4-N3	41.4(4)	O34-Ta4-N3	81.5(4)	N4-Ta4-N41	136.9(4)
O34-Ta4-N41	94.5(4)	N3-Ta4-N41	97.4(4)	N4-Ta4-N42	93.4(4)
O34-Ta4-N42	141.5(3)	N3-Ta4-N42	77.0(4)	N41-Ta4-N42	57.8(4)
N4-Ta4-C82	78.9(4)	O34-Ta4-C82	96.0(4)	N3-Ta4-C82	119.9(4)
N41-Ta4-C82	142.4(5)	N42-Ta4-C82	122.4(4)	N4-Ta4-C81	83.6(4)
O34-Ta4-C81	129.4(4)	N3-Ta4-C81	120.7(4)	N41-Ta4-C81	122.9(4)
N42-Ta4-C81	89.1(4)	C82-Ta4-C81	33.5(4)	N4-Ta4-C83	109.4(4)
O34-Ta4-C83	79.8(4)	N3-Ta4-C83	144.7(4)	N41-Ta4-C83	113.6(5)
N42-Ta4-C83	133.5(4)	C82-Ta4-C83	34.5(5)	C81-Ta4-C83	55.5(4)
N4-Ta4-C84	134.9(4)	O34-Ta4-C84	100.6(4)	N3-Ta4-C84	176.1(4)
N41-Ta4-C84	85.8(4)	N42-Ta4-C84	103.0(4)	C82-Ta4-C84	56.8(5)
C81-Ta4-C84	55.4(4)	C83-Ta4-C84	33.7(4)	N4-Ta4-C80	115.5(4)
O34-Ta4-C80	132.7(4)	N3-Ta4-C80	144.1(4)	N41-Ta4-C80	91.1(4)
N42-Ta4-C80	78.4(4)	C82-Ta4-C80	56.1(4)	C81-Ta4-C80	33.3(4)
C83-Ta4-C80	55.3(5)	C84-Ta4-C80	33.1(4)	N4-Ta4-C40	114.7(4)
O34-Ta4-C40	117.4(4)	N3-Ta4-C40	83.6(4)	N41-Ta4-C40	29.0(4)
N42-Ta4-C40	29.2(4)	C82-Ta4-C40	142.5(4)	C81-Ta4-C40	110.3(4)
C83-Ta4-C40	131.6(4)	C84-Ta4-C40	98.2(4)	C80-Ta4-C40	87.5(4)
N4-Ta4-Ta3	51.5(3)	O34-Ta4-Ta3	42.7(2)	N3-Ta4-Ta3	42.5(3)
N41-Ta4-Ta3	111.3(3)	N42-Ta4-Ta3	118.5(3)	C82-Ta4-Ta3	100.6(3)
C81-Ta4-Ta3	125.6(3)	C83-Ta4-Ta3	107.2(3)	C84-Ta4-Ta3	138.2(3)
C80-Ta4-Ta3	156.6(3)	C40-Ta4-Ta3	115.3(3)	Ta3-O34-Ta4	93.8(3)
N4-N3-Ta3	80.5(7)	N4-N3-Ta4	58.4(6)	Ta3-N3-Ta4	86.4(5)
N3-N4-Ta4	80.2(6)	N3-N4-Ta3	58.3(6)	Ta4-N4-Ta3	86.2(4)
C30-N31-C32	118.9(12)	C30-N31-Ta3	93.4(8)	C32-N31-Ta3	141.8(9)
C30-N32-C35	121.1(11)	C30-N32-Ta3	97.0(8)	C35-N32-Ta3	140.2(9)
N31-C30-N32	110.4(11)	N31-C30-C31	127.0(13)	N32-C30-C31	122.6(13)
N31-C32-C33	108.1(11)	N31-C32-C34	110.3(10)	C33-C32-C34	109.9(14)
N32-C35-C36	110.3(11)	N32-C35-C37	111.2(11)	C36-C35-C37	110.0(12)
C40-N41-C42	123.6(11)	C40-N41-Ta4	93.7(8)	C42-N41-Ta4	141.7(9)
C40-N42-C45	120.8(11)	C40-N42-Ta4	93.4(8)	C45-N42-Ta4	139.3(8)
N41-C40-N42	113.6(11)	N41-C40-C41	122.7(12)	N42-C40-C41	123.6(12)
N41-C40-Ta4	57.3(7)	N42-C40-Ta4	57.4(6)	C41-C40-Ta4	168.2(10)
C43-C42-C44	110.5(13)	C43-C42-N41	111.2(11)	C44-C42-N41	112.6(12)
N42-C45-C46	111.8(10)	N42-C45-C47	111.9(13)	C46-C45-C47	108.3(13)
C74-C70-C71	108.6(12)	C74-C70-C75	125.1(12)	C71-C70-C75	125.6(12)
C74-C70-Ta3	74.8(8)	C71-C70-Ta3	72.3(7)	C75-C70-Ta3	126.5(8)
C70-C71-C72	105.3(11)	C70-C71-C76	129.5(12)	C72-C71-C76	124.6(12)
C70-C71-Ta3	74.1(7)	C72-C71-Ta3	71.4(7)	C76-C71-Ta3	125.7(9)
C73-C72-C71	109.2(11)	C73-C72-C77	129.2(12)	C71-C72-C77	121.4(11)
C73-C72-Ta3	75.9(7)	C71-C72-Ta3	74.2(7)	C77-C72-Ta3	120.5(8)
C74-C73-C72	107.0(12)	C74-C73-C78	128.0(13)	C72-C73-C78	124.9(12)
C74-C73-Ta3	74.8(8)	C72-C73-Ta3	70.4(7)	C78-C73-Ta3	122.5(9)
C73-C74-C70	109.8(12)	C73-C74-C79	126.5(13)	C70-C74-C79	122.6(13)
C73-C74-Ta3	73.1(8)	C70-C74-Ta3	72.4(8)	C79-C74-Ta3	130.3(9)

C81-C80-C84	107.3(12)	C81-C80-C85	129.5(13)	C84-C80-C85	123.0(13)
C81-C80-Ta4	70.5(7)	C84-C80-Ta4	72.6(8)	C85-C80-Ta4	125.1(9)
C82-C81-C80	110.3(12)	C82-C81-C86	122.6(13)	C80-C81-C86	126.7(13)
C82-C81-Ta4	72.1(7)	C80-C81-Ta4	76.1(7)	C86-C81-Ta4	124.1(9)
C81-C82-C83	106.4(12)	C81-C82-C87	127.8(13)	C83-C82-C87	125.3(13)
C81-C82-Ta4	74.4(7)	C83-C82-Ta4	73.9(7)	C87-C82-Ta4	123.1(9)
C84-C83-C82	108.6(12)	C84-C83-C88	122.1(13)	C82-C83-C88	129.3(13)
C84-C83-Ta4	75.0(8)	C82-C83-Ta4	71.5(7)	C88-C83-Ta4	122.0(9)
C80-C84-C83	107.4(12)	C80-C84-C89	125.8(13)	C83-C84-C89	125.6(13)
C80-C84-Ta4	74.3(8)	C83-C84-Ta4	71.3(8)	C89-C84-Ta4	129.5(9)

Table 6. Torsion angles (°) for **9a**.

N2-Ta2-O12-Ta1	-19.0(4)	N22-Ta2-O12-Ta1	71.3(7)	N21-Ta2-O12-Ta1	115.2(4)
N1-Ta2-O12-Ta1	19.8(4)	C52-Ta2-O12-Ta1	-99.9(4)	C51-Ta2-O12-Ta1	-103.7(5)
C53-Ta2-O12-Ta1	-129.5(4)	C54-Ta2-O12-Ta1	-155.5(4)	C50-Ta2-O12-Ta1	-147.4(4)
C20-Ta2-O12-Ta1	95.2(4)	N1-Ta1-O12-Ta2	-23.6(4)	N12-Ta1-O12-Ta2	76.4(6)
N2-Ta1-O12-Ta2	16.1(3)	N11-Ta1-O12-Ta2	116.8(4)	C62-Ta1-O12-Ta2	-107.6(4)
C61-Ta1-O12-Ta2	-102.0(5)	C63-Ta1-O12-Ta2	-139.9(4)	C60-Ta1-O12-Ta2	-142.2(5)
C64-Ta1-O12-Ta2	-160.3(4)	C10-Ta1-O12-Ta2	102.5(4)	O12-Ta1-N1-N2	77.3(6)
N12-Ta1-N1-N2	-62.2(7)	N11-Ta1-N1-N2	-15.3(11)	C62-Ta1-N1-N2	170.4(7)
C61-Ta1-N1-N2	-156.9(7)	C63-Ta1-N1-N2	160.9(6)	C60-Ta1-N1-N2	-140.7(6)
C64-Ta1-N1-N2	-165.3(6)	C10-Ta1-N1-N2	-45.7(8)	Ta2-Ta1-N1-N2	57.1(5)
O12-Ta1-N1-Ta2	20.2(3)	N12-Ta1-N1-Ta2	-119.3(4)	N2-Ta1-N1-Ta2	-57.1(5)
N11-Ta1-N1-Ta2	-72.4(7)	C62-Ta1-N1-Ta2	113.3(4)	C61-Ta1-N1-Ta2	146.0(4)
C63-Ta1-N1-Ta2	103.8(4)	C60-Ta1-N1-Ta2	162.3(4)	C64-Ta1-N1-Ta2	137.7(5)
C10-Ta1-N1-Ta2	-102.8(4)	O12-Ta2-N1-N2	-104.7(6)	N22-Ta2-N1-N2	106.1(7)
N21-Ta2-N1-N2	162.1(6)	C52-Ta2-N1-N2	-10.7(8)	C51-Ta2-N1-N2	28.6(8)
C53-Ta2-N1-N2	-43.5(10)	C50-Ta2-N1-N2	59.1(10)	C20-Ta2-N1-N2	134.9(7)
Ta1-Ta2-N1-N2	-84.1(7)	N2-Ta2-N1-Ta1	84.1(6)	O12-Ta2-N1-Ta1	-20.6(4)
N22-Ta2-N1-Ta1	-169.8(5)	N21-Ta2-N1-Ta1	-113.8(4)	C52-Ta2-N1-Ta1	73.4(5)
C51-Ta2-N1-Ta1	112.7(5)	C53-Ta2-N1-Ta1	40.5(8)	C50-Ta2-N1-Ta1	143.2(6)
C20-Ta2-N1-Ta1	-141.1(4)	Ta1-N1-N2-Ta2	-90.1(4)	Ta2-N1-N2-Ta1	90.1(4)
O12-Ta2-N2-N1	73.1(6)	N22-Ta2-N2-N1	-67.9(6)	N21-Ta2-N2-N1	-25.0(9)
C52-Ta2-N2-N1	170.7(7)	C51-Ta2-N2-N1	-155.6(7)	C53-Ta2-N2-N1	154.9(6)
C54-Ta2-N2-N1	-178.4(6)	C50-Ta2-N2-N1	-146.5(6)	C20-Ta2-N2-N1	-48.2(7)
Ta1-Ta2-N2-N1	56.6(6)	O12-Ta2-N2-Ta1	16.4(3)	N22-Ta2-N2-Ta1	-124.5(4)
N21-Ta2-N2-Ta1	-81.7(6)	N1-Ta2-N2-Ta1	-56.6(6)	C52-Ta2-N2-Ta1	114.1(4)
C51-Ta2-N2-Ta1	147.8(4)	C53-Ta2-N2-Ta1	98.3(4)	C54-Ta2-N2-Ta1	125.0(5)
C50-Ta2-N2-Ta1	156.9(4)	C20-Ta2-N2-Ta1	-104.8(4)	O12-Ta1-N2-N1	-100.4(7)
N12-Ta1-N2-N1	115.4(7)	N11-Ta1-N2-N1	170.1(7)	C62-Ta1-N2-N1	-11.6(8)
C61-Ta1-N2-N1	25.7(8)	C63-Ta1-N2-N1	-39.4(12)	C60-Ta1-N2-N1	59.2(9)
C64-Ta1-N2-N1	63(2)	C10-Ta1-N2-N1	142.2(7)	Ta2-Ta1-N2-N1	-83.9(7)
N1-Ta1-N2-Ta2	83.9(7)	O12-Ta1-N2-Ta2	-16.4(4)	N12-Ta1-N2-Ta2	-160.7(4)
N11-Ta1-N2-Ta2	-106.0(4)	C62-Ta1-N2-Ta2	72.3(5)	C61-Ta1-N2-Ta2	109.6(5)
C63-Ta1-N2-Ta2	44.5(10)	C60-Ta1-N2-Ta2	143.1(5)	C64-Ta1-N2-Ta2	147.3(18)
C10-Ta1-N2-Ta2	-133.9(4)	N1-Ta1-N11-C10	-61.1(11)	O12-Ta1-N11-C10	-153.6(8)
N12-Ta1-N11-C10	-3.3(7)	N2-Ta1-N11-C10	-71.1(8)	C62-Ta1-N11-C10	110.9(9)
C61-Ta1-N11-C10	67.3(9)	C63-Ta1-N11-C10	122.4(8)	C60-Ta1-N11-C10	67.6(8)
C64-Ta1-N11-C10	97.3(8)	Ta2-Ta1-N11-C10	-113.7(7)	N1-Ta1-N11-C12	141.7(13)
O12-Ta1-N11-C12	49.2(14)	N12-Ta1-N11-C12	-160.5(15)	N2-Ta1-N11-C12	131.7(14)
C62-Ta1-N11-C12	-46.3(16)	C61-Ta1-N11-C12	-89.9(15)	C63-Ta1-N11-C12	-34.8(15)
C60-Ta1-N11-C12	-89.6(14)	C64-Ta1-N11-C12	-59.9(14)	C10-Ta1-N11-C12	-157.2(19)
Ta2-Ta1-N11-C12	89.0(14)	N1-Ta1-N12-C10	150.5(8)	O12-Ta1-N12-C10	52.3(10)
N2-Ta1-N12-C10	114.3(8)	N11-Ta1-N12-C10	3.3(7)	C62-Ta1-N12-C10	-122.7(8)
C61-Ta1-N12-C10	-129.0(8)	C63-Ta1-N12-C10	-80.0(9)	C60-Ta1-N12-C10	-102.5(8)
C64-Ta1-N12-C10	-75.2(8)	Ta2-Ta1-N12-C10	100.0(8)	N1-Ta1-N12-C15	-13.5(13)
O12-Ta1-N12-C15	-111.7(13)	N2-Ta1-N12-C15	-49.7(13)	N11-Ta1-N12-C15	-160.7(14)
C62-Ta1-N12-C15	73.3(14)	C61-Ta1-N12-C15	66.9(13)	C63-Ta1-N12-C15	115.9(13)
C60-Ta1-N12-C15	93.5(13)	C64-Ta1-N12-C15	120.8(13)	C10-Ta1-N12-C15	-164.0(18)
Ta2-Ta1-N12-C15	-64.0(13)	C12-N11-C10-N12	168.4(11)	Ta1-N11-C10-N12	5.0(11)

C12-N11-C10-C11	-8.8(19)	Ta1-N11-C10-C11	-172.2(12)	C12-N11-C10-Ta1	163.4(13)
C15-N12-C10-N11	163.0(11)	Ta1-N12-C10-N11	-5.3(12)	C15-N12-C10-C11	-20(2)
Ta1-N12-C10-C11	171.7(12)	C15-N12-C10-Ta1	168.3(13)	N1-Ta1-C10-N11	139.3(8)
O12-Ta1-C10-N11	30.0(9)	N12-Ta1-C10-N11	174.2(13)	N2-Ta1-C10-N11	111.6(8)
C62-Ta1-C10-N11	-101.7(9)	C61-Ta1-C10-N11	-128.5(8)	C63-Ta1-C10-N11	-67.6(8)
C60-Ta1-C10-N11	-112.8(8)	C64-Ta1-C10-N11	-80.2(8)	Ta2-Ta1-C10-N11	78.7(8)
N1-Ta1-C10-N12	-34.9(9)	O12-Ta1-C10-N12	-144.3(7)	N2-Ta1-C10-N12	-62.7(8)
N11-Ta1-C10-N12	-174.2(13)	C62-Ta1-C10-N12	84.1(10)	C61-Ta1-C10-N12	57.3(9)
C63-Ta1-C10-N12	118.2(8)	C60-Ta1-C10-N12	72.9(8)	C64-Ta1-C10-N12	105.6(8)
Ta2-Ta1-C10-N12	-95.6(8)	C10-N11-C12-C13	-162.0(13)	Ta1-N11-C12-C13	-10(2)
C10-N11-C12-C14	73.1(17)	Ta1-N11-C12-C14	-134.5(13)	C10-N12-C15-C17	-66.0(17)
Ta1-N12-C15-C17	95.4(16)	C10-N12-C15-C16	171.1(12)	Ta1-N12-C15-C16	-27.5(19)
N2-Ta2-N21-C20	-46.4(10)	O12-Ta2-N21-C20	-143.8(8)	N22-Ta2-N21-C20	5.7(7)
N1-Ta2-N21-C20	-62.4(8)	C52-Ta2-N21-C20	107.3(9)	C51-Ta2-N21-C20	70.1(9)
C53-Ta2-N21-C20	133.6(8)	C54-Ta2-N21-C20	115.0(8)	C50-Ta2-N21-C20	83.0(8)
Ta1-Ta2-N21-C20	-102.5(7)	N2-Ta2-N21-C22	124.9(15)	O12-Ta2-N21-C22	27.5(15)
N22-Ta2-N21-C22	177.0(17)	N1-Ta2-N21-C22	108.9(15)	C52-Ta2-N21-C22	-81.4(16)
C51-Ta2-N21-C22	-118.6(15)	C53-Ta2-N21-C22	-55.1(16)	C54-Ta2-N21-C22	-73.7(15)
C50-Ta2-N21-C22	-105.7(15)	C20-Ta2-N21-C22	171(2)	Ta1-Ta2-N21-C22	68.8(15)
N2-Ta2-N22-C20	139.2(8)	O12-Ta2-N22-C20	47.4(11)	N21-Ta2-N22-C20	-6.0(8)
N1-Ta2-N22-C20	100.8(9)	C52-Ta2-N22-C20	-142.7(8)	C51-Ta2-N22-C20	-136.3(9)
C53-Ta2-N22-C20	-103.1(9)	C54-Ta2-N22-C20	-84.6(9)	C50-Ta2-N22-C20	-104.8(9)
Ta1-Ta2-N22-C20	93.3(8)	N2-Ta2-N22-C25	-19.0(12)	O12-Ta2-N22-C25	-110.8(12)
N21-Ta2-N22-C25	-164.3(14)	N1-Ta2-N22-C25	-57.5(12)	C52-Ta2-N22-C25	59.1(13)
C51-Ta2-N22-C25	65.4(12)	C53-Ta2-N22-C25	98.6(13)	C54-Ta2-N22-C25	117.2(12)
C50-Ta2-N22-C25	96.9(12)	C20-Ta2-N22-C25	-158.3(17)	Ta1-Ta2-N22-C25	-64.9(12)
C25-N22-C20-N21	169.9(12)	Ta2-N22-C20-N21	9.3(12)	C25-N22-C20-C21	-10(2)
Ta2-N22-C20-C21	-170.4(13)	C25-N22-C20-Ta2	160.6(15)	C22-N21-C20-N22	177.3(12)
Ta2-N21-C20-N22	-9.0(11)	C22-N21-C20-C21	-3(2)	Ta2-N21-C20-C21	170.7(11)
C22-N21-C20-Ta2	-173.7(15)	N2-Ta2-C20-N22	-44.0(9)	O12-Ta2-C20-N22	-148.2(8)
N21-Ta2-C20-N22	169.8(13)	N1-Ta2-C20-N22	-73.2(9)	C52-Ta2-C20-N22	56.1(11)
C51-Ta2-C20-N22	46.6(9)	C53-Ta2-C20-N22	105.6(9)	C54-Ta2-C20-N22	102.4(9)
C50-Ta2-C20-N22	72.5(9)	Ta1-Ta2-C20-N22	-100.1(8)	N2-Ta2-C20-N21	146.2(8)
O12-Ta2-C20-N21	41.9(9)	N22-Ta2-C20-N21	-169.8(13)	N1-Ta2-C20-N21	117.0(8)
C52-Ta2-C20-N21	-113.8(9)	C51-Ta2-C20-N21	-123.2(8)	C53-Ta2-C20-N21	-64.2(9)
C54-Ta2-C20-N21	-67.4(8)	C50-Ta2-C20-N21	-97.3(8)	Ta1-Ta2-C20-N21	90.0(8)
C20-N21-C22-C24	-66.6(17)	Ta2-N21-C22-C24	124.0(14)	C20-N21-C22-C23	169.2(13)
Ta2-N21-C22-C23	0(2)	C20-N22-C25-C26	-56.3(19)	Ta2-N22-C25-C26	96.5(14)
C20-N22-C25-C27	74.5(17)	Ta2-N22-C25-C27	-132.8(11)	N2-Ta2-C50-C51	-17.2(9)
O12-Ta2-C50-C51	102.8(9)	N22-Ta2-C50-C51	-100.7(8)	N21-Ta2-C50-C51	-159.1(8)
N1-Ta2-C50-C51	-55.1(11)	C52-Ta2-C50-C51	38.6(8)	C53-Ta2-C50-C51	80.8(9)
C54-Ta2-C50-C51	117.9(12)	C20-Ta2-C50-C51	-128.7(8)	Ta1-Ta2-C50-C51	34.1(13)
N2-Ta2-C50-C54	-135.2(7)	O12-Ta2-C50-C54	-15.1(10)	N22-Ta2-C50-C54	141.3(8)
N21-Ta2-C50-C54	82.9(8)	N1-Ta2-C50-C54	-173.1(7)	C52-Ta2-C50-C54	-79.3(8)
C51-Ta2-C50-C54	-117.9(12)	C53-Ta2-C50-C54	-37.2(7)	C20-Ta2-C50-C54	113.4(8)
Ta1-Ta2-C50-C54	-83.9(11)	N2-Ta2-C50-C55	105.3(12)	O12-Ta2-C50-C55	-134.7(11)
N22-Ta2-C50-C55	21.7(11)	N21-Ta2-C50-C55	-36.7(12)	N1-Ta2-C50-C55	67.4(14)
C52-Ta2-C50-C55	161.1(14)	C51-Ta2-C50-C55	122.5(15)	C53-Ta2-C50-C55	-156.8(14)
C54-Ta2-C50-C55	-119.6(15)	C20-Ta2-C50-C55	-6.2(12)	Ta1-Ta2-C50-C55	156.5(8)
C54-C50-C51-C52	-3.0(16)	C55-C50-C51-C52	174.0(13)	Ta2-C50-C51-C52	-66.3(9)
C54-C50-C51-C56	-176.7(13)	C55-C50-C51-C56	0(2)	Ta2-C50-C51-C56	120.0(14)
C54-C50-C51-Ta2	63.3(10)	C55-C50-C51-Ta2	-119.7(14)	N2-Ta2-C51-C50	164.4(8)
O12-Ta2-C51-C50	-107.2(9)	N22-Ta2-C51-C50	75.9(8)	N21-Ta2-C51-C50	24.9(10)
N1-Ta2-C51-C50	146.2(8)	C52-Ta2-C51-C50	-114.0(11)	C53-Ta2-C51-C50	-75.5(9)
C54-Ta2-C51-C50	-35.5(8)	C20-Ta2-C51-C50	55.3(9)	Ta1-Ta2-C51-C50	-163.8(7)
N2-Ta2-C51-C52	-81.6(8)	O12-Ta2-C51-C52	6.7(10)	N22-Ta2-C51-C52	-170.1(8)
N21-Ta2-C51-C52	138.9(7)	N1-Ta2-C51-C52	-99.8(8)	C53-Ta2-C51-C52	38.4(7)
C54-Ta2-C51-C52	78.5(8)	C50-Ta2-C51-C52	114.0(11)	C20-Ta2-C51-C52	169.2(7)
Ta1-Ta2-C51-C52	-49.9(8)	N2-Ta2-C51-C56	36.9(11)	O12-Ta2-C51-C56	125.3(10)
N22-Ta2-C51-C56	-51.6(11)	N21-Ta2-C51-C56	-102.6(11)	N1-Ta2-C51-C56	18.8(13)
C52-Ta2-C51-C56	118.5(14)	C53-Ta2-C51-C56	157.0(13)	C54-Ta2-C51-C56	-162.9(13)
C50-Ta2-C51-C56	-127.5(15)	C20-Ta2-C51-C56	-72.2(11)	Ta1-Ta2-C51-C56	68.7(11)

C50-C51-C52-C53	1.0(15)	C56-C51-C52-C53	175.1(12)	Ta2-C51-C52-C53	-68.5(8)
C50-C51-C52-C57	-175.2(12)	C56-C51-C52-C57	-1(2)	Ta2-C51-C52-C57	115.3(12)
C50-C51-C52-Ta2	69.4(10)	C56-C51-C52-Ta2	-116.5(13)	N2-Ta2-C52-C51	93.9(8)
O12-Ta2-C52-C51	-174.9(7)	N22-Ta2-C52-C51	11.5(9)	N21-Ta2-C52-C51	-67.2(10)
N1-Ta2-C52-C51	100.8(8)	C53-Ta2-C52-C51	-113.3(11)	C54-Ta2-C52-C51	-76.6(8)
C50-Ta2-C52-C51	-36.8(7)	C20-Ta2-C52-C51	-16.4(11)	Ta1-Ta2-C52-C51	141.3(7)
N2-Ta2-C52-C53	-152.8(8)	O12-Ta2-C52-C53	-61.6(8)	N22-Ta2-C52-C53	124.8(8)
N21-Ta2-C52-C53	46.1(11)	N1-Ta2-C52-C53	-145.9(7)	C51-Ta2-C52-C53	113.3(11)
C54-Ta2-C52-C53	36.7(7)	C50-Ta2-C52-C53	76.5(8)	C20-Ta2-C52-C53	96.9(9)
Ta1-Ta2-C52-C53	-105.4(7)	N2-Ta2-C52-C57	-27.3(10)	O12-Ta2-C52-C57	63.9(10)
N22-Ta2-C52-C57	-109.7(10)	N21-Ta2-C52-C57	171.6(8)	N1-Ta2-C52-C57	-20.3(12)
C51-Ta2-C52-C57	-121.2(13)	C53-Ta2-C52-C57	125.5(14)	C54-Ta2-C52-C57	162.2(12)
C50-Ta2-C52-C57	-158.0(12)	C20-Ta2-C52-C57	-137.5(9)	Ta1-Ta2-C52-C57	20.2(10)
C51-C52-C53-C54	1.4(14)	C57-C52-C53-C54	177.5(11)	Ta2-C52-C53-C54	-66.2(9)
C51-C52-C53-C58	-178.2(13)	C57-C52-C53-C58	-2(2)	Ta2-C52-C53-C58	114.1(13)
C51-C52-C53-Ta2	67.6(9)	C57-C52-C53-Ta2	-116.3(12)	N2-Ta2-C53-C54	143.5(7)
O12-Ta2-C53-C54	-127.0(8)	N22-Ta2-C53-C54	34.7(10)	N21-Ta2-C53-C54	-36.5(8)
N1-Ta2-C53-C54	172.0(7)	C52-Ta2-C53-C54	114.7(11)	C51-Ta2-C53-C54	76.5(8)
C50-Ta2-C53-C54	36.8(7)	C20-Ta2-C53-C54	-5.8(10)	Ta1-Ta2-C53-C54	-161.0(6)
N2-Ta2-C53-C52	28.8(9)	O12-Ta2-C53-C52	118.3(8)	N22-Ta2-C53-C52	-80.0(9)
N21-Ta2-C53-C52	-151.2(7)	N1-Ta2-C53-C52	57.3(11)	C51-Ta2-C53-C52	-38.3(7)
C54-Ta2-C53-C52	-114.7(11)	C50-Ta2-C53-C52	-77.9(8)	C20-Ta2-C53-C52	-120.6(8)
Ta1-Ta2-C53-C52	84.3(7)	N2-Ta2-C53-C58	-93.6(11)	O12-Ta2-C53-C58	-4.1(10)
N22-Ta2-C53-C58	157.6(10)	N21-Ta2-C53-C58	86.4(11)	N1-Ta2-C53-C58	-65.1(13)
C52-Ta2-C53-C58	-122.4(14)	C51-Ta2-C53-C58	-160.7(13)	C54-Ta2-C53-C58	122.9(14)
C50-Ta2-C53-C58	159.7(13)	C20-Ta2-C53-C58	117.0(11)	Ta1-Ta2-C53-C58	-38.1(11)
C51-C50-C54-C53	4.0(15)	C55-C50-C54-C53	-173.2(12)	Ta2-C50-C54-C53	66.0(9)
C51-C50-C54-C59	169.6(12)	C55-C50-C54-C59	-8(2)	Ta2-C50-C54-C59	-128.4(12)
C51-C50-C54-Ta2	-62.0(10)	C55-C50-C54-Ta2	120.8(13)	C52-C53-C54-C50	-3.3(14)
C58-C53-C54-C50	176.4(13)	Ta2-C53-C54-C50	-67.2(9)	C52-C53-C54-C59	-169.1(11)
C58-C53-C54-C59	11(2)	Ta2-C53-C54-C59	127.0(12)	C52-C53-C54-Ta2	63.9(8)
C58-C53-C54-Ta2	-116.4(13)	N2-Ta2-C54-C50	63.7(10)	O12-Ta2-C54-C50	168.7(7)
N22-Ta2-C54-C50	-39.8(8)	N21-Ta2-C54-C50	-97.4(8)	C52-Ta2-C54-C50	76.9(8)
C51-Ta2-C54-C50	35.3(8)	C53-Ta2-C54-C50	115.1(11)	C20-Ta2-C54-C50	-69.2(8)
Ta1-Ta2-C54-C50	143.1(6)	N2-Ta2-C54-C53	-51.4(9)	O12-Ta2-C54-C53	53.7(8)
N22-Ta2-C54-C53	-154.9(7)	N21-Ta2-C54-C53	147.5(7)	C52-Ta2-C54-C53	-38.1(7)
C51-Ta2-C54-C53	-79.7(8)	C50-Ta2-C54-C53	-115.1(11)	C20-Ta2-C54-C53	175.7(7)
Ta1-Ta2-C54-C53	28.0(9)	N2-Ta2-C54-C59	-172.3(11)	O12-Ta2-C54-C59	-67.3(12)
N22-Ta2-C54-C59	84.2(12)	N21-Ta2-C54-C59	26.6(12)	C52-Ta2-C54-C59	-159.1(14)
C51-Ta2-C54-C59	159.3(14)	C53-Ta2-C54-C59	-121.0(15)	C50-Ta2-C54-C59	124.0(15)
C20-Ta2-C54-C59	54.7(12)	Ta1-Ta2-C54-C59	-92.9(12)	N1-Ta1-C60-C61	-31.2(10)
O12-Ta1-C60-C61	81.5(10)	N12-Ta1-C60-C61	-123.3(9)	N2-Ta1-C60-C61	-67.1(10)
N11-Ta1-C60-C61	-179.6(9)	C62-Ta1-C60-C61	36.9(8)	C63-Ta1-C60-C61	78.6(9)
C64-Ta1-C60-C61	114.5(12)	C10-Ta1-C60-C61	-152.3(9)	Ta2-Ta1-C60-C61	3.3(14)
N1-Ta1-C60-C64	-145.7(8)	O12-Ta1-C60-C64	-33.0(11)	N12-Ta1-C60-C64	122.2(8)
N2-Ta1-C60-C64	178.4(7)	N11-Ta1-C60-C64	65.9(8)	C62-Ta1-C60-C64	-77.6(8)
C61-Ta1-C60-C64	-114.5(12)	C63-Ta1-C60-C64	-35.9(7)	C10-Ta1-C60-C64	93.2(8)
Ta2-Ta1-C60-C64	-111.2(9)	N1-Ta1-C60-C65	95.4(13)	O12-Ta1-C60-C65	-151.9(11)
N12-Ta1-C60-C65	3.3(12)	N2-Ta1-C60-C65	59.5(14)	N11-Ta1-C60-C65	-53.0(13)
C62-Ta1-C60-C65	163.5(15)	C61-Ta1-C60-C65	126.6(17)	C63-Ta1-C60-C65	-154.8(14)
C64-Ta1-C60-C65	-118.9(16)	C10-Ta1-C60-C65	-25.7(13)	Ta2-Ta1-C60-C65	129.9(10)
C64-C60-C61-C62	1.8(16)	C65-C60-C61-C62	174.4(14)	Ta1-C60-C61-C62	-64.3(10)
C64-C60-C61-C66	-171.4(14)	C65-C60-C61-C66	1(3)	Ta1-C60-C61-C66	122.5(15)
C64-C60-C61-Ta1	66.1(10)	C65-C60-C61-Ta1	-121.3(16)	N1-Ta1-C61-C62	-94.4(8)
O12-Ta1-C61-C62	-10.4(10)	N12-Ta1-C61-C62	170.7(8)	N2-Ta1-C61-C62	-111.0(8)
N11-Ta1-C61-C62	116.2(8)	C63-Ta1-C61-C62	38.1(8)	C60-Ta1-C61-C62	115.7(12)
C64-Ta1-C61-C62	78.1(9)	C10-Ta1-C61-C62	146.0(8)	Ta2-Ta1-C61-C62	-62.6(8)
N1-Ta1-C61-C60	150.0(9)	O12-Ta1-C61-C60	-126.1(8)	N12-Ta1-C61-C60	55.0(9)
N2-Ta1-C61-C60	133.3(8)	N11-Ta1-C61-C60	0.5(11)	C62-Ta1-C61-C60	-115.7(12)
C63-Ta1-C61-C60	-77.6(9)	C64-Ta1-C61-C60	-37.6(8)	C10-Ta1-C61-C60	30.3(10)
Ta2-Ta1-C61-C60	-178.3(7)	N1-Ta1-C61-C66	23.4(11)	O12-Ta1-C61-C66	107.3(11)
N12-Ta1-C61-C66	-71.6(12)	N2-Ta1-C61-C66	6.7(13)	N11-Ta1-C61-C66	-126.1(11)

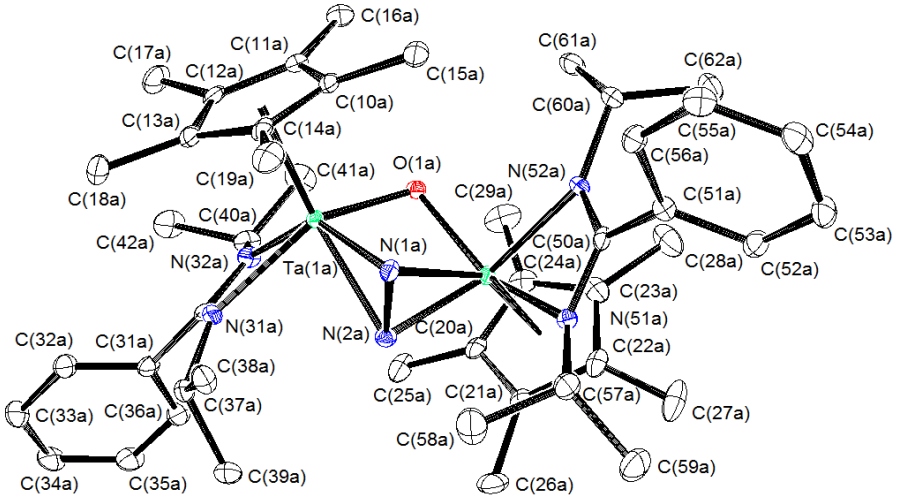
C62-Ta1-C61-C66	117.7(15)	C63-Ta1-C61-C66	155.8(13)	C60-Ta1-C61-C66	-126.6(16)
C64-Ta1-C61-C66	-164.2(14)	C10-Ta1-C61-C66	-96.3(11)	Ta2-Ta1-C61-C66	55.1(12)
C60-C61-C62-C63	-1.8(16)	C66-C61-C62-C63	171.7(12)	Ta1-C61-C62-C63	-69.5(8)
C60-C61-C62-C67	-175.8(11)	C66-C61-C62-C67	-2(2)	Ta1-C61-C62-C67	116.5(12)
C60-C61-C62-Ta1	67.7(10)	C66-C61-C62-Ta1	-118.8(13)	N1-Ta1-C62-C61	80.9(8)
O12-Ta1-C62-C61	171.5(8)	N12-Ta1-C62-C61	-11.7(10)	N2-Ta1-C62-C61	88.5(8)
N11-Ta1-C62-C61	-93.9(9)	C63-Ta1-C62-C61	-114.5(12)	C60-Ta1-C62-C61	-36.4(8)
C64-Ta1-C62-C61	-77.1(8)	C10-Ta1-C62-C61	-50.2(11)	Ta2-Ta1-C62-C61	129.5(7)
N1-Ta1-C62-C63	-164.5(9)	O12-Ta1-C62-C63	-73.9(8)	N12-Ta1-C62-C63	102.8(9)
N2-Ta1-C62-C63	-157.0(7)	N11-Ta1-C62-C63	20.6(11)	C61-Ta1-C62-C63	114.5(12)
C60-Ta1-C62-C63	78.1(9)	C64-Ta1-C62-C63	37.4(8)	C10-Ta1-C62-C63	64.4(10)
Ta2-Ta1-C62-C63	-116.0(7)	N1-Ta1-C62-C67	-40.3(10)	O12-Ta1-C62-C67	50.3(10)
N12-Ta1-C62-C67	-133.0(10)	N2-Ta1-C62-C67	-32.8(12)	N11-Ta1-C62-C67	144.8(9)
C61-Ta1-C62-C67	-121.3(14)	C63-Ta1-C62-C67	124.2(14)	C60-Ta1-C62-C67	-157.7(12)
C64-Ta1-C62-C67	161.6(12)	C10-Ta1-C62-C67	-171.5(9)	Ta2-Ta1-C62-C67	8.2(11)
C61-C62-C63-C64	1.0(14)	C67-C62-C63-C64	174.8(12)	Ta1-C62-C63-C64	-68.6(9)
C61-C62-C63-C68	-178.5(12)	C67-C62-C63-C68	-5(2)	Ta1-C62-C63-C68	111.9(12)
C61-C62-C63-Ta1	69.6(9)	C67-C62-C63-Ta1	-116.6(12)	N1-Ta1-C63-C64	130.2(8)
O12-Ta1-C63-C64	-141.7(8)	N12-Ta1-C63-C64	9.1(10)	N2-Ta1-C63-C64	157.6(9)
N11-Ta1-C63-C64	-52.2(8)	C62-Ta1-C63-C64	113.0(12)	C61-Ta1-C63-C64	76.1(8)
C60-Ta1-C63-C64	36.3(8)	C10-Ta1-C63-C64	-24.2(9)	Ta2-Ta1-C63-C64	-171.0(7)
N1-Ta1-C63-C62	17.2(9)	O12-Ta1-C63-C62	105.2(8)	N12-Ta1-C63-C62	-104.0(8)
N2-Ta1-C63-C62	44.6(13)	N11-Ta1-C63-C62	-165.3(8)	C61-Ta1-C63-C62	-36.9(8)
C60-Ta1-C63-C62	-76.7(9)	C64-Ta1-C63-C62	-113.0(12)	C10-Ta1-C63-C62	-137.2(8)
Ta2-Ta1-C63-C62	76.0(8)	N1-Ta1-C63-C68	-104.9(10)	O12-Ta1-C63-C68	-16.8(10)
N12-Ta1-C63-C68	134.0(10)	N2-Ta1-C63-C68	-77.5(13)	N11-Ta1-C63-C68	72.7(10)
C62-Ta1-C63-C68	-122.1(14)	C61-Ta1-C63-C68	-159.0(12)	C60-Ta1-C63-C68	161.2(12)
C64-Ta1-C63-C68	124.9(14)	C10-Ta1-C63-C68	100.7(10)	Ta2-Ta1-C63-C68	-46.1(10)
C62-C63-C64-C60	0.1(14)	C68-C63-C64-C60	179.6(12)	Ta1-C63-C64-C60	-64.4(10)
C62-C63-C64-C69	-169.0(13)	C68-C63-C64-C69	11(2)	Ta1-C63-C64-C69	126.5(14)
C62-C63-C64-Ta1	64.5(8)	C68-C63-C64-Ta1	-115.9(12)	C61-C60-C64-C63	-1.1(15)
C65-C60-C64-C63	-174.4(13)	Ta1-C60-C64-C63	63.3(9)	C61-C60-C64-C69	168.5(13)
C65-C60-C64-C69	-5(2)	Ta1-C60-C64-C69	-127.1(13)	C61-C60-C64-Ta1	-64.4(10)
C65-C60-C64-Ta1	122.3(14)	N1-Ta1-C64-C63	-69.6(10)	O12-Ta1-C64-C63	40.7(8)
N12-Ta1-C64-C63	-172.8(8)	N2-Ta1-C64-C63	-122.2(19)	N11-Ta1-C64-C63	129.2(8)
C62-Ta1-C64-C63	-39.0(7)	C61-Ta1-C64-C63	-79.8(8)	C60-Ta1-C64-C63	-116.8(11)
C10-Ta1-C64-C63	158.6(8)	Ta2-Ta1-C64-C63	15.3(11)	N1-Ta1-C64-C60	47.2(10)
O12-Ta1-C64-C60	157.4(8)	N12-Ta1-C64-C60	-56.0(8)	N2-Ta1-C64-C60	-5(2)
N11-Ta1-C64-C60	-114.0(8)	C62-Ta1-C64-C60	77.7(9)	C61-Ta1-C64-C60	37.0(8)
C63-Ta1-C64-C60	116.8(11)	C10-Ta1-C64-C60	-84.6(8)	Ta2-Ta1-C64-C60	132.1(7)
N1-Ta1-C64-C69	166.9(12)	O12-Ta1-C64-C69	-82.9(13)	N12-Ta1-C64-C69	63.7(13)
N2-Ta1-C64-C69	114(2)	N11-Ta1-C64-C69	5.7(13)	C62-Ta1-C64-C69	-162.6(15)
C61-Ta1-C64-C69	156.7(15)	C63-Ta1-C64-C69	-123.5(17)	C60-Ta1-C64-C69	119.7(17)
C10-Ta1-C64-C69	35.1(13)	Ta2-Ta1-C64-C69	-108.2(13)	N3-Ta3-O34-Ta4	-23.2(4)
N32-Ta3-O34-Ta4	79.2(6)	N4-Ta3-O34-Ta4	17.4(3)	N31-Ta3-O34-Ta4	117.6(4)
C72-Ta3-O34-Ta4	-106.1(4)	C71-Ta3-O34-Ta4	-100.0(5)	C70-Ta3-O34-Ta4	-142.4(4)
C73-Ta3-O34-Ta4	-138.7(4)	C74-Ta3-O34-Ta4	-159.2(4)	N4-Ta4-O34-Ta3	-20.2(4)
N3-Ta4-O34-Ta3	20.2(4)	N41-Ta4-O34-Ta3	117.0(4)	N42-Ta4-O34-Ta3	76.6(6)
C82-Ta4-O34-Ta3	-99.2(4)	C81-Ta4-O34-Ta3	-102.8(5)	C83-Ta4-O34-Ta3	-129.8(4)
C84-Ta4-O34-Ta3	-156.4(4)	C80-Ta4-O34-Ta3	-147.3(4)	C40-Ta4-O34-Ta3	98.4(4)
O34-Ta3-N3-N4	78.9(6)	N32-Ta3-N3-N4	-61.0(7)	N31-Ta3-N3-N4	-12.7(10)
C72-Ta3-N3-N4	170.1(7)	C71-Ta3-N3-N4	-155.3(7)	C70-Ta3-N3-N4	-140.3(6)
C73-Ta3-N3-N4	160.4(6)	C74-Ta3-N3-N4	-166.8(6)	Ta4-Ta3-N3-N4	58.5(5)
O34-Ta3-N3-Ta4	20.4(3)	N32-Ta3-N3-Ta4	-119.5(4)	N4-Ta3-N3-Ta4	-58.5(5)
N31-Ta3-N3-Ta4	-71.3(7)	C72-Ta3-N3-Ta4	111.5(4)	C71-Ta3-N3-Ta4	146.1(4)
C70-Ta3-N3-Ta4	161.2(4)	C73-Ta3-N3-Ta4	101.9(4)	C74-Ta3-N3-Ta4	134.6(5)
O34-Ta4-N3-N4	-101.4(6)	N41-Ta4-N3-N4	165.2(6)	N42-Ta4-N3-N4	110.8(6)
C82-Ta4-N3-N4	-9.3(8)	C81-Ta4-N3-N4	29.7(8)	C83-Ta4-N3-N4	-42.8(10)
C80-Ta4-N3-N4	62.9(10)	C40-Ta4-N3-N4	139.6(7)	Ta3-Ta4-N3-N4	-81.1(6)
N4-Ta4-N3-Ta3	81.1(6)	O34-Ta4-N3-Ta3	-20.3(3)	N41-Ta4-N3-Ta3	-113.7(4)
N42-Ta4-N3-Ta3	-168.1(4)	C82-Ta4-N3-Ta3	71.8(5)	C81-Ta4-N3-Ta3	110.8(5)
C83-Ta4-N3-Ta3	38.3(8)	C80-Ta4-N3-Ta3	144.0(6)	C40-Ta4-N3-Ta3	-139.3(4)

Ta3-N3-N4-Ta4	-91.6(4)	Ta4-N3-N4-Ta3	91.6(4)	O34-Ta4-N4-N3	75.9(6)
N41-Ta4-N4-N3	-21.8(9)	N42-Ta4-N4-N3	-65.8(6)	C82-Ta4-N4-N3	171.8(7)
C81-Ta4-N4-N3	-154.6(7)	C83-Ta4-N4-N3	155.4(6)	C84-Ta4-N4-N3	-178.0(6)
C80-Ta4-N4-N3	-144.6(6)	C40-Ta4-N4-N3	-45.1(7)	Ta3-Ta4-N4-N3	58.5(5)
O34-Ta4-N4-Ta3	17.4(3)	N3-Ta4-N4-Ta3	-58.5(5)	N41-Ta4-N4-Ta3	-80.2(6)
N42-Ta4-N4-Ta3	-124.3(4)	C82-Ta4-N4-Ta3	113.3(4)	C81-Ta4-N4-Ta3	146.9(4)
C83-Ta4-N4-Ta3	97.0(4)	C84-Ta4-N4-Ta3	123.6(5)	C80-Ta4-N4-Ta3	156.9(4)
C40-Ta4-N4-Ta3	-103.6(4)	O34-Ta3-N4-N3	-98.7(7)	N32-Ta3-N4-N3	117.4(7)
N31-Ta3-N4-N3	171.9(7)	C72-Ta3-N4-N3	-11.8(8)	C71-Ta3-N4-N3	27.2(8)
C70-Ta3-N4-N3	61.3(8)	C73-Ta3-N4-N3	-40.1(11)	C74-Ta3-N4-N3	64(2)
Ta4-Ta3-N4-N3	-80.8(7)	N3-Ta3-N4-Ta4	80.8(7)	O34-Ta3-N4-Ta4	-17.9(3)
N32-Ta3-N4-Ta4	-161.8(4)	N31-Ta3-N4-Ta4	-107.3(4)	C72-Ta3-N4-Ta4	69.0(5)
C71-Ta3-N4-Ta4	108.0(4)	C70-Ta3-N4-Ta4	142.1(5)	C73-Ta3-N4-Ta4	40.7(10)
C74-Ta3-N4-Ta4	144(2)	N3-Ta3-N31-C30	-64.8(11)	O34-Ta3-N31-C30	-156.4(8)
N32-Ta3-N31-C30	-4.8(7)	N4-Ta3-N31-C30	-73.3(8)	C72-Ta3-N31-C30	111.2(9)
C71-Ta3-N31-C30	64.2(9)	C70-Ta3-N31-C30	66.3(8)	C73-Ta3-N31-C30	121.6(8)
C74-Ta3-N31-C30	96.5(8)	Ta4-Ta3-N31-C30	-116.1(7)	N3-Ta3-N31-C32	146.0(14)
O34-Ta3-N31-C32	54.4(14)	N32-Ta3-N31-C32	-154.0(16)	N4-Ta3-N31-C32	137.5(14)
C72-Ta3-N31-C32	-38.0(17)	C71-Ta3-N31-C32	-84.9(15)	C70-Ta3-N31-C32	-82.9(15)
C73-Ta3-N31-C32	-27.6(15)	C74-Ta3-N31-C32	-52.7(15)	Ta4-Ta3-N31-C32	94.7(14)
N3-Ta3-N32-C30	151.2(8)	O34-Ta3-N32-C30	51.5(10)	N4-Ta3-N32-C30	115.1(8)
N31-Ta3-N32-C30	4.7(7)	C72-Ta3-N32-C30	-121.6(8)	C71-Ta3-N32-C30	-129.2(8)
C70-Ta3-N32-C30	-100.8(8)	C73-Ta3-N32-C30	-78.1(9)	C74-Ta3-N32-C30	-73.6(8)
Ta4-Ta3-N32-C30	101.3(7)	N3-Ta3-N32-C35	-13.0(13)	O34-Ta3-N32-C35	-112.7(12)
N4-Ta3-N32-C35	-49.1(12)	N31-Ta3-N32-C35	-159.4(14)	C72-Ta3-N32-C35	74.2(14)
C71-Ta3-N32-C35	66.7(13)	C70-Ta3-N32-C35	95.0(13)	C73-Ta3-N32-C35	117.7(12)
C74-Ta3-N32-C35	122.2(13)	Ta4-Ta3-N32-C35	-62.8(13)	C32-N31-C30-N32	165.9(11)
Ta3-N31-C30-N32	7.1(10)	C32-N31-C30-C31	-11.2(19)	Ta3-N31-C30-C31	-170.0(12)
C35-N32-C30-N31	160.8(11)	Ta3-N32-C30-N31	-7.5(11)	C35-N32-C30-C31	-21.9(18)
Ta3-N32-C30-C31	169.8(11)	C30-N31-C32-C33	-163.0(12)	Ta3-N31-C32-C33	-19(2)
C30-N31-C32-C34	76.8(17)	Ta3-N31-C32-C34	-138.9(13)	C30-N32-C35-C36	172.2(12)
Ta3-N32-C35-C36	-26.2(18)	C30-N32-C35-C37	-65.5(15)	Ta3-N32-C35-C37	96.0(15)
N4-Ta4-N41-C40	-48.0(11)	O34-Ta4-N41-C40	-144.3(8)	N3-Ta4-N41-C40	-62.4(9)
N42-Ta4-N41-C40	7.1(8)	C82-Ta4-N41-C40	109.8(10)	C81-Ta4-N41-C40	71.8(10)
C83-Ta4-N41-C40	134.9(8)	C84-Ta4-N41-C40	115.3(9)	C80-Ta4-N41-C40	82.7(9)
Ta3-Ta4-N41-C40	-103.9(8)	N4-Ta4-N41-C42	119.6(15)	O34-Ta4-N41-C42	23.3(15)
N3-Ta4-N41-C42	105.3(15)	N42-Ta4-N41-C42	174.8(17)	C82-Ta4-N41-C42	-82.5(16)
C81-Ta4-N41-C42	-120.6(14)	C83-Ta4-N41-C42	-57.5(16)	C84-Ta4-N41-C42	-77.0(15)
C80-Ta4-N41-C42	-109.7(15)	C40-Ta4-N41-C42	168(2)	Ta3-Ta4-N41-C42	63.7(15)
N4-Ta4-N42-C40	138.7(8)	O34-Ta4-N42-C40	42.7(11)	N3-Ta4-N42-C40	100.4(8)
N41-Ta4-N42-C40	-7.1(8)	C82-Ta4-N42-C40	-142.3(8)	C81-Ta4-N42-C40	-137.7(9)
C83-Ta4-N42-C40	-100.3(9)	C84-Ta4-N42-C40	-83.6(9)	C80-Ta4-N42-C40	-105.9(9)
Ta3-Ta4-N42-C40	91.3(8)	N4-Ta4-N42-C45	-10.3(14)	O34-Ta4-N42-C45	-106.3(13)
N3-Ta4-N42-C45	-48.6(14)	N41-Ta4-N42-C45	-156.1(15)	C82-Ta4-N42-C45	68.7(15)
C81-Ta4-N42-C45	73.3(14)	C83-Ta4-N42-C45	110.7(14)	C84-Ta4-N42-C45	127.4(14)
C80-Ta4-N42-C45	105.1(14)	C40-Ta4-N42-C45	-149.0(18)	Ta3-Ta4-N42-C45	-57.7(14)
C42-N41-C40-N42	177.7(12)	Ta4-N41-C40-N42	-11.5(12)	C42-N41-C40-C41	-5(2)
Ta4-N41-C40-C41	166.0(12)	C42-N41-C40-Ta4	-170.8(15)	C45-N42-C40-N41	168.4(12)
Ta4-N42-C40-N41	11.4(12)	C45-N42-C40-C41	-9(2)	Ta4-N42-C40-C41	-166.0(12)
C45-N42-C40-Ta4	157.0(13)	N4-Ta4-C40-N41	146.0(8)	O34-Ta4-C40-N41	40.9(9)
N3-Ta4-C40-N41	117.9(9)	N42-Ta4-C40-N41	-167.5(13)	C82-Ta4-C40-N41	-109.5(10)
C81-Ta4-C40-N41	-121.7(8)	C83-Ta4-C40-N41	-60.3(10)	C84-Ta4-C40-N41	-65.6(9)
C80-Ta4-C40-N41	-97.0(9)	Ta3-Ta4-C40-N41	88.7(8)	N4-Ta4-C40-N42	-46.5(9)
O34-Ta4-C40-N42	-151.6(8)	N3-Ta4-C40-N42	-74.6(8)	N41-Ta4-C40-N42	167.5(13)
C82-Ta4-C40-N42	58.0(12)	C81-Ta4-C40-N42	45.8(9)	C83-Ta4-C40-N42	107.3(9)
C84-Ta4-C40-N42	101.9(9)	C80-Ta4-C40-N42	70.5(9)	Ta3-Ta4-C40-N42	-103.7(8)
N4-Ta4-C40-C41	52(5)	O34-Ta4-C40-C41	-53(5)	N3-Ta4-C40-C41	24(5)
N41-Ta4-C40-C41	-94(5)	N42-Ta4-C40-C41	99(5)	C82-Ta4-C40-C41	157(5)
C81-Ta4-C40-C41	145(5)	C83-Ta4-C40-C41	-154(5)	C84-Ta4-C40-C41	-159(5)
C80-Ta4-C40-C41	169(5)	Ta3-Ta4-C40-C41	-5(5)	C40-N41-C42-C43	169.0(13)
Ta4-N41-C42-C43	4(2)	C40-N41-C42-C44	-66.5(18)	Ta4-N41-C42-C44	128.4(14)
C40-N42-C45-C46	-144.9(13)	Ta4-N42-C45-C46	-2(2)	C40-N42-C45-C47	93.3(16)

Ta4-N42-C45-C47	-123.5(13)	N3-Ta3-C70-C74	-143.1(8)	O34-Ta3-C70-C74	-30.7(10)
N32-Ta3-C70-C74	123.0(8)	N4-Ta3-C70-C74	179.2(7)	N31-Ta3-C70-C74	67.1(8)
C72-Ta3-C70-C74	-76.5(8)	C71-Ta3-C70-C74	-115.7(11)	C73-Ta3-C70-C74	-35.1(7)
Ta4-Ta3-C70-C74	-107.5(9)	N3-Ta3-C70-C71	-27.4(9)	O34-Ta3-C70-C71	85.1(9)
N32-Ta3-C70-C71	-121.3(8)	N4-Ta3-C70-C71	-65.0(9)	N31-Ta3-C70-C71	-177.1(8)
C72-Ta3-C70-C71	39.2(7)	C73-Ta3-C70-C71	80.6(8)	C74-Ta3-C70-C71	115.7(11)
Ta4-Ta3-C70-C71	8.2(13)	N3-Ta3-C70-C75	94.2(11)	O34-Ta3-C70-C75	-153.3(9)
N32-Ta3-C70-C75	0.3(11)	N4-Ta3-C70-C75	56.6(13)	N31-Ta3-C70-C75	-55.5(11)
C72-Ta3-C70-C75	160.9(13)	C71-Ta3-C70-C75	121.6(15)	C73-Ta3-C70-C75	-157.8(13)
C74-Ta3-C70-C75	-122.6(14)	Ta4-Ta3-C70-C75	129.8(9)	C74-C70-C71-C72	1.5(14)
C75-C70-C71-C72	172.4(11)	Ta3-C70-C71-C72	-65.0(8)	C74-C70-C71-C76	-170.0(13)
C75-C70-C71-C76	1(2)	Ta3-C70-C71-C76	123.5(14)	C74-C70-C71-Ta3	66.5(9)
C75-C70-C71-Ta3	-122.6(12)	N3-Ta3-C71-C70	153.7(8)	O34-Ta3-C71-C70	-123.5(7)
N32-Ta3-C71-C70	57.0(8)	N4-Ta3-C71-C70	135.9(7)	N31-Ta3-C71-C70	3.7(10)
C72-Ta3-C71-C70	-112.7(10)	C73-Ta3-C71-C70	-75.6(8)	C74-Ta3-C71-C70	-36.4(8)
Ta4-Ta3-C71-C70	-175.9(6)	N3-Ta3-C71-C72	-93.6(8)	O34-Ta3-C71-C72	-10.8(9)
N32-Ta3-C71-C72	169.7(7)	N4-Ta3-C71-C72	-111.4(7)	N31-Ta3-C71-C72	116.4(8)
C70-Ta3-C71-C72	112.7(10)	C73-Ta3-C71-C72	37.1(7)	C74-Ta3-C71-C72	76.3(8)
Ta4-Ta3-C71-C72	-63.2(7)	N3-Ta3-C71-C76	26.2(11)	O34-Ta3-C71-C76	108.9(11)
N32-Ta3-C71-C76	-70.6(11)	N4-Ta3-C71-C76	8.3(13)	N31-Ta3-C71-C76	-123.8(11)
C72-Ta3-C71-C76	119.7(15)	C70-Ta3-C71-C76	-127.6(15)	C73-Ta3-C71-C76	156.9(13)
C74-Ta3-C71-C76	-164.0(14)	Ta4-Ta3-C71-C76	56.6(12)	C70-C71-C72-C73	-1.5(13)
C76-C71-C72-C73	170.5(12)	Ta3-C71-C72-C73	-68.5(8)	C70-C71-C72-C77	-176.5(11)
C76-C71-C72-C77	-4.6(19)	Ta3-C71-C72-C77	116.5(11)	C70-C71-C72-Ta3	67.0(8)
C76-C71-C72-Ta3	-121.1(13)	N3-Ta3-C72-C73	-164.1(8)	O34-Ta3-C72-C73	-73.8(8)
N32-Ta3-C72-C73	101.7(8)	N4-Ta3-C72-C73	-156.3(7)	N31-Ta3-C72-C73	18.4(10)
C71-Ta3-C72-C73	115.0(10)	C70-Ta3-C72-C73	76.8(8)	C74-Ta3-C72-C73	36.4(7)
Ta4-Ta3-C72-C73	-116.4(7)	N3-Ta3-C72-C71	80.8(8)	O34-Ta3-C72-C71	171.1(7)
N32-Ta3-C72-C71	-13.4(9)	N4-Ta3-C72-C71	88.7(8)	N31-Ta3-C72-C71	-96.6(9)
C70-Ta3-C72-C71	-38.3(7)	C73-Ta3-C72-C71	-115.0(10)	C74-Ta3-C72-C71	-78.6(8)
Ta4-Ta3-C72-C71	128.6(7)	N3-Ta3-C72-C77	-36.7(10)	O34-Ta3-C72-C77	53.6(10)
N32-Ta3-C72-C77	-130.9(9)	N4-Ta3-C72-C77	-28.9(11)	N31-Ta3-C72-C77	145.8(9)
C71-Ta3-C72-C77	-117.5(13)	C70-Ta3-C72-C77	-155.8(12)	C73-Ta3-C72-C77	127.4(14)
C74-Ta3-C72-C77	163.9(12)	Ta4-Ta3-C72-C77	11.0(10)	C71-C72-C73-C74	1.0(14)
C77-C72-C73-C74	175.5(13)	Ta3-C72-C73-C74	-66.4(9)	C71-C72-C73-C78	-176.0(12)
C77-C72-C73-C78	-2(2)	Ta3-C72-C73-C78	116.5(12)	C71-C72-C73-Ta3	67.4(8)
C77-C72-C73-Ta3	-118.1(13)	N3-Ta3-C73-C74	132.2(8)	O34-Ta3-C73-C74	-141.0(8)
N32-Ta3-C73-C74	8.4(10)	N4-Ta3-C73-C74	160.2(8)	N31-Ta3-C73-C74	-52.2(8)
C72-Ta3-C73-C74	114.8(11)	C71-Ta3-C73-C74	76.8(8)	C70-Ta3-C73-C74	35.9(7)
Ta4-Ta3-C73-C74	-171.0(7)	N3-Ta3-C73-C72	17.5(9)	O34-Ta3-C73-C72	104.2(8)
N32-Ta3-C73-C72	-106.3(8)	N4-Ta3-C73-C72	45.5(12)	N31-Ta3-C73-C72	-167.0(7)
C71-Ta3-C73-C72	-37.9(7)	C70-Ta3-C73-C72	-78.9(8)	C74-Ta3-C73-C72	-114.8(11)
Ta4-Ta3-C73-C72	74.2(7)	N3-Ta3-C73-C78	-102.2(11)	O34-Ta3-C73-C78	-15.4(10)
N32-Ta3-C73-C78	134.0(10)	N4-Ta3-C73-C78	-74.2(14)	N31-Ta3-C73-C78	73.4(11)
C72-Ta3-C73-C78	-119.6(14)	C71-Ta3-C73-C78	-157.6(13)	C70-Ta3-C73-C78	161.5(13)
C74-Ta3-C73-C78	125.6(14)	Ta4-Ta3-C73-C78	-45.4(11)	C72-C73-C74-C70	-0.1(15)
C78-C73-C74-C70	176.9(12)	Ta3-C73-C74-C70	-63.6(10)	C72-C73-C74-C79	-168.5(13)
C78-C73-C74-C79	8(2)	Ta3-C73-C74-C79	128.0(14)	C72-C73-C74-Ta3	63.5(8)
C78-C73-C74-Ta3	-119.6(13)	C71-C70-C74-C73	-0.9(15)	C75-C70-C74-C73	-171.9(12)
Ta3-C70-C74-C73	64.0(10)	C71-C70-C74-C79	168.0(12)	C75-C70-C74-C79	-3(2)
Ta3-C70-C74-C79	-127.1(13)	C71-C70-C74-Ta3	-64.9(9)	C75-C70-C74-Ta3	124.1(12)
N3-Ta3-C74-C73	-66.8(10)	O34-Ta3-C74-C73	40.7(8)	N32-Ta3-C74-C73	-173.3(8)
N4-Ta3-C74-C73	-121(2)	N31-Ta3-C74-C73	129.3(8)	C72-Ta3-C74-C73	-38.2(7)
C71-Ta3-C74-C73	-80.6(8)	C70-Ta3-C74-C73	-117.9(11)	Ta4-Ta3-C74-C73	14.7(10)
N3-Ta3-C74-C70	51.1(10)	O34-Ta3-C74-C70	158.6(7)	N32-Ta3-C74-C70	-55.4(8)
N4-Ta3-C74-C70	-3(3)	N31-Ta3-C74-C70	-112.8(8)	C72-Ta3-C74-C70	79.7(8)
C71-Ta3-C74-C70	37.3(7)	C73-Ta3-C74-C70	117.9(11)	Ta4-Ta3-C74-C70	132.7(7)
N3-Ta3-C74-C79	169.3(11)	O34-Ta3-C74-C79	-83.2(13)	N32-Ta3-C74-C79	62.8(13)
N4-Ta3-C74-C79	115(2)	N31-Ta3-C74-C79	5.5(13)	C72-Ta3-C74-C79	-162.1(15)
C71-Ta3-C74-C79	155.6(15)	C70-Ta3-C74-C79	118.2(16)	C73-Ta3-C74-C79	-123.9(16)
Ta4-Ta3-C74-C79	-109.1(12)	N4-Ta4-C80-C81	-18.3(9)	O34-Ta4-C80-C81	99.6(9)
N3-Ta4-C80-C81	-59.0(11)	N41-Ta4-C80-C81	-163.2(8)	N42-Ta4-C80-C81	-106.5(8)

C82-Ta4-C80-C81	36.4(8)	C83-Ta4-C80-C81	78.5(9)	C84-Ta4-C80-C81	116.2(11)
C40-Ta4-C80-C81	-134.5(8)	Ta3-Ta4-C80-C81	32.4(14)	N4-Ta4-C80-C84	-134.4(8)
O34-Ta4-C80-C84	-16.6(10)	N3-Ta4-C80-C84	-175.2(7)	N41-Ta4-C80-C84	80.6(8)
N42-Ta4-C80-C84	137.3(8)	C82-Ta4-C80-C84	-79.8(8)	C81-Ta4-C80-C84	-116.2(11)
C83-Ta4-C80-C84	-37.7(7)	C40-Ta4-C80-C84	109.3(8)	Ta3-Ta4-C80-C84	-83.8(11)
N4-Ta4-C80-C85	107.0(12)	O34-Ta4-C80-C85	-135.1(11)	N3-Ta4-C80-C85	66.2(15)
N41-Ta4-C80-C85	-38.0(12)	N42-Ta4-C80-C85	18.7(12)	C82-Ta4-C80-C85	161.6(14)
C81-Ta4-C80-C85	125.2(16)	C83-Ta4-C80-C85	-156.3(14)	C84-Ta4-C80-C85	-118.6(15)
C40-Ta4-C80-C85	-9.2(12)	Ta3-Ta4-C80-C85	157.6(9)	C84-C80-C81-C82	-0.8(15)
C85-C80-C81-C82	175.5(13)	Ta4-C80-C81-C82	-64.6(9)	C84-C80-C81-C86	-173.8(12)
C85-C80-C81-C86	3(2)	Ta4-C80-C81-C86	122.5(13)	C84-C80-C81-Ta4	63.8(10)
C85-C80-C81-Ta4	-119.9(14)	N4-Ta4-C81-C82	-79.5(9)	O34-Ta4-C81-C82	6.6(10)
N3-Ta4-C81-C82	-98.7(9)	N41-Ta4-C81-C82	137.1(8)	N42-Ta4-C81-C82	-173.0(8)
C83-Ta4-C81-C82	39.4(8)	C84-Ta4-C81-C82	80.6(9)	C80-Ta4-C81-C82	117.1(12)
C40-Ta4-C81-C82	166.5(8)	Ta3-Ta4-C81-C82	-47.8(9)	N4-Ta4-C81-C80	163.5(9)
O34-Ta4-C81-C80	-110.5(8)	N3-Ta4-C81-C80	144.2(8)	N41-Ta4-C81-C80	20.1(10)
N42-Ta4-C81-C80	69.9(8)	C82-Ta4-C81-C80	-117.1(12)	C83-Ta4-C81-C80	-77.7(9)
C84-Ta4-C81-C80	-36.5(8)	C40-Ta4-C81-C80	49.5(9)	Ta3-Ta4-C81-C80	-164.8(7)
N4-Ta4-C81-C86	38.3(12)	O34-Ta4-C81-C86	124.4(11)	N3-Ta4-C81-C86	19.0(13)
N41-Ta4-C81-C86	-105.1(12)	N42-Ta4-C81-C86	-55.3(12)	C82-Ta4-C81-C86	117.7(15)
C83-Ta4-C81-C86	157.1(14)	C84-Ta4-C81-C86	-161.7(14)	C80-Ta4-C81-C86	-125.2(16)
C40-Ta4-C81-C86	-75.7(12)	Ta3-Ta4-C81-C86	70.0(12)	C80-C81-C82-C83	-0.4(14)
C86-C81-C82-C83	172.9(11)	Ta4-C81-C82-C83	-67.6(8)	C80-C81-C82-C87	-172.7(13)
C86-C81-C82-C87	1(2)	Ta4-C81-C82-C87	120.1(14)	C80-C81-C82-Ta4	67.2(9)
C86-C81-C82-Ta4	-119.6(12)	N4-Ta4-C82-C81	95.3(8)	O34-Ta4-C82-C81	-174.9(8)
N3-Ta4-C82-C81	101.5(8)	N41-Ta4-C82-C81	-69.5(11)	N42-Ta4-C82-C81	8.3(10)
C83-Ta4-C82-C81	-112.7(11)	C84-Ta4-C82-C81	-76.1(8)	C80-Ta4-C82-C81	-36.1(8)
C40-Ta4-C82-C81	-21.0(12)	Ta3-Ta4-C82-C81	142.2(7)	N4-Ta4-C82-C83	-152.0(8)
O34-Ta4-C82-C83	-62.1(8)	N3-Ta4-C82-C83	-145.8(7)	N41-Ta4-C82-C83	43.2(11)
N42-Ta4-C82-C83	121.0(8)	C81-Ta4-C82-C83	112.7(11)	C84-Ta4-C82-C83	36.6(7)
C80-Ta4-C82-C83	76.6(9)	C40-Ta4-C82-C83	91.7(10)	Ta3-Ta4-C82-C83	-105.0(7)
N4-Ta4-C82-C87	-30.0(12)	O34-Ta4-C82-C87	59.8(12)	N3-Ta4-C82-C87	-23.8(14)
N41-Ta4-C82-C87	165.2(10)	N42-Ta4-C82-C87	-117.0(12)	C81-Ta4-C82-C87	-125.3(16)
C83-Ta4-C82-C87	122.0(15)	C84-Ta4-C82-C87	158.6(14)	C80-Ta4-C82-C87	-161.5(14)
C40-Ta4-C82-C87	-146.3(11)	Ta3-Ta4-C82-C87	16.9(12)	C81-C82-C83-C84	1.5(14)
C87-C82-C83-C84	174.0(12)	Ta4-C82-C83-C84	-66.4(10)	C81-C82-C83-C88	-175.5(13)
C87-C82-C83-C88	-3(2)	Ta4-C82-C83-C88	116.7(14)	C81-C82-C83-Ta4	67.9(8)
C87-C82-C83-Ta4	-119.6(13)	N4-Ta4-C83-C84	145.1(8)	O34-Ta4-C83-C84	-127.4(8)
N3-Ta4-C83-C84	173.6(7)	N41-Ta4-C83-C84	-37.0(8)	N42-Ta4-C83-C84	30.2(10)
C82-Ta4-C83-C84	115.9(11)	C81-Ta4-C83-C84	77.7(8)	C80-Ta4-C83-C84	37.0(7)
C40-Ta4-C83-C84	-9.6(10)	Ta3-Ta4-C83-C84	-160.4(7)	N4-Ta4-C83-C82	29.2(8)
O34-Ta4-C83-C82	116.7(8)	N3-Ta4-C83-C82	57.7(10)	N41-Ta4-C83-C82	-152.9(7)
N42-Ta4-C83-C82	-85.7(9)	C81-Ta4-C83-C82	-38.2(7)	C84-Ta4-C83-C82	-115.9(11)
C80-Ta4-C83-C82	-78.9(8)	C40-Ta4-C83-C82	-125.5(8)	Ta3-Ta4-C83-C82	83.7(7)
N4-Ta4-C83-C88	-96.1(12)	O34-Ta4-C83-C88	-8.7(11)	N3-Ta4-C83-C88	-67.7(14)
N41-Ta4-C83-C88	81.8(12)	N42-Ta4-C83-C88	149.0(10)	C82-Ta4-C83-C88	-125.3(15)
C81-Ta4-C83-C88	-163.5(14)	C84-Ta4-C83-C88	118.7(15)	C80-Ta4-C83-C88	155.7(13)
C40-Ta4-C83-C88	109.1(11)	Ta3-Ta4-C83-C88	-41.7(12)	C81-C80-C84-C83	1.7(15)
C85-C80-C84-C83	-174.9(12)	Ta4-C80-C84-C83	64.1(10)	C81-C80-C84-C89	169.8(13)
C85-C80-C84-C89	-7(2)	Ta4-C80-C84-C89	-127.8(14)	C81-C80-C84-Ta4	-62.4(9)
C85-C80-C84-Ta4	121.0(12)	C82-C83-C84-C80	-2.0(15)	C88-C83-C84-C80	175.2(12)
Ta4-C83-C84-C80	-66.1(10)	C82-C83-C84-C89	-170.1(13)	C88-C83-C84-C89	7(2)
Ta4-C83-C84-C89	125.8(14)	C82-C83-C84-Ta4	64.1(9)	C88-C83-C84-Ta4	-118.7(12)
N4-Ta4-C84-C80	65.4(10)	O34-Ta4-C84-C80	167.7(7)	N41-Ta4-C84-C80	-98.5(8)
N42-Ta4-C84-C80	-43.0(8)	C82-Ta4-C84-C80	77.4(8)	C81-Ta4-C84-C80	36.8(8)
C83-Ta4-C84-C80	115.0(11)	C40-Ta4-C84-C80	-72.3(8)	Ta3-Ta4-C84-C80	143.7(6)
N4-Ta4-C84-C83	-49.6(10)	O34-Ta4-C84-C83	52.7(8)	N41-Ta4-C84-C83	146.5(8)
N42-Ta4-C84-C83	-158.0(7)	C82-Ta4-C84-C83	-37.5(7)	C81-Ta4-C84-C83	-78.2(8)
C80-Ta4-C84-C83	-115.0(11)	C40-Ta4-C84-C83	172.7(7)	Ta3-Ta4-C84-C83	28.7(10)
N4-Ta4-C84-C89	-170.8(11)	O34-Ta4-C84-C89	-68.5(13)	N41-Ta4-C84-C89	25.2(13)
N42-Ta4-C84-C89	80.8(13)	C82-Ta4-C84-C89	-158.8(15)	C81-Ta4-C84-C89	160.6(15)
C83-Ta4-C84-C89	-121.2(16)	C80-Ta4-C84-C89	123.8(16)	C40-Ta4-C84-C89	51.5(13)

{Cp*Ta[N(iPr)C(Ph)N(iPr]}$_2$(μ-η^2:η^2-N$_2$)(μ-O) (9b)



A clear light pink-orange plate-like specimen of $C_{46}H_{68}N_6OTa_2$, approximate dimensions 0.02 mm x 0.12 mm x 0.25 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker Smart Apex2, CCD system equipped with a graphite monochromator and a MoK_α fine focus sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 20.71 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 48359 reflections to a maximum θ angle of 27.50° (0.77 Å resolution), of which 20406 were independent (average redundancy 2.370, completeness = 99.6%, R_{int} = 2.59%, R_{sig} = 3.60%) and 17028 (83.45%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.3290(13) Å, b = 17.301(2) Å, c = 25.090(3) Å, α = 95.3168(19)°, β = 93.183(2)°, γ = 92.545(2)°, volume = 4451.9(10) Å^3, are based upon the refinement of the XYZ-centroids of 9985 reflections above 20 σ(I) with 4.506° < 2θ < 63.54°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.4790 and 0.9060.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 4 for the formula unit, $C_{46}H_{68}N_6OTa_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 1027 variables converged at R1 = 2.46%, for the observed data and wR2 = 4.62% for all data. The goodness-of-fit was 1.001. The largest peak in the final difference electron density synthesis was 1.000 e$^-$/Å^3 and the largest hole was -0.970 e$^-$/Å^3 with an RMS deviation of 0.111 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.616 g/cm^3 and F(000), 2160 e$^-$.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)
SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2008/4 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 9b.

Identification code	**9b**	
Chemical formula	$C_{46}H_{68}N_6OTa_2$	
Formula weight	1082.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal size	0.02 x 0.12 x 0.25 mm	
Crystal habit	clear light pink-orange plate	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.3290(13) Å	α = 95.3168(19)°
	b = 17.301(2) Å	β = 93.183(2)°
	c = 25.090(3) Å	γ = 92.545(2)°
Volume	4451.9(10) $Å^3$	
Z	4	
Density (calculated)	1.616 Mg/cm^3	
Absorption coefficient	4.952 mm^{-1}	
F(000)	2160	

Table 2. Data collection and structure refinement for 9b.

Diffractometer	Bruker Smart Apex2, CCD	
Radiation source	fine focus sealed tube, MoK_α	
Theta range for data collection	1.92 to 27.50°	
Index ranges	-13<=h<=13, -22<=k<=22, -32<=l<=31	
Reflections collected	48359	
Independent reflections	20406 [R(int) = 0.0259]	
Coverage of independent reflections	99.6%	
Absorption correction	multi-scan	
Max. and min. transmission	0.9060 and 0.4790	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-97 (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	20406 / 0 / 1027	
Goodness-of-fit on F^2	1.001	
Δ/σ_{max}	0.005	
Final R indices	17028 data; I>2σ(I)	R1 = 0.0246, wR2 = 0.0443
	all data	R1 = 0.0351, wR2 = 0.0462
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.01P)^2+5.818P]$, $P=(\max(F_o^2,0)+2F_c^2)/3$	
Largest diff. peak and hole	1.000 and -0.970 $eÅ^{-3}$	

R.M.S. deviation from mean 0.111 eÅ^{-3}

$R_{int} = \Sigma|F_o^2 - F_o^2(mean)| / \Sigma[F_o^2]$ $R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$

$GOOF = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$ $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 9b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Ta1A	0.248129(12)	0.802271(7)	0.697997(5)	0.01488(3)
Ta2A	0.312123(12)	0.867371(7)	0.807086(5)	0.01550(3)
O1A	0.1539(2)	0.83481(12)	0.76190(8)	0.0173(5)
N1A	0.3976(2)	0.79014(15)	0.74649(10)	0.0183(6)
N2A	0.4030(2)	0.87636(15)	0.74228(10)	0.0187(6)
C10A	0.1858(3)	0.66805(18)	0.71089(13)	0.0215(7)
C11A	0.0723(3)	0.69717(19)	0.68760(14)	0.0235(7)
C12A	0.0979(3)	0.71136(19)	0.63451(13)	0.0235(7)
C13A	0.2258(3)	0.68993(19)	0.62477(13)	0.0225(7)
C14A	0.2803(3)	0.66278(18)	0.67215(13)	0.0215(7)
C15A	0.2041(4)	0.6376(2)	0.76467(14)	0.0310(9)
C16A	0.9462(3)	0.7082(2)	0.71359(15)	0.0342(9)
C17A	0.0013(4)	0.7312(2)	0.59172(15)	0.0380(10)
C18A	0.2815(4)	0.6863(2)	0.57070(14)	0.0348(9)
C19A	0.4084(4)	0.6262(2)	0.68043(15)	0.0325(9)
C20A	0.2658(3)	0.00328(18)	0.80086(14)	0.0240(7)
C21A	0.3884(3)	0.00383(19)	0.82966(14)	0.0239(7)
C22A	0.3672(4)	0.97664(19)	0.87991(14)	0.0278(8)
C23A	0.2329(4)	0.9593(2)	0.88259(15)	0.0305(8)
C24A	0.1689(3)	0.97606(19)	0.83407(16)	0.0293(8)
C25A	0.2440(4)	0.0361(2)	0.74860(15)	0.0387(10)
C26A	0.5130(4)	0.0344(2)	0.80982(17)	0.0382(10)
C27A	0.4623(5)	0.9776(2)	0.92748(16)	0.0476(12)
C28A	0.1688(5)	0.9408(2)	0.93233(17)	0.0542(13)
C29A	0.0246(4)	0.9687(2)	0.82192(19)	0.0470(12)
N31A	0.3562(2)	0.84763(16)	0.63196(10)	0.0192(6)
N32A	0.1647(3)	0.89379(16)	0.64810(11)	0.0223(6)
C30A	0.2692(3)	0.89897(18)	0.61978(12)	0.0187(7)
C31A	0.2890(3)	0.9559(2)	0.57908(14)	0.0245(8)
C32A	0.3060(3)	0.9294(2)	0.52601(14)	0.0286(8)
C33A	0.3219(4)	0.9823(2)	0.48805(15)	0.0358(9)
C34A	0.3211(4)	0.0609(2)	0.50292(16)	0.0383(10)
C35A	0.3062(4)	0.0877(2)	0.55558(16)	0.0354(9)
C36A	0.2898(3)	0.0353(2)	0.59344(15)	0.0300(8)
C37A	0.4926(3)	0.8565(2)	0.61808(13)	0.0224(7)

	x/a	y/b	z/c	U(eq)
C38A	0.5690(3)	0.7903(2)	0.63734(14)	0.0275(8)
C39A	0.5599(3)	0.9337(2)	0.64219(15)	0.0302(8)
C40A	0.0505(3)	0.9412(2)	0.64116(15)	0.0286(8)
C41A	0.9493(3)	0.9171(3)	0.67818(17)	0.0410(10)
C42A	0.9888(4)	0.9381(3)	0.58365(17)	0.0428(11)
N51A	0.4884(2)	0.82305(15)	0.85367(10)	0.0185(6)
N52A	0.2879(2)	0.77738(15)	0.86466(10)	0.0177(6)
C50A	0.4152(3)	0.77047(18)	0.87491(12)	0.0187(7)
C51A	0.4685(3)	0.70881(19)	0.90705(13)	0.0204(7)
C52A	0.5282(3)	0.7280(2)	0.95798(14)	0.0259(8)
C53A	0.5722(3)	0.6709(2)	0.98864(15)	0.0304(8)
C54A	0.5563(3)	0.5939(2)	0.96847(15)	0.0298(8)
C55A	0.4986(3)	0.5738(2)	0.91809(15)	0.0282(8)
C56A	0.4550(3)	0.63068(19)	0.88709(14)	0.0232(7)
C57A	0.6293(3)	0.8134(2)	0.85024(14)	0.0271(8)
C58A	0.6740(4)	0.8194(3)	0.79452(16)	0.0487(12)
C59A	0.7117(4)	0.8706(3)	0.88956(16)	0.0438(11)
C60A	0.1869(3)	0.7279(2)	0.88604(13)	0.0217(7)
C61A	0.0547(3)	0.7510(2)	0.86467(15)	0.0287(8)
C62A	0.1885(4)	0.7305(2)	0.94694(14)	0.0348(9)
Ta1B	0.840386(12)	0.344423(8)	0.693326(5)	0.01616(3)
Ta2B	0.815319(12)	0.38107(7)	0.806854(5)	0.01521(3)
O1B	0.8777(2)	0.43549(12)	0.74728(8)	0.0185(5)
N1B	0.8487(2)	0.27827(15)	0.75137(11)	0.0193(6)
N2B	0.7158(2)	0.30745(16)	0.75535(11)	0.0207(6)
C10B	0.0766(3)	0.3350(2)	0.68878(13)	0.0232(7)
C11B	0.0224(3)	0.2649(2)	0.66129(14)	0.0244(7)
C12B	0.9548(3)	0.2835(2)	0.61378(13)	0.0239(7)
C13B	0.9663(3)	0.3652(2)	0.61218(13)	0.0218(7)
C14B	0.0431(3)	0.3972(2)	0.65893(13)	0.0231(7)
C15B	0.1673(3)	0.3379(3)	0.73768(15)	0.0394(10)
C16B	0.0491(4)	0.1857(2)	0.67764(17)	0.0407(10)
C17B	0.8987(4)	0.2287(2)	0.56766(15)	0.0360(9)
C18B	0.9269(4)	0.4063(2)	0.56433(14)	0.0347(9)
C19B	0.0889(4)	0.4808(2)	0.67179(15)	0.0346(9)
C20B	0.6085(3)	0.4444(2)	0.80987(14)	0.0251(8)
C21B	0.6124(3)	0.3957(2)	0.85250(13)	0.0220(7)
C22B	0.7109(3)	0.42686(19)	0.89081(13)	0.0206(7)
C23B	0.7668(3)	0.49538(19)	0.87203(14)	0.0231(7)
C24B	0.7022(3)	0.5063(2)	0.82261(14)	0.0275(8)
C25B	0.5108(4)	0.4347(3)	0.76252(15)	0.0403(10)
C26B	0.5180(3)	0.3279(2)	0.85586(16)	0.0327(9)
C27B	0.7428(4)	0.3999(2)	0.94505(14)	0.0304(8)

	x/a	y/b	z/c	U(eq)
C28B	0.8586(4)	0.5535(2)	0.90486(17)	0.0398(10)
C29B	0.7274(5)	0.5756(2)	0.79255(18)	0.0471(11)
N31B	0.6830(3)	0.39886(16)	0.64494(11)	0.0218(6)
N32B	0.6832(3)	0.27175(16)	0.64561(11)	0.0226(6)
C30B	0.6215(3)	0.3305(2)	0.62850(13)	0.0218(7)
C31B	0.5003(3)	0.3205(2)	0.59254(13)	0.0252(8)
C32B	0.3846(4)	0.3483(3)	0.60887(16)	0.0442(11)
C33B	0.2748(4)	0.3409(3)	0.57379(17)	0.0618(16)
C34B	0.2819(4)	0.3064(3)	0.52242(16)	0.0476(12)
C35B	0.3955(4)	0.2787(2)	0.50604(15)	0.0347(9)
C36B	0.5047(3)	0.2850(2)	0.54110(14)	0.0281(8)
C37B	0.6393(3)	0.4751(2)	0.63085(14)	0.0293(8)
C38B	0.7431(4)	0.5373(2)	0.65088(16)	0.0385(10)
C39B	0.6049(4)	0.4829(2)	0.57128(16)	0.0418(10)
C40B	0.6171(4)	0.1940(2)	0.64656(15)	0.0307(9)
C41B	0.7133(4)	0.1362(2)	0.66480(17)	0.0422(11)
C42B	0.5028(4)	0.1955(3)	0.68297(17)	0.0428(11)
N51B	0.0026(2)	0.37100(15)	0.85405(10)	0.0182(6)
N52B	0.8460(2)	0.28222(15)	0.85893(10)	0.0181(6)
C50B	0.9711(3)	0.30130(18)	0.86981(12)	0.0182(7)
C51B	0.0666(3)	0.25152(18)	0.89517(13)	0.0210(7)
C52B	0.1675(3)	0.22109(19)	0.86711(15)	0.0275(8)
C53B	0.2539(4)	0.1742(2)	0.89089(18)	0.0371(10)
C54B	0.2412(4)	0.1573(2)	0.94284(19)	0.0436(12)
C55B	0.1433(4)	0.1882(2)	0.97189(17)	0.0391(10)
C56B	0.0563(3)	0.2353(2)	0.94828(14)	0.0277(8)
C57B	0.1298(3)	0.41152(19)	0.86824(13)	0.0215(7)
C58B	0.1403(3)	0.4852(2)	0.83980(15)	0.0285(8)
C59B	0.1575(4)	0.4312(2)	0.92850(14)	0.0323(9)
C60B	0.7833(3)	0.20328(19)	0.85498(13)	0.0232(7)
C61B	0.8621(3)	0.1393(2)	0.82944(15)	0.0298(8)
C62B	0.7366(4)	0.1810(2)	0.90880(15)	0.0322(9)

Table 4. Bond lengths (Å) for 9b.

Ta1A-N1A	1.943(2)	Ta1A-O1A	1.972(2)
Ta1A-N2A	2.189(3)	Ta1A-N31A	2.231(3)
Ta1A-N32A	2.277(3)	Ta1A-C10A	2.437(3)
Ta1A-C14A	2.482(3)	Ta1A-C11A	2.498(3)
Ta1A-C13A	2.541(3)	Ta1A-C12A	2.542(3)
Ta1A-Ta2A	2.8912(4)	Ta2A-N2A	1.937(3)
Ta2A-O1A	1.967(2)	Ta2A-N1A	2.180(3)
Ta2A-N52A	2.235(3)	Ta2A-N51A	2.307(3)

Ta2A-C20A	2.438(3)	Ta2A-C21A	2.460(3)
Ta2A-C24A	2.511(3)	Ta2A-C22A	2.527(3)
Ta2A-C23A	2.553(3)	N1A-N2A	1.504(4)
C10A-C11A	1.414(5)	C10A-C14A	1.415(5)
C10A-C15A	1.499(4)	C11A-C12A	1.414(5)
C11A-C16A	1.500(5)	C12A-C13A	1.416(5)
C12A-C17A	1.499(4)	C13A-C14A	1.416(4)
C13A-C18A	1.500(5)	C14A-C19A	1.504(5)
C15A-H15A	0.98	C15A-H15B	0.98
C15A-H15C	0.98	C16A-H16A	0.98
C16A-H16B	0.98	C16A-H16C	0.98
C17A-H17A	0.98	C17A-H17B	0.98
C17A-H17C	0.98	C18A-H18A	0.98
C18A-H18B	0.98	C18A-H18C	0.98
C19A-H19A	0.98	C19A-H19B	0.98
C19A-H19C	0.98	C20A-C21A	1.422(5)
C20A-C24A	1.428(5)	C20A-C25A	1.486(5)
C21A-C22A	1.411(5)	C21A-C26A	1.498(5)
C22A-C23A	1.412(5)	C22A-C27A	1.501(5)
C23A-C24A	1.413(5)	C23A-C28A	1.498(5)
C24A-C29A	1.502(5)	C25A-H25A	0.98
C25A-H25B	0.98	C25A-H25C	0.98
C26A-H26A	0.98	C26A-H26B	0.98
C26A-H26C	0.98	C27A-H27A	0.98
C27A-H27B	0.98	C27A-H27C	0.98
C28A-H28A	0.98	C28A-H28B	0.98
C28A-H28C	0.98	C29A-H29A	0.98
C29A-H29B	0.98	C29A-H29C	0.98
N31A-C30A	1.334(4)	N31A-C37A	1.475(4)
N32A-C30A	1.330(4)	N32A-C40A	1.477(4)
C30A-C31A	1.498(4)	C31A-C36A	1.388(5)
C31A-C32A	1.390(5)	C32A-C33A	1.391(5)
C32A-H32A	0.95	C33A-C34A	1.377(6)
C33A-H33A	0.95	C34A-C35A	1.378(6)
C34A-H34A	0.95	C35A-C36A	1.384(5)
C35A-H35A	0.95	C36A-H36A	0.95
C37A-C38A	1.520(5)	C37A-C39A	1.535(5)
C37A-H37A	1.0	C38A-H38A	0.98
C38A-H38B	0.98	C38A-H38C	0.98
C39A-H39A	0.98	C39A-H39B	0.98
C39A-H39C	0.98	C40A-C41A	1.507(5)
C40A-C42A	1.540(5)	C40A-H40A	1.0
C41A-H41A	0.98	C41A-H41B	0.98
C41A-H41C	0.98	C42A-H42A	0.98

C42A-H42B	0.98	C42A-H42C	0.98
N51A-C50A	1.326(4)	N51A-C57A	1.478(4)
N52A-C50A	1.338(4)	N52A-C60A	1.475(4)
C50A-C51A	1.501(4)	C51A-C52A	1.393(4)
C51A-C56A	1.395(4)	C52A-C53A	1.385(5)
C52A-H52A	0.95	C53A-C54A	1.380(5)
C53A-H53A	0.95	C54A-C55A	1.375(5)
C54A-H54A	0.95	C55A-C56A	1.385(5)
C55A-H55A	0.95	C56A-H56A	0.95
C57A-C58A	1.507(5)	C57A-C59A	1.525(5)
C57A-H57A	1.0	C58A-H58A	0.98
C58A-H58B	0.98	C58A-H58C	0.98
C59A-H59A	0.98	C59A-H59B	0.98
C59A-H59C	0.98	C60A-C61A	1.523(4)
C60A-C62A	1.524(5)	C60A-H60A	1.0
C61A-H61A	0.98	C61A-H61B	0.98
C61A-H61C	0.98	C62A-H62A	0.98
C62A-H62B	0.98	C62A-H62C	0.98
Ta1B-N1B	1.934(3)	Ta1B-O1B	1.989(2)
Ta1B-N2B	2.196(3)	Ta1B-N32B	2.230(3)
Ta1B-N31B	2.266(3)	Ta1B-C10B	2.461(3)
Ta1B-C14B	2.478(3)	Ta1B-C11B	2.503(3)
Ta1B-C13B	2.521(3)	Ta1B-C12B	2.544(3)
Ta1B-Ta2B	2.8887(4)	Ta2B-N2B	1.944(3)
Ta2B-O1B	1.962(2)	Ta2B-N1B	2.207(3)
Ta2B-N51B	2.233(2)	Ta2B-N52B	2.269(3)
Ta2B-C20B	2.445(3)	Ta2B-C21B	2.455(3)
Ta2B-C22B	2.500(3)	Ta2B-C24B	2.516(3)
Ta2B-C23B	2.533(3)	N1B-N2B	1.489(4)
C10B-C14B	1.411(5)	C10B-C11B	1.415(5)
C10B-C15B	1.498(4)	C11B-C12B	1.418(5)
C11B-C16B	1.499(5)	C12B-C13B	1.418(5)
C12B-C17B	1.498(5)	C13B-C14B	1.432(4)
C13B-C18B	1.498(5)	C14B-C19B	1.502(5)
C15B-H15D	0.98	C15B-H15E	0.98
C15B-H15F	0.98	C16B-H16D	0.98
C16B-H16E	0.98	C16B-H16F	0.98
C17B-H17D	0.98	C17B-H17E	0.98
C17B-H17F	0.98	C18B-H18D	0.98
C18B-H18E	0.98	C18B-H18F	0.98
C19B-H19D	0.98	C19B-H19E	0.98
C19B-H19F	0.98	C20B-C24B	1.413(5)
C20B-C21B	1.421(5)	C20B-C25B	1.508(5)
C21B-C22B	1.413(4)	C21B-C26B	1.503(5)

C22B-C23B	1.426(5)	C22B-C27B	1.503(5)
C23B-C24B	1.407(5)	C23B-C28B	1.504(5)
C24B-C29B	1.496(5)	C25B-H25D	0.98
C25B-H25E	0.98	C25B-H25F	0.98
C26B-H26D	0.98	C26B-H26E	0.98
C26B-H26F	0.98	C27B-H27D	0.98
C27B-H27E	0.98	C27B-H27F	0.98
C28B-H28D	0.98	C28B-H28E	0.98
C28B-H28F	0.98	C29B-H29D	0.98
C29B-H29E	0.98	C29B-H29F	0.98
N31B-C30B	1.337(4)	N31B-C37B	1.480(4)
N32B-C30B	1.315(4)	N32B-C40B	1.484(4)
C30B-C31B	1.496(4)	C31B-C32B	1.377(5)
C31B-C36B	1.381(5)	C32B-C33B	1.390(5)
C32B-H32B	0.95	C33B-C34B	1.376(6)
C33B-H33B	0.95	C34B-C35B	1.358(6)
C34B-H34B	0.95	C35B-C36B	1.385(5)
C35B-H35B	0.95	C36B-H36B	0.95
C37B-C38B	1.516(5)	C37B-C39B	1.536(5)
C37B-H37B	1.0	C38B-H38D	0.98
C38B-H38E	0.98	C38B-H38F	0.98
C39B-H39D	0.98	C39B-H39E	0.98
C39B-H39F	0.98	C40B-C41B	1.522(5)
C40B-C42B	1.533(5)	C40B-H40B	1.0
C41B-H41D	0.98	C41B-H41E	0.98
C41B-H41F	0.98	C42B-H42D	0.98
C42B-H42E	0.98	C42B-H42F	0.98
N51B-C50B	1.336(4)	N51B-C57B	1.471(4)
N52B-C50B	1.326(4)	N52B-C60B	1.478(4)
C50B-C51B	1.492(4)	C51B-C52B	1.386(5)
C51B-C56B	1.396(5)	C52B-C53B	1.380(5)
C52B-H52B	0.95	C53B-C54B	1.374(6)
C53B-H53B	0.95	C54B-C55B	1.377(6)
C54B-H54B	0.95	C55B-C56B	1.385(5)
C55B-H55B	0.95	C56B-H56B	0.95
C57B-C58B	1.520(5)	C57B-C59B	1.527(5)
C57B-H57B	1.0	C58B-H58D	0.98
C58B-H58E	0.98	C58B-H58F	0.98
C59B-H59D	0.98	C59B-H59E	0.98
C59B-H59F	0.98	C60B-C61B	1.518(5)
C60B-C62B	1.535(5)	C60B-H60B	1.0
C61B-H61D	0.98	C61B-H61E	0.98
C61B-H61F	0.98	C62B-H62D	0.98
C62B-H62E	0.98	C62B-H62F	0.98

Table 5. Bond angles (°) for 9b.

N1A-Ta1A-O1A	87.32(10)	N1A-Ta1A-N2A	42.16(10)
O1A-Ta1A-N2A	81.60(9)	N1A-Ta1A-N31A	97.37(10)
O1A-Ta1A-N31A	143.01(9)	N2A-Ta1A-N31A	77.88(10)
N1A-Ta1A-N32A	139.01(10)	O1A-Ta1A-N32A	94.44(9)
N2A-Ta1A-N32A	97.53(10)	N31A-Ta1A-N32A	58.70(10)
N1A-Ta1A-C10A	86.07(11)	O1A-Ta1A-C10A	88.14(10)
N2A-Ta1A-C10A	127.29(10)	N31A-Ta1A-C10A	128.69(11)
N32A-Ta1A-C10A	134.89(10)	N1A-Ta1A-C14A	81.75(11)
O1A-Ta1A-C14A	120.81(10)	N2A-Ta1A-C14A	120.61(10)
N31A-Ta1A-C14A	96.15(11)	N32A-Ta1A-C14A	129.62(10)
C10A-Ta1A-C14A	33.42(11)	N1A-Ta1A-C11A	118.10(11)
O1A-Ta1A-C11A	81.56(10)	N2A-Ta1A-C11A	154.60(10)
N31A-Ta1A-C11A	126.06(10)	N32A-Ta1A-C11A	102.60(10)
C10A-Ta1A-C11A	33.28(11)	C14A-Ta1A-C11A	54.98(11)
N1A-Ta1A-C13A	110.09(11)	O1A-Ta1A-C13A	135.72(10)
N2A-Ta1A-C13A	138.31(11)	N31A-Ta1A-C13A	76.81(10)
N32A-Ta1A-C13A	96.91(10)	C10A-Ta1A-C13A	54.58(11)
C14A-Ta1A-C13A	32.71(10)	C11A-Ta1A-C13A	54.21(11)
N1A-Ta1A-C12A	135.49(11)	O1A-Ta1A-C12A	108.48(10)
N2A-Ta1A-C12A	169.90(11)	N31A-Ta1A-C12A	93.68(10)
N32A-Ta1A-C12A	82.48(10)	C10A-Ta1A-C12A	54.42(11)
C14A-Ta1A-C12A	54.19(11)	C11A-Ta1A-C12A	32.56(11)
C13A-Ta1A-C12A	32.35(11)	N1A-Ta1A-Ta2A	48.93(8)
O1A-Ta1A-Ta2A	42.70(6)	N2A-Ta1A-Ta2A	42.06(7)
N31A-Ta1A-Ta2A	119.01(7)	N32A-Ta1A-Ta2A	110.54(7)
C10A-Ta1A-Ta2A	101.57(7)	C14A-Ta1A-Ta2A	119.80(7)
C11A-Ta1A-Ta2A	114.93(8)	C13A-Ta1A-Ta2A	152.46(7)
C12A-Ta1A-Ta2A	147.13(8)	N2A-Ta2A-O1A	88.50(10)
N2A-Ta2A-N1A	42.33(10)	O1A-Ta2A-N1A	81.18(9)
N2A-Ta2A-N52A	135.95(10)	O1A-Ta2A-N52A	95.81(9)
N1A-Ta2A-N52A	94.97(10)	N2A-Ta2A-N51A	94.10(10)
O1A-Ta2A-N51A	144.15(9)	N1A-Ta2A-N51A	77.07(9)
N52A-Ta2A-N51A	58.61(9)	N2A-Ta2A-C20A	85.18(12)
O1A-Ta2A-C20A	90.14(10)	N1A-Ta2A-C20A	126.59(11)
N52A-Ta2A-C20A	138.41(11)	N51A-Ta2A-C20A	125.71(10)
N2A-Ta2A-C21A	84.33(11)	O1A-Ta2A-C21A	123.77(10)
N1A-Ta2A-C21A	123.05(11)	N52A-Ta2A-C21A	126.41(10)
N51A-Ta2A-C21A	92.04(10)	C20A-Ta2A-C21A	33.75(11)
N2A-Ta2A-C24A	116.37(12)	O1A-Ta2A-C24A	79.61(10)
N1A-Ta2A-C24A	151.66(11)	N52A-Ta2A-C24A	107.51(11)
N51A-Ta2A-C24A	129.36(11)	C20A-Ta2A-C24A	33.51(12)

C21A-Ta2A-C24A	55.29(12)	N2A-Ta2A-C22A	114.26(12)
O1A-Ta2A-C22A	133.47(10)	N1A-Ta2A-C22A	142.86(11)
N52A-Ta2A-C22A	94.02(11)	N51A-Ta2A-C22A	77.20(10)
C20A-Ta2A-C22A	54.79(11)	C21A-Ta2A-C22A	32.83(11)
C24A-Ta2A-C22A	54.11(12)	N2A-Ta2A-C23A	137.09(11)
O1A-Ta2A-C23A	104.13(11)	N1A-Ta2A-C23A	174.67(11)
N52A-Ta2A-C23A	84.18(11)	N51A-Ta2A-C23A	98.07(11)
C20A-Ta2A-C23A	54.56(12)	C21A-Ta2A-C23A	54.37(12)
C24A-Ta2A-C23A	32.39(12)	C22A-Ta2A-C23A	32.28(12)
N2A-Ta2A-Ta1A	49.21(8)	O1A-Ta2A-Ta1A	42.85(6)
N1A-Ta2A-Ta1A	42.21(7)	N52A-Ta2A-Ta1A	111.06(7)
N51A-Ta2A-Ta1A	118.89(7)	C20A-Ta2A-Ta1A	101.11(8)
C21A-Ta2A-Ta1A	122.51(8)	C24A-Ta2A-Ta1A	111.53(9)
C22A-Ta2A-Ta1A	154.59(8)	C23A-Ta2A-Ta1A	142.87(9)
Ta2A-O1A-Ta1A	94.45(9)	N2A-N1A-Ta1A	77.72(15)
N2A-N1A-Ta2A	60.17(14)	Ta1A-N1A-Ta2A	88.86(10)
N1A-N2A-Ta2A	77.49(15)	N1A-N2A-Ta1A	60.12(13)
Ta2A-N2A-Ta1A	88.73(10)	C11A-C10A-C14A	108.6(3)
C11A-C10A-C15A	128.0(3)	C14A-C10A-C15A	123.0(3)
C11A-C10A-Ta1A	75.69(19)	C14A-C10A-Ta1A	75.02(18)
C15A-C10A-Ta1A	121.2(2)	C12A-C11A-C10A	107.4(3)
C12A-C11A-C16A	126.1(3)	C10A-C11A-C16A	126.4(3)
C12A-C11A-Ta1A	75.46(18)	C10A-C11A-Ta1A	71.02(18)
C16A-C11A-Ta1A	120.8(2)	C11A-C12A-C13A	108.5(3)
C11A-C12A-C17A	126.7(3)	C13A-C12A-C17A	123.9(3)
C11A-C12A-Ta1A	71.98(18)	C13A-C12A-Ta1A	73.78(18)
C17A-C12A-Ta1A	128.8(2)	C14A-C13A-C12A	107.9(3)
C14A-C13A-C18A	127.5(3)	C12A-C13A-C18A	124.0(3)
C14A-C13A-Ta1A	71.35(18)	C12A-C13A-Ta1A	73.87(18)
C18A-C13A-Ta1A	127.4(2)	C10A-C14A-C13A	107.6(3)
C10A-C14A-C19A	123.8(3)	C13A-C14A-C19A	128.2(3)
C10A-C14A-Ta1A	71.56(18)	C13A-C14A-Ta1A	75.94(19)
C19A-C14A-Ta1A	123.0(2)	C10A-C15A-H15A	109.5
C10A-C15A-H15B	109.5	H15A-C15A-H15B	109.5
C10A-C15A-H15C	109.5	H15A-C15A-H15C	109.5
H15B-C15A-H15C	109.5	C11A-C16A-H16A	109.5
C11A-C16A-H16B	109.5	H16A-C16A-H16B	109.5
C11A-C16A-H16C	109.5	H16A-C16A-H16C	109.5
H16B-C16A-H16C	109.5	C12A-C17A-H17A	109.5
C12A-C17A-H17B	109.5	H17A-C17A-H17B	109.5
C12A-C17A-H17C	109.5	H17A-C17A-H17C	109.5
H17B-C17A-H17C	109.5	C13A-C18A-H18A	109.5
C13A-C18A-H18B	109.5	H18A-C18A-H18B	109.5
C13A-C18A-H18C	109.5	H18A-C18A-H18C	109.5

H18B-C18A-H18C	109.5	C14A-C19A-H19A	109.5
C14A-C19A-H19B	109.5	H19A-C19A-H19B	109.5
C14A-C19A-H19C	109.5	H19A-C19A-H19C	109.5
H19B-C19A-H19C	109.5	C21A-C20A-C24A	108.1(3)
C21A-C20A-C25A	124.4(3)	C24A-C20A-C25A	127.0(3)
C21A-C20A-Ta2A	73.99(18)	C24A-C20A-Ta2A	76.05(19)
C25A-C20A-Ta2A	122.4(2)	C22A-C21A-C20A	107.6(3)
C22A-C21A-C26A	128.1(3)	C20A-C21A-C26A	124.1(3)
C22A-C21A-Ta2A	76.19(19)	C20A-C21A-Ta2A	72.26(18)
C26A-C21A-Ta2A	120.8(2)	C21A-C22A-C23A	108.5(3)
C21A-C22A-C27A	127.8(4)	C23A-C22A-C27A	122.9(4)
C21A-C22A-Ta2A	70.98(19)	C23A-C22A-Ta2A	74.9(2)
C27A-C22A-Ta2A	128.1(2)	C22A-C23A-C24A	108.4(3)
C22A-C23A-C28A	124.7(4)	C24A-C23A-C28A	126.0(4)
C22A-C23A-Ta2A	72.8(2)	C24A-C23A-Ta2A	72.2(2)
C28A-C23A-Ta2A	129.4(2)	C23A-C24A-C20A	107.4(3)
C23A-C24A-C29A	125.0(4)	C20A-C24A-C29A	127.6(4)
C23A-C24A-Ta2A	75.4(2)	C20A-C24A-Ta2A	70.44(19)
C29A-C24A-Ta2A	121.4(2)	C20A-C25A-H25A	109.5
C20A-C25A-H25B	109.5	H25A-C25A-H25B	109.5
C20A-C25A-H25C	109.5	H25A-C25A-H25C	109.5
H25B-C25A-H25C	109.5	C21A-C26A-H26A	109.5
C21A-C26A-H26B	109.5	H26A-C26A-H26B	109.5
C21A-C26A-H26C	109.5	H26A-C26A-H26C	109.5
H26B-C26A-H26C	109.5	C22A-C27A-H27A	109.5
C22A-C27A-H27B	109.5	H27A-C27A-H27B	109.5
C22A-C27A-H27C	109.5	H27A-C27A-H27C	109.5
H27B-C27A-H27C	109.5	C23A-C28A-H28A	109.5
C23A-C28A-H28B	109.5	H28A-C28A-H28B	109.5
C23A-C28A-H28C	109.5	H28A-C28A-H28C	109.5
H28B-C28A-H28C	109.5	C24A-C29A-H29A	109.5
C24A-C29A-H29B	109.5	H29A-C29A-H29B	109.5
C24A-C29A-H29C	109.5	H29A-C29A-H29C	109.5
H29B-C29A-H29C	109.5	C30A-N31A-C37A	121.6(3)
C30A-N31A-Ta1A	95.5(2)	C37A-N31A-Ta1A	137.2(2)
C30A-N32A-C40A	123.8(3)	C30A-N32A-Ta1A	93.48(19)
C40A-N32A-Ta1A	142.7(2)	N32A-C30A-N31A	112.1(3)
N32A-C30A-C31A	124.5(3)	N31A-C30A-C31A	123.3(3)
C36A-C31A-C32A	119.0(3)	C36A-C31A-C30A	120.9(3)
C32A-C31A-C30A	120.1(3)	C31A-C32A-C33A	120.1(4)
C31A-C32A-H32A	120.0	C33A-C32A-H32A	120.0
C34A-C33A-C32A	120.1(4)	C34A-C33A-H33A	119.9
C32A-C33A-H33A	119.9	C33A-C34A-C35A	120.2(3)
C33A-C34A-H34A	119.9	C35A-C34A-H34A	119.9

C34A-C35A-C36A	119.8(4)	C34A-C35A-H35A	120.1
C36A-C35A-H35A	120.1	C35A-C36A-C31A	120.7(4)
C35A-C36A-H36A	119.6	C31A-C36A-H36A	119.6
N31A-C37A-C38A	110.0(3)	N31A-C37A-C39A	113.1(3)
C38A-C37A-C39A	108.6(3)	N31A-C37A-H37A	108.4
C38A-C37A-H37A	108.4	C39A-C37A-H37A	108.4
C37A-C38A-H38A	109.5	C37A-C38A-H38B	109.5
H38A-C38A-H38B	109.5	C37A-C38A-H38C	109.5
H38A-C38A-H38C	109.5	H38B-C38A-H38C	109.5
C37A-C39A-H39A	109.5	C37A-C39A-H39B	109.5
H39A-C39A-H39B	109.5	C37A-C39A-H39C	109.5
H39A-C39A-H39C	109.5	H39B-C39A-H39C	109.5
N32A-C40A-C41A	108.9(3)	N32A-C40A-C42A	115.7(3)
C41A-C40A-C42A	109.3(3)	N32A-C40A-H40A	107.5
C41A-C40A-H40A	107.5	C42A-C40A-H40A	107.5
C40A-C41A-H41A	109.5	C40A-C41A-H41B	109.5
H41A-C41A-H41B	109.5	C40A-C41A-H41C	109.5
H41A-C41A-H41C	109.5	H41B-C41A-H41C	109.5
C40A-C42A-H42A	109.5	C40A-C42A-H42B	109.5
H42A-C42A-H42B	109.5	C40A-C42A-H42C	109.5
H42A-C42A-H42C	109.5	H42B-C42A-H42C	109.5
C50A-N51A-C57A	120.2(3)	C50A-N51A-Ta2A	92.30(19)
C57A-N51A-Ta2A	141.4(2)	C50A-N52A-C60A	123.3(3)
C50A-N52A-Ta2A	95.19(19)	C60A-N52A-Ta2A	141.2(2)
N51A-C50A-N52A	113.2(3)	N51A-C50A-C51A	123.8(3)
N52A-C50A-C51A	122.9(3)	C52A-C51A-C56A	118.7(3)
C52A-C51A-C50A	120.8(3)	C56A-C51A-C50A	120.4(3)
C53A-C52A-C51A	120.9(3)	C53A-C52A-H52A	119.6
C51A-C52A-H52A	119.6	C54A-C53A-C52A	119.5(3)
C54A-C53A-H53A	120.2	C52A-C53A-H53A	120.2
C55A-C54A-C53A	120.5(3)	C55A-C54A-H54A	119.8
C53A-C54A-H54A	119.8	C54A-C55A-C56A	120.3(3)
C54A-C55A-H55A	119.8	C56A-C55A-H55A	119.8
C55A-C56A-C51A	120.1(3)	C55A-C56A-H56A	120.0
C51A-C56A-H56A	120.0	N51A-C57A-C58A	112.9(3)
N51A-C57A-C59A	112.9(3)	C58A-C57A-C59A	109.0(3)
N51A-C57A-H57A	107.2	C58A-C57A-H57A	107.2
C59A-C57A-H57A	107.2	C57A-C58A-H58A	109.5
C57A-C58A-H58B	109.5	H58A-C58A-H58B	109.5
C57A-C58A-H58C	109.5	H58A-C58A-H58C	109.5
H58B-C58A-H58C	109.5	C57A-C59A-H59A	109.5
C57A-C59A-H59B	109.5	H59A-C59A-H59B	109.5
C57A-C59A-H59C	109.5	H59A-C59A-H59C	109.5
H59B-C59A-H59C	109.5	N52A-C60A-C61A	108.4(3)

N52A-C60A-C62A	115.7(3)	C61A-C60A-C62A	109.1(3)
N52A-C60A-H60A	107.8	C61A-C60A-H60A	107.8
C62A-C60A-H60A	107.8	C60A-C61A-H61A	109.5
C60A-C61A-H61B	109.5	H61A-C61A-H61B	109.5
C60A-C61A-H61C	109.5	H61A-C61A-H61C	109.5
H61B-C61A-H61C	109.5	C60A-C62A-H62A	109.5
C60A-C62A-H62B	109.5	H62A-C62A-H62B	109.5
C60A-C62A-H62C	109.5	H62A-C62A-H62C	109.5
H62B-C62A-H62C	109.5	N1B-Ta1B-O1B	88.38(10)
N1B-Ta1B-N2B	41.67(10)	O1B-Ta1B-N2B	81.83(9)
N1B-Ta1B-N32B	94.55(10)	O1B-Ta1B-N32B	144.51(10)
N2B-Ta1B-N32B	77.28(10)	N1B-Ta1B-N31B	136.73(11)
O1B-Ta1B-N31B	96.13(9)	N2B-Ta1B-N31B	96.30(10)
N32B-Ta1B-N31B	58.62(10)	N1B-Ta1B-C10B	87.98(11)
O1B-Ta1B-C10B	87.46(10)	N2B-Ta1B-C10B	128.40(10)
N32B-Ta1B-C10B	127.95(11)	N31B-Ta1B-C10B	135.10(11)
N1B-Ta1B-C14B	120.03(11)	O1B-Ta1B-C14B	80.81(10)
N2B-Ta1B-C14B	155.12(10)	N32B-Ta1B-C14B	126.28(10)
N31B-Ta1B-C14B	103.14(11)	C10B-Ta1B-C14B	33.21(11)
N1B-Ta1B-C11B	82.65(11)	O1B-Ta1B-C11B	119.80(10)
N2B-Ta1B-C11B	121.65(11)	N32B-Ta1B-C11B	95.62(11)
N31B-Ta1B-C11B	129.20(11)	C10B-Ta1B-C11B	33.12(11)
C14B-Ta1B-C11B	54.90(12)	N1B-Ta1B-C13B	136.88(11)
O1B-Ta1B-C13B	108.49(10)	N2B-Ta1B-C13B	169.65(10)
N32B-Ta1B-C13B	93.27(10)	N31B-Ta1B-C13B	82.05(10)
C10B-Ta1B-C13B	54.81(11)	C14B-Ta1B-C13B	33.28(10)
C11B-Ta1B-C13B	54.38(11)	N1B-Ta1B-C12B	110.07(11)
O1B-Ta1B-C12B	135.28(10)	N2B-Ta1B-C12B	138.58(11)
N32B-Ta1B-C12B	76.38(10)	N31B-Ta1B-C12B	96.59(10)
C10B-Ta1B-C12B	54.44(11)	C14B-Ta1B-C12B	54.56(11)
C11B-Ta1B-C12B	32.61(11)	C13B-Ta1B-C12B	32.50(11)
N1B-Ta1B-Ta2B	49.77(8)	O1B-Ta1B-Ta2B	42.65(6)
N2B-Ta1B-Ta2B	42.28(7)	N32B-Ta1B-Ta2B	118.90(7)
N31B-Ta1B-Ta2B	110.78(7)	C10B-Ta1B-Ta2B	101.92(8)
C14B-Ta1B-Ta2B	114.81(7)	C11B-Ta1B-Ta2B	120.00(8)
C13B-Ta1B-Ta2B	147.66(7)	C12B-Ta1B-Ta2B	152.59(8)
N2B-Ta2B-O1B	89.30(10)	N2B-Ta2B-N1B	41.45(10)
O1B-Ta2B-N1B	81.79(9)	N2B-Ta2B-N51B	131.38(10)
O1B-Ta2B-N51B	100.17(9)	N1B-Ta2B-N51B	92.52(9)
N2B-Ta2B-N52B	88.05(10)	O1B-Ta2B-N52B	146.09(9)
N1B-Ta2B-N52B	74.03(10)	N51B-Ta2B-N52B	58.41(9)
N2B-Ta2B-C20B	82.45(11)	O1B-Ta2B-C20B	95.20(10)
N1B-Ta2B-C20B	123.63(11)	N51B-Ta2B-C20B	142.46(11)
N52B-Ta2B-C20B	117.89(11)	N2B-Ta2B-C21B	86.08(11)

O1B-Ta2B-C21B	128.86(10)	N1B-Ta2B-C21B	122.35(11)
N51B-Ta2B-C21B	120.40(10)	N52B-Ta2B-C21B	84.65(10)
C20B-Ta2B-C21B	33.71(11)	N2B-Ta2B-C22B	117.72(11)
O1B-Ta2B-C22B	132.52(10)	N1B-Ta2B-C22B	144.41(10)
N51B-Ta2B-C22B	90.15(10)	N52B-Ta2B-C22B	77.35(10)
C20B-Ta2B-C22B	55.13(11)	C21B-Ta2B-C22B	33.12(10)
N2B-Ta2B-C24B	111.47(12)	O1B-Ta2B-C24B	80.23(10)
N1B-Ta2B-C24B	147.54(11)	N51B-Ta2B-C24B	117.11(11)
N52B-Ta2B-C24B	131.72(11)	C20B-Ta2B-C24B	33.06(12)
C21B-Ta2B-C24B	54.98(11)	C22B-Ta2B-C24B	54.39(11)
N2B-Ta2B-C23B	136.41(11)	O1B-Ta2B-C23B	100.55(10)
N1B-Ta2B-C23B	177.06(10)	N51B-Ta2B-C23B	88.83(10)
N52B-Ta2B-C23B	104.54(10)	C20B-Ta2B-C23B	54.59(11)
C21B-Ta2B-C23B	54.77(11)	C22B-Ta2B-C23B	32.91(10)
C24B-Ta2B-C23B	32.37(11)	N2B-Ta2B-Ta1B	49.44(8)
O1B-Ta2B-Ta1B	43.39(6)	N1B-Ta2B-Ta1B	42.02(7)
N51B-Ta2B-Ta1B	111.77(7)	N52B-Ta2B-Ta1B	115.97(7)
C20B-Ta2B-Ta1B	102.94(8)	C21B-Ta2B-Ta1B	126.72(8)
C22B-Ta2B-Ta1B	157.89(7)	C24B-Ta2B-Ta1B	109.74(8)
C23B-Ta2B-Ta1B	139.49(8)	Ta2B-O1B-Ta1B	93.96(9)
N2B-N1B-Ta1B	78.60(15)	N2B-N1B-Ta2B	59.80(14)
Ta1B-N1B-Ta2B	88.21(10)	N1B-N2B-Ta2B	78.75(15)
N1B-N2B-Ta1B	59.73(14)	Ta2B-N2B-Ta1B	88.27(10)
C14B-C10B-C11B	108.7(3)	C14B-C10B-C15B	127.6(3)
C11B-C10B-C15B	123.3(3)	C14B-C10B-Ta1B	74.07(18)
C11B-C10B-Ta1B	75.10(18)	C15B-C10B-Ta1B	122.8(2)
C10B-C11B-C12B	107.9(3)	C10B-C11B-C16B	124.1(3)
C12B-C11B-C16B	127.6(3)	C10B-C11B-Ta1B	71.78(18)
C12B-C11B-Ta1B	75.28(19)	C16B-C11B-Ta1B	124.5(2)
C13B-C12B-C11B	108.1(3)	C13B-C12B-C17B	123.3(3)
C11B-C12B-C17B	127.9(3)	C13B-C12B-Ta1B	72.82(19)
C11B-C12B-Ta1B	72.10(19)	C17B-C12B-Ta1B	128.4(2)
C12B-C13B-C14B	107.8(3)	C12B-C13B-C18B	124.3(3)
C14B-C13B-C18B	126.9(3)	C12B-C13B-Ta1B	74.68(19)
C14B-C13B-Ta1B	71.73(18)	C18B-C13B-Ta1B	128.5(2)
C10B-C14B-C13B	107.5(3)	C10B-C14B-C19B	126.0(3)
C13B-C14B-C19B	126.3(3)	C10B-C14B-Ta1B	72.72(18)
C13B-C14B-Ta1B	74.99(18)	C19B-C14B-Ta1B	121.6(2)
C10B-C15B-H15D	109.5	C10B-C15B-H15E	109.5
H15D-C15B-H15E	109.5	C10B-C15B-H15F	109.5
H15D-C15B-H15F	109.5	H15E-C15B-H15F	109.5
C11B-C16B-H16D	109.5	C11B-C16B-H16E	109.5
H16D-C16B-H16E	109.5	C11B-C16B-H16F	109.5
H16D-C16B-H16F	109.5	H16E-C16B-H16F	109.5

C12B-C17B-H17D	109.5	C12B-C17B-H17E	109.5
H17D-C17B-H17E	109.5	C12B-C17B-H17F	109.5
H17D-C17B-H17F	109.5	H17E-C17B-H17F	109.5
C13B-C18B-H18D	109.5	C13B-C18B-H18E	109.5
H18D-C18B-H18E	109.5	C13B-C18B-H18F	109.5
H18D-C18B-H18F	109.5	H18E-C18B-H18F	109.5
C14B-C19B-H19D	109.5	C14B-C19B-H19E	109.5
H19D-C19B-H19E	109.5	C14B-C19B-H19F	109.5
H19D-C19B-H19F	109.5	H19E-C19B-H19F	109.5
C24B-C20B-C21B	108.2(3)	C24B-C20B-C25B	126.8(3)
C21B-C20B-C25B	124.7(3)	C24B-C20B-Ta2B	76.24(19)
C21B-C20B-Ta2B	73.56(18)	C25B-C20B-Ta2B	121.0(2)
C22B-C21B-C20B	107.7(3)	C22B-C21B-C26B	128.4(3)
C20B-C21B-C26B	123.7(3)	C22B-C21B-Ta2B	75.15(19)
C20B-C21B-Ta2B	72.73(18)	C26B-C21B-Ta2B	121.7(2)
C21B-C22B-C23B	107.9(3)	C21B-C22B-C27B	127.2(3)
C23B-C22B-C27B	124.5(3)	C21B-C22B-Ta2B	71.72(19)
C23B-C22B-Ta2B	74.84(19)	C27B-C22B-Ta2B	124.8(2)
C24B-C23B-C22B	108.0(3)	C24B-C23B-C28B	126.1(3)
C22B-C23B-C28B	124.9(3)	C24B-C23B-Ta2B	73.1(2)
C22B-C23B-Ta2B	72.25(19)	C28B-C23B-Ta2B	129.7(2)
C23B-C24B-C20B	108.2(3)	C23B-C24B-C29B	123.5(4)
C20B-C24B-C29B	128.2(4)	C23B-C24B-Ta2B	74.49(19)
C20B-C24B-Ta2B	70.71(19)	C29B-C24B-Ta2B	123.7(2)
C20B-C25B-H25D	109.5	C20B-C25B-H25E	109.5
H25D-C25B-H25E	109.5	C20B-C25B-H25F	109.5
H25D-C25B-H25F	109.5	H25E-C25B-H25F	109.5
C21B-C26B-H26D	109.5	C21B-C26B-H26E	109.5
H26D-C26B-H26E	109.5	C21B-C26B-H26F	109.5
H26D-C26B-H26F	109.5	H26E-C26B-H26F	109.5
C22B-C27B-H27D	109.5	C22B-C27B-H27E	109.5
H27D-C27B-H27E	109.5	C22B-C27B-H27F	109.5
H27D-C27B-H27F	109.5	H27E-C27B-H27F	109.5
C23B-C28B-H28D	109.5	C23B-C28B-H28E	109.5
H28D-C28B-H28E	109.5	C23B-C28B-H28F	109.5
H28D-C28B-H28F	109.5	H28E-C28B-H28F	109.5
C24B-C29B-H29D	109.5	C24B-C29B-H29E	109.5
H29D-C29B-H29E	109.5	C24B-C29B-H29F	109.5
H29D-C29B-H29F	109.5	H29E-C29B-H29F	109.5
C30B-N31B-C37B	124.7(3)	C30B-N31B-Ta1B	93.45(19)
C37B-N31B-Ta1B	141.9(2)	C30B-N32B-C40B	121.5(3)
C30B-N32B-Ta1B	95.7(2)	C40B-N32B-Ta1B	137.7(2)
N32B-C30B-N31B	112.2(3)	N32B-C30B-C31B	123.2(3)
N31B-C30B-C31B	124.6(3)	C32B-C31B-C36B	118.8(3)

C32B-C31B-C30B	121.5(3)	C36B-C31B-C30B	119.6(3)
C31B-C32B-C33B	120.2(4)	C31B-C32B-H32B	119.9
C33B-C32B-H32B	119.9	C34B-C33B-C32B	120.0(4)
C34B-C33B-H33B	120.0	C32B-C33B-H33B	120.0
C35B-C34B-C33B	120.2(3)	C35B-C34B-H34B	119.9
C33B-C34B-H34B	119.9	C34B-C35B-C36B	120.0(4)
C34B-C35B-H35B	120.0	C36B-C35B-H35B	120.0
C31B-C36B-C35B	120.8(3)	C31B-C36B-H36B	119.6
C35B-C36B-H36B	119.6	N31B-C37B-C38B	108.8(3)
N31B-C37B-C39B	117.0(3)	C38B-C37B-C39B	108.4(3)
N31B-C37B-H37B	107.4	C38B-C37B-H37B	107.4
C39B-C37B-H37B	107.4	C37B-C38B-H38D	109.5
C37B-C38B-H38E	109.5	H38D-C38B-H38E	109.5
C37B-C38B-H38F	109.5	H38D-C38B-H38F	109.5
H38E-C38B-H38F	109.5	C37B-C39B-H39D	109.5
C37B-C39B-H39E	109.5	H39D-C39B-H39E	109.5
C37B-C39B-H39F	109.5	H39D-C39B-H39F	109.5
H39E-C39B-H39F	109.5	N32B-C40B-C41B	110.3(3)
N32B-C40B-C42B	112.6(3)	C41B-C40B-C42B	109.3(3)
N32B-C40B-H40B	108.2	C41B-C40B-H40B	108.2
C42B-C40B-H40B	108.2	C40B-C41B-H41D	109.5
C40B-C41B-H41E	109.5	H41D-C41B-H41E	109.5
C40B-C41B-H41F	109.5	H41D-C41B-H41F	109.5
H41E-C41B-H41F	109.5	C40B-C42B-H42D	109.5
C40B-C42B-H42E	109.5	H42D-C42B-H42E	109.5
C40B-C42B-H42F	109.5	H42D-C42B-H42F	109.5
H42E-C42B-H42F	109.5	C50B-N51B-C57B	122.6(3)
C50B-N51B-Ta2B	95.13(18)	C57B-N51B-Ta2B	142.2(2)
C50B-N52B-C60B	126.7(3)	C50B-N52B-Ta2B	93.81(19)
C60B-N52B-Ta2B	130.31(19)	N52B-C50B-N51B	111.2(3)
N52B-C50B-C51B	125.2(3)	N51B-C50B-C51B	123.5(3)
C52B-C51B-C56B	118.5(3)	C52B-C51B-C50B	121.3(3)
C56B-C51B-C50B	120.2(3)	C53B-C52B-C51B	120.5(4)
C53B-C52B-H52B	119.7	C51B-C52B-H52B	119.7
C54B-C53B-C52B	120.4(4)	C54B-C53B-H53B	119.8
C52B-C53B-H53B	119.8	C53B-C54B-C55B	120.1(3)
C53B-C54B-H54B	119.9	C55B-C54B-H54B	119.9
C54B-C55B-C56B	119.8(4)	C54B-C55B-H55B	120.1
C56B-C55B-H55B	120.1	C55B-C56B-C51B	120.6(4)
C55B-C56B-H56B	119.7	C51B-C56B-H56B	119.7
N51B-C57B-C58B	109.8(3)	N51B-C57B-C59B	113.6(3)
C58B-C57B-C59B	109.8(3)	N51B-C57B-H57B	107.8
C58B-C57B-H57B	107.8	C59B-C57B-H57B	107.8
C57B-C58B-H58D	109.5	C57B-C58B-H58E	109.5

H58D-C58B-H58E	109.5	C57B-C58B-H58F	109.5
H58D-C58B-H58F	109.5	H58E-C58B-H58F	109.5
C57B-C59B-H59D	109.5	C57B-C59B-H59E	109.5
H59D-C59B-H59E	109.5	C57B-C59B-H59F	109.5
H59D-C59B-H59F	109.5	H59E-C59B-H59F	109.5
N52B-C60B-C61B	115.2(3)	N52B-C60B-C62B	112.8(3)
C61B-C60B-C62B	110.2(3)	N52B-C60B-H60B	106.0
C61B-C60B-H60B	106.0	C62B-C60B-H60B	106.0
C60B-C61B-H61D	109.5	C60B-C61B-H61E	109.5
H61D-C61B-H61E	109.5	C60B-C61B-H61F	109.5
H61D-C61B-H61F	109.5	H61E-C61B-H61F	109.5
C60B-C62B-H62D	109.5	C60B-C62B-H62E	109.5
H62D-C62B-H62E	109.5	C60B-C62B-H62F	109.5
H62D-C62B-H62F	109.5	H62E-C62B-H62F	109.5

Table 6. Torsion angles (°) for 9b.

N1A-Ta1A-Ta2A-N2A	59.87(14)	O1A-Ta1A-Ta2A-N2A	-151.59(13)
N31A-Ta1A-Ta2A-N2A	-13.35(13)	N32A-Ta1A-Ta2A-N2A	-78.09(12)
C10A-Ta1A-Ta2A-N2A	134.13(13)	C14A-Ta1A-Ta2A-N2A	103.96(14)
C11A-Ta1A-Ta2A-N2A	166.37(13)	C13A-Ta1A-Ta2A-N2A	106.6(2)
C12A-Ta1A-Ta2A-N2A	173.09(17)	N1A-Ta1A-Ta2A-O1A	-148.54(14)
N2A-Ta1A-Ta2A-O1A	151.59(13)	N31A-Ta1A-Ta2A-O1A	138.24(12)
N32A-Ta1A-Ta2A-O1A	73.49(11)	C10A-Ta1A-Ta2A-O1A	-74.29(12)
C14A-Ta1A-Ta2A-O1A	-104.46(13)	C11A-Ta1A-Ta2A-O1A	-42.05(13)
C13A-Ta1A-Ta2A-O1A	-101.82(19)	C12A-Ta1A-Ta2A-O1A	-35.32(17)
O1A-Ta1A-Ta2A-N1A	148.54(14)	N2A-Ta1A-Ta2A-N1A	-59.87(14)
N31A-Ta1A-Ta2A-N1A	-73.22(13)	N32A-Ta1A-Ta2A-N1A	-137.96(13)
C10A-Ta1A-Ta2A-N1A	74.26(13)	C14A-Ta1A-Ta2A-N1A	44.08(14)
C11A-Ta1A-Ta2A-N1A	106.50(14)	C13A-Ta1A-Ta2A-N1A	46.7(2)
C12A-Ta1A-Ta2A-N1A	113.22(18)	N1A-Ta1A-Ta2A-N52A	-73.36(13)
O1A-Ta1A-Ta2A-N52A	75.18(11)	N2A-Ta1A-Ta2A-N52A	-133.23(12)
N31A-Ta1A-Ta2A-N52A	-146.58(11)	N32A-Ta1A-Ta2A-N52A	148.67(10)
C10A-Ta1A-Ta2A-N52A	0.89(11)	C14A-Ta1A-Ta2A-N52A	-29.28(12)
C11A-Ta1A-Ta2A-N52A	33.13(11)	C13A-Ta1A-Ta2A-N52A	-26.64(18)
C12A-Ta1A-Ta2A-N52A	39.86(16)	N1A-Ta1A-Ta2A-N51A	-8.51(13)
O1A-Ta1A-Ta2A-N51A	140.03(12)	N2A-Ta1A-Ta2A-N51A	-68.39(12)
N31A-Ta1A-Ta2A-N51A	-81.73(11)	N32A-Ta1A-Ta2A-N51A	-146.48(10)
C10A-Ta1A-Ta2A-N51A	65.74(11)	C14A-Ta1A-Ta2A-N51A	35.57(12)
C11A-Ta1A-Ta2A-N51A	97.98(12)	C13A-Ta1A-Ta2A-N51A	38.21(18)
C12A-Ta1A-Ta2A-N51A	104.70(16)	N1A-Ta1A-Ta2A-C20A	133.46(13)
O1A-Ta1A-Ta2A-C20A	-78.00(12)	N2A-Ta1A-Ta2A-C20A	73.58(13)
N31A-Ta1A-Ta2A-C20A	60.24(12)	N32A-Ta1A-Ta2A-C20A	-4.51(11)
C10A-Ta1A-Ta2A-C20A	-152.29(12)	C14A-Ta1A-Ta2A-C20A	177.54(13)

C11A-Ta1A-Ta2A-C20A	-120.05(12)	C13A-Ta1A-Ta2A-C20A	-179.82(19)
C12A-Ta1A-Ta2A-C20A	-113.32(17)	N1A-Ta1A-Ta2A-C21A	105.06(14)
O1A-Ta1A-Ta2A-C21A	-106.39(13)	N2A-Ta1A-Ta2A-C21A	45.19(14)
N31A-Ta1A-Ta2A-C21A	31.84(12)	N32A-Ta1A-Ta2A-C21A	-32.90(12)
C10A-Ta1A-Ta2A-C21A	179.32(13)	C14A-Ta1A-Ta2A-C21A	149.15(13)
C11A-Ta1A-Ta2A-C21A	-148.44(13)	C13A-Ta1A-Ta2A-C21A	151.78(19)
C12A-Ta1A-Ta2A-C21A	-141.72(17)	N1A-Ta1A-Ta2A-C24A	166.74(14)
O1A-Ta1A-Ta2A-C24A	-44.72(13)	N2A-Ta1A-Ta2A-C24A	106.87(14)
N31A-Ta1A-Ta2A-C24A	93.52(12)	N32A-Ta1A-Ta2A-C24A	28.77(12)
C10A-Ta1A-Ta2A-C24A	-119.00(12)	C14A-Ta1A-Ta2A-C24A	-149.18(13)
C11A-Ta1A-Ta2A-C24A	-86.77(13)	C13A-Ta1A-Ta2A-C24A	-146.54(19)
C12A-Ta1A-Ta2A-C24A	-80.04(17)	N1A-Ta1A-Ta2A-C22A	116.4(2)
O1A-Ta1A-Ta2A-C22A	-95.1(2)	N2A-Ta1A-Ta2A-C22A	56.5(2)
N31A-Ta1A-Ta2A-C22A	43.2(2)	N32A-Ta1A-Ta2A-C22A	-21.6(2)
C10A-Ta1A-Ta2A-C22A	-169.4(2)	C14A-Ta1A-Ta2A-C22A	160.5(2)
C11A-Ta1A-Ta2A-C22A	-137.1(2)	C13A-Ta1A-Ta2A-C22A	163.1(3)
C12A-Ta1A-Ta2A-C22A	-130.4(3)	N1A-Ta1A-Ta2A-C23A	177.45(17)
O1A-Ta1A-Ta2A-C23A	-34.01(16)	N2A-Ta1A-Ta2A-C23A	117.58(17)
N31A-Ta1A-Ta2A-C23A	104.23(16)	N32A-Ta1A-Ta2A-C23A	39.48(16)
C10A-Ta1A-Ta2A-C23A	-108.30(16)	C14A-Ta1A-Ta2A-C23A	-138.47(16)
C11A-Ta1A-Ta2A-C23A	-76.06(16)	C13A-Ta1A-Ta2A-C23A	-135.8(2)
C12A-Ta1A-Ta2A-C23A	-69.3(2)	N2A-Ta2A-O1A-Ta1A	21.12(10)
N1A-Ta2A-O1A-Ta1A	-20.78(9)	N52A-Ta2A-O1A-Ta1A	-114.93(9)
N51A-Ta2A-O1A-Ta1A	-73.81(17)	C20A-Ta2A-O1A-Ta1A	106.30(11)
C21A-Ta2A-O1A-Ta1A	103.28(12)	C24A-Ta2A-O1A-Ta1A	138.28(12)
C22A-Ta2A-O1A-Ta1A	143.91(12)	C23A-Ta2A-O1A-Ta1A	159.62(10)
N1A-Ta1A-O1A-Ta2A	23.20(10)	N2A-Ta1A-O1A-Ta2A	-18.80(9)
N31A-Ta1A-O1A-Ta2A	-75.51(15)	N32A-Ta1A-O1A-Ta2A	-115.77(9)
C10A-Ta1A-O1A-Ta2A	109.34(10)	C14A-Ta1A-O1A-Ta2A	101.94(11)
C11A-Ta1A-O1A-Ta2A	142.12(11)	C13A-Ta1A-O1A-Ta2A	139.60(12)
C12A-Ta1A-O1A-Ta2A	160.68(9)	O1A-Ta1A-N1A-N2A	-80.43(15)
N31A-Ta1A-N1A-N2A	62.72(16)	N32A-Ta1A-N1A-N2A	13.3(2)
C10A-Ta1A-N1A-N2A	-168.75(16)	C14A-Ta1A-N1A-N2A	157.91(16)
C11A-Ta1A-N1A-N2A	-159.38(15)	C13A-Ta1A-N1A-N2A	141.32(15)
C12A-Ta1A-N1A-N2A	165.67(16)	Ta2A-Ta1A-N1A-N2A	-59.68(13)
O1A-Ta1A-N1A-Ta2A	-20.75(9)	N2A-Ta1A-N1A-Ta2A	59.68(13)
N31A-Ta1A-N1A-Ta2A	122.41(10)	N32A-Ta1A-N1A-Ta2A	72.94(17)
C10A-Ta1A-N1A-Ta2A	-109.07(11)	C14A-Ta1A-N1A-Ta2A	-142.41(11)
C11A-Ta1A-N1A-Ta2A	-99.70(12)	C13A-Ta1A-N1A-Ta2A	-159.00(9)
C12A-Ta1A-N1A-Ta2A	-134.65(13)	O1A-Ta2A-N1A-N2A	97.53(15)
N52A-Ta2A-N1A-N2A	-167.35(14)	N51A-Ta2A-N1A-N2A	-111.16(15)
C20A-Ta2A-N1A-N2A	13.96(19)	C21A-Ta2A-N1A-N2A	-27.24(18)
C24A-Ta2A-N1A-N2A	49.8(3)	C22A-Ta2A-N1A-N2A	-64.0(2)
Ta1A-Ta2A-N1A-N2A	76.48(14)	N2A-Ta2A-N1A-Ta1A	-76.48(14)

O1A-Ta2A-N1A-Ta1A	21.05(9)	N52A-Ta2A-N1A-Ta1A	116.17(10)
N51A-Ta2A-N1A-Ta1A	172.36(11)	C20A-Ta2A-N1A-Ta1A	-62.52(15)
C21A-Ta2A-N1A-Ta1A	-103.71(12)	C24A-Ta2A-N1A-Ta1A	-26.7(3)
C22A-Ta2A-N1A-Ta1A	-140.45(14)	Ta1A-N1A-N2A-Ta2A	95.82(9)
Ta2A-N1A-N2A-Ta1A	-95.82(9)	O1A-Ta2A-N2A-N1A	-78.52(14)
N52A-Ta2A-N2A-N1A	18.3(2)	N51A-Ta2A-N2A-N1A	65.68(14)
C20A-Ta2A-N2A-N1A	-168.79(15)	C21A-Ta2A-N2A-N1A	157.33(15)
C24A-Ta2A-N2A-N1A	-156.14(14)	C22A-Ta2A-N2A-N1A	143.48(14)
C23A-Ta2A-N2A-N1A	172.17(16)	Ta1A-Ta2A-N2A-N1A	-59.63(12)
O1A-Ta2A-N2A-Ta1A	-18.89(9)	N1A-Ta2A-N2A-Ta1A	59.63(12)
N52A-Ta2A-N2A-Ta1A	77.92(14)	N51A-Ta2A-N2A-Ta1A	125.31(9)
C20A-Ta2A-N2A-Ta1A	-109.16(10)	C21A-Ta2A-N2A-Ta1A	-143.04(11)
C24A-Ta2A-N2A-Ta1A	-96.51(12)	C22A-Ta2A-N2A-Ta1A	-156.89(9)
C23A-Ta2A-N2A-Ta1A	-128.19(15)	O1A-Ta1A-N2A-N1A	95.32(15)
N31A-Ta1A-N2A-N1A	-115.64(16)	N32A-Ta1A-N2A-N1A	-171.27(15)
C10A-Ta1A-N2A-N1A	14.2(2)	C14A-Ta1A-N2A-N1A	-25.62(19)
C11A-Ta1A-N2A-N1A	46.4(3)	C13A-Ta1A-N2A-N1A	-61.9(2)
C12A-Ta1A-N2A-N1A	-81.9(6)	Ta2A-Ta1A-N2A-N1A	76.28(15)
N1A-Ta1A-N2A-Ta2A	-76.28(15)	O1A-Ta1A-N2A-Ta2A	19.04(9)
N31A-Ta1A-N2A-Ta2A	168.08(11)	N32A-Ta1A-N2A-Ta2A	112.45(10)
C10A-Ta1A-N2A-Ta2A	-62.12(15)	C14A-Ta1A-N2A-Ta2A	-101.90(12)
C11A-Ta1A-N2A-Ta2A	-29.9(3)	C13A-Ta1A-N2A-Ta2A	-138.22(13)
C12A-Ta1A-N2A-Ta2A	-158.1(5)	N1A-Ta1A-C10A-C11A	164.8(2)
O1A-Ta1A-C10A-C11A	77.4(2)	N2A-Ta1A-C10A-C11A	155.36(18)
N31A-Ta1A-C10A-C11A	-98.9(2)	N32A-Ta1A-C10A-C11A	-17.0(3)
C14A-Ta1A-C10A-C11A	-114.2(3)	C13A-Ta1A-C10A-C11A	-77.0(2)
C12A-Ta1A-C10A-C11A	-37.02(19)	Ta2A-Ta1A-C10A-C11A	118.17(18)
N1A-Ta1A-C10A-C14A	-80.97(19)	O1A-Ta1A-C10A-C14A	-168.41(19)
N2A-Ta1A-C10A-C14A	-90.4(2)	N31A-Ta1A-C10A-C14A	15.3(2)
N32A-Ta1A-C10A-C14A	97.2(2)	C11A-Ta1A-C10A-C14A	114.2(3)
C13A-Ta1A-C10A-C14A	37.16(18)	C12A-Ta1A-C10A-C14A	77.2(2)
Ta2A-Ta1A-C10A-C14A	-127.63(17)	N1A-Ta1A-C10A-C15A	38.8(3)
O1A-Ta1A-C10A-C15A	-48.6(3)	N2A-Ta1A-C10A-C15A	29.4(3)
N31A-Ta1A-C10A-C15A	135.1(3)	N32A-Ta1A-C10A-C15A	-143.0(3)
C14A-Ta1A-C10A-C15A	119.8(4)	C11A-Ta1A-C10A-C15A	-126.0(4)
C13A-Ta1A-C10A-C15A	157.0(3)	C12A-Ta1A-C10A-C15A	-163.0(3)
Ta2A-Ta1A-C10A-C15A	-7.8(3)	C14A-C10A-C11A-C12A	-1.1(4)
C15A-C10A-C11A-C12A	-174.0(3)	Ta1A-C10A-C11A-C12A	67.3(2)
C14A-C10A-C11A-C16A	176.7(3)	C15A-C10A-C11A-C16A	3.8(6)
Ta1A-C10A-C11A-C16A	-114.8(3)	C14A-C10A-C11A-Ta1A	-68.4(2)
C15A-C10A-C11A-Ta1A	118.7(3)	N1A-Ta1A-C11A-C12A	-131.7(2)
O1A-Ta1A-C11A-C12A	145.9(2)	N2A-Ta1A-C11A-C12A	-165.2(2)
N31A-Ta1A-C11A-C12A	-7.1(2)	N32A-Ta1A-C11A-C12A	53.2(2)
C10A-Ta1A-C11A-C12A	-114.5(3)	C14A-Ta1A-C11A-C12A	-76.7(2)

C13A-Ta1A-C11A-C12A	-36.28(19)	Ta2A-Ta1A-C11A-C12A	173.22(17)
N1A-Ta1A-C11A-C10A	-17.2(2)	O1A-Ta1A-C11A-C10A	-99.6(2)
N2A-Ta1A-C11A-C10A	-50.6(3)	N31A-Ta1A-C11A-C10A	107.5(2)
N32A-Ta1A-C11A-C10A	167.73(19)	C14A-Ta1A-C11A-C10A	37.84(19)
C13A-Ta1A-C11A-C10A	78.3(2)	C12A-Ta1A-C11A-C10A	114.5(3)
Ta2A-Ta1A-C11A-C10A	-72.2(2)	N1A-Ta1A-C11A-C16A	104.6(3)
O1A-Ta1A-C11A-C16A	22.2(3)	N2A-Ta1A-C11A-C16A	71.1(4)
N31A-Ta1A-C11A-C16A	-130.8(3)	N32A-Ta1A-C11A-C16A	-70.5(3)
C10A-Ta1A-C11A-C16A	121.8(4)	C14A-Ta1A-C11A-C16A	159.6(3)
C13A-Ta1A-C11A-C16A	-160.0(3)	C12A-Ta1A-C11A-C16A	-123.7(4)
Ta2A-Ta1A-C11A-C16A	49.5(3)	C10A-C11A-C12A-C13A	0.9(4)
C16A-C11A-C12A-C13A	-176.9(3)	Ta1A-C11A-C12A-C13A	65.3(2)
C10A-C11A-C12A-C17A	170.3(3)	C16A-C11A-C12A-C17A	-7.6(6)
Ta1A-C11A-C12A-C17A	-125.4(4)	C10A-C11A-C12A-Ta1A	-64.3(2)
C16A-C11A-C12A-Ta1A	117.8(3)	N1A-Ta1A-C12A-C11A	69.9(3)
O1A-Ta1A-C12A-C11A	-35.8(2)	N2A-Ta1A-C12A-C11A	141.3(5)
N31A-Ta1A-C12A-C11A	174.3(2)	N32A-Ta1A-C12A-C11A	-128.0(2)
C10A-Ta1A-C12A-C11A	37.87(19)	C14A-Ta1A-C12A-C11A	79.3(2)
C13A-Ta1A-C12A-C11A	116.2(3)	Ta2A-Ta1A-C12A-C11A	-11.4(3)
N1A-Ta1A-C12A-C13A	-46.4(3)	O1A-Ta1A-C12A-C13A	-152.00(18)
N2A-Ta1A-C12A-C13A	25.0(7)	N31A-Ta1A-C12A-C13A	58.1(2)
N32A-Ta1A-C12A-C13A	115.8(2)	C10A-Ta1A-C12A-C13A	-78.3(2)
C14A-Ta1A-C12A-C13A	-36.87(19)	C11A-Ta1A-C12A-C13A	-116.2(3)
Ta2A-Ta1A-C12A-C13A	-127.58(18)	N1A-Ta1A-C12A-C17A	-167.1(3)
O1A-Ta1A-C12A-C17A	87.2(3)	N2A-Ta1A-C12A-C17A	-95.7(6)
N31A-Ta1A-C12A-C17A	-62.7(3)	N32A-Ta1A-C12A-C17A	-5.0(3)
C10A-Ta1A-C12A-C17A	160.9(4)	C14A-Ta1A-C12A-C17A	-157.6(4)
C11A-Ta1A-C12A-C17A	123.0(4)	C13A-Ta1A-C12A-C17A	-120.8(4)
Ta2A-Ta1A-C12A-C17A	111.7(3)	C11A-C12A-C13A-C14A	-0.4(4)
C17A-C12A-C13A-C14A	-170.1(3)	Ta1A-C12A-C13A-C14A	63.7(2)
C11A-C12A-C13A-C18A	171.3(3)	C17A-C12A-C13A-C18A	1.6(5)
Ta1A-C12A-C13A-C18A	-124.6(3)	C11A-C12A-C13A-Ta1A	-64.1(2)
C17A-C12A-C13A-Ta1A	126.2(3)	N1A-Ta1A-C13A-C14A	31.5(2)
O1A-Ta1A-C13A-C14A	-76.2(2)	N2A-Ta1A-C13A-C14A	70.6(3)
N31A-Ta1A-C13A-C14A	124.7(2)	N32A-Ta1A-C13A-C14A	-179.8(2)
C10A-Ta1A-C13A-C14A	-38.0(2)	C11A-Ta1A-C13A-C14A	-79.2(2)
C12A-Ta1A-C13A-C14A	-115.8(3)	Ta2A-Ta1A-C13A-C14A	-4.2(3)
N1A-Ta1A-C13A-C12A	147.31(19)	O1A-Ta1A-C13A-C12A	39.6(2)
N2A-Ta1A-C13A-C12A	-173.59(18)	N31A-Ta1A-C13A-C12A	-119.6(2)
N32A-Ta1A-C13A-C12A	-64.0(2)	C10A-Ta1A-C13A-C12A	77.8(2)
C14A-Ta1A-C13A-C12A	115.8(3)	C11A-Ta1A-C13A-C12A	36.54(19)
Ta2A-Ta1A-C13A-C12A	111.5(2)	N1A-Ta1A-C13A-C18A	-91.9(3)
O1A-Ta1A-C13A-C18A	160.4(3)	N2A-Ta1A-C13A-C18A	-52.8(4)
N31A-Ta1A-C13A-C18A	1.2(3)	N32A-Ta1A-C13A-C18A	56.7(3)

C10A-Ta1A-C13A-C18A	-161.5(3)	C14A-Ta1A-C13A-C18A	-123.5(4)
C11A-Ta1A-C13A-C18A	157.3(3)	C12A-Ta1A-C13A-C18A	120.8(4)
Ta2A-Ta1A-C13A-C18A	-127.7(3)	C11A-C10A-C14A-C13A	0.9(4)
C15A-C10A-C14A-C13A	174.2(3)	Ta1A-C10A-C14A-C13A	-68.0(2)
C11A-C10A-C14A-C19A	-173.2(3)	C15A-C10A-C14A-C19A	0.1(5)
Ta1A-C10A-C14A-C19A	117.9(3)	C11A-C10A-C14A-Ta1A	68.9(2)
C15A-C10A-C14A-Ta1A	-117.8(3)	C12A-C13A-C14A-C10A	-0.3(4)
C18A-C13A-C14A-C10A	-171.6(3)	Ta1A-C13A-C14A-C10A	65.1(2)
C12A-C13A-C14A-C19A	173.4(3)	C18A-C13A-C14A-C19A	2.1(6)
Ta1A-C13A-C14A-C19A	-121.2(3)	C12A-C13A-C14A-Ta1A	-65.4(2)
C18A-C13A-C14A-Ta1A	123.3(3)	N1A-Ta1A-C14A-C10A	95.4(2)
O1A-Ta1A-C14A-C10A	13.5(2)	N2A-Ta1A-C14A-C10A	112.44(19)
N31A-Ta1A-C14A-C10A	-168.03(18)	N32A-Ta1A-C14A-C10A	-114.1(2)
C11A-Ta1A-C14A-C10A	-37.68(18)	C13A-Ta1A-C14A-C10A	-114.4(3)
C12A-Ta1A-C14A-C10A	-77.9(2)	Ta2A-Ta1A-C14A-C10A	63.4(2)
N1A-Ta1A-C14A-C13A	-150.3(2)	O1A-Ta1A-C14A-C13A	127.88(19)
N2A-Ta1A-C14A-C13A	-133.2(2)	N31A-Ta1A-C14A-C13A	-53.7(2)
N32A-Ta1A-C14A-C13A	0.2(3)	C10A-Ta1A-C14A-C13A	114.4(3)
C11A-Ta1A-C14A-C13A	76.7(2)	C12A-Ta1A-C14A-C13A	36.45(19)
Ta2A-Ta1A-C14A-C13A	177.74(17)	N1A-Ta1A-C14A-C19A	-23.5(3)
O1A-Ta1A-C14A-C19A	-105.4(3)	N2A-Ta1A-C14A-C19A	-6.5(3)
N31A-Ta1A-C14A-C19A	73.1(3)	N32A-Ta1A-C14A-C19A	127.0(3)
C10A-Ta1A-C14A-C19A	-118.9(4)	C11A-Ta1A-C14A-C19A	-156.6(3)
C13A-Ta1A-C14A-C19A	126.7(4)	C12A-Ta1A-C14A-C19A	163.2(3)
Ta2A-Ta1A-C14A-C19A	-55.5(3)	N2A-Ta2A-C20A-C21A	-87.0(2)
O1A-Ta2A-C20A-C21A	-175.5(2)	N1A-Ta2A-C20A-C21A	-96.4(2)
N52A-Ta2A-C20A-C21A	85.6(2)	N51A-Ta2A-C20A-C21A	4.6(3)
C24A-Ta2A-C20A-C21A	113.8(3)	C22A-Ta2A-C20A-C21A	37.3(2)
C23A-Ta2A-C20A-C21A	77.2(2)	Ta1A-Ta2A-C20A-C21A	-133.79(19)
N2A-Ta2A-C20A-C24A	159.2(2)	O1A-Ta2A-C20A-C24A	70.7(2)
N1A-Ta2A-C20A-C24A	149.80(19)	N52A-Ta2A-C20A-C24A	-28.2(3)
N51A-Ta2A-C20A-C24A	-109.2(2)	C21A-Ta2A-C20A-C24A	-113.8(3)
C22A-Ta2A-C20A-C24A	-76.5(2)	C23A-Ta2A-C20A-C24A	-36.6(2)
Ta1A-Ta2A-C20A-C24A	112.40(19)	N2A-Ta2A-C20A-C25A	33.9(3)
O1A-Ta2A-C20A-C25A	-54.5(3)	N1A-Ta2A-C20A-C25A	24.6(3)
N52A-Ta2A-C20A-C25A	-153.5(3)	N51A-Ta2A-C20A-C25A	125.5(3)
C21A-Ta2A-C20A-C25A	120.9(4)	C24A-Ta2A-C20A-C25A	-125.2(4)
C22A-Ta2A-C20A-C25A	158.3(4)	C23A-Ta2A-C20A-C25A	-161.9(4)
Ta1A-Ta2A-C20A-C25A	-12.8(3)	C24A-C20A-C21A-C22A	0.4(4)
C25A-C20A-C21A-C22A	172.8(3)	Ta2A-C20A-C21A-C22A	-68.6(2)
C24A-C20A-C21A-C26A	-175.3(3)	C25A-C20A-C21A-C26A	-3.0(5)
Ta2A-C20A-C21A-C26A	115.7(3)	C24A-C20A-C21A-Ta2A	69.1(2)
C25A-C20A-C21A-Ta2A	-118.6(3)	N2A-Ta2A-C21A-C22A	-156.3(2)
O1A-Ta2A-C21A-C22A	119.4(2)	N1A-Ta2A-C21A-C22A	-138.2(2)

N52A-Ta2A-C21A-C22A	-10.8(3)	N51A-Ta2A-C21A-C22A	-62.3(2)
C20A-Ta2A-C21A-C22A	113.9(3)	C24A-Ta2A-C21A-C22A	76.0(2)
C23A-Ta2A-C21A-C22A	36.1(2)	Ta1A-Ta2A-C21A-C22A	171.06(17)
N2A-Ta2A-C21A-C20A	89.8(2)	O1A-Ta2A-C21A-C20A	5.4(2)
N1A-Ta2A-C21A-C20A	107.8(2)	N52A-Ta2A-C21A-C20A	-124.7(2)
N51A-Ta2A-C21A-C20A	-176.3(2)	C24A-Ta2A-C21A-C20A	-37.9(2)
C22A-Ta2A-C21A-C20A	-113.9(3)	C23A-Ta2A-C21A-C20A	-77.8(2)
Ta1A-Ta2A-C21A-C20A	57.1(2)	N2A-Ta2A-C21A-C26A	-29.8(3)
O1A-Ta2A-C21A-C26A	-114.2(3)	N1A-Ta2A-C21A-C26A	-11.8(3)
N52A-Ta2A-C21A-C26A	115.7(3)	N51A-Ta2A-C21A-C26A	64.1(3)
C20A-Ta2A-C21A-C26A	-119.6(4)	C24A-Ta2A-C21A-C26A	-157.6(3)
C22A-Ta2A-C21A-C26A	126.4(4)	C23A-Ta2A-C21A-C26A	162.6(3)
Ta1A-Ta2A-C21A-C26A	-62.5(3)	C20A-C21A-C22A-C23A	0.0(4)
C26A-C21A-C22A-C23A	175.5(3)	Ta2A-C21A-C22A-C23A	-66.0(2)
C20A-C21A-C22A-C27A	-170.1(3)	C26A-C21A-C22A-C27A	5.4(6)
Ta2A-C21A-C22A-C27A	123.9(4)	C20A-C21A-C22A-Ta2A	66.0(2)
C26A-C21A-C22A-Ta2A	-118.5(4)	N2A-Ta2A-C22A-C21A	26.1(2)
O1A-Ta2A-C22A-C21A	-86.8(2)	N1A-Ta2A-C22A-C21A	67.6(3)
N52A-Ta2A-C22A-C21A	171.3(2)	N51A-Ta2A-C22A-C21A	114.8(2)
C20A-Ta2A-C22A-C21A	-38.4(2)	C24A-Ta2A-C22A-C21A	-79.9(2)
C23A-Ta2A-C22A-C21A	-116.2(3)	Ta1A-Ta2A-C22A-C21A	-17.8(3)
N2A-Ta2A-C22A-C23A	142.3(2)	O1A-Ta2A-C22A-C23A	29.4(3)
N1A-Ta2A-C22A-C23A	-176.15(19)	N52A-Ta2A-C22A-C23A	-72.5(2)
N51A-Ta2A-C22A-C23A	-129.0(2)	C20A-Ta2A-C22A-C23A	77.8(2)
C21A-Ta2A-C22A-C23A	116.2(3)	C24A-Ta2A-C22A-C23A	36.3(2)
Ta1A-Ta2A-C22A-C23A	98.4(3)	N2A-Ta2A-C22A-C27A	-97.6(4)
O1A-Ta2A-C22A-C27A	149.6(3)	N1A-Ta2A-C22A-C27A	-56.0(4)
N52A-Ta2A-C22A-C27A	47.7(4)	N51A-Ta2A-C22A-C27A	-8.8(4)
C20A-Ta2A-C22A-C27A	-162.1(4)	C21A-Ta2A-C22A-C27A	-123.6(5)
C24A-Ta2A-C22A-C27A	156.5(4)	C23A-Ta2A-C22A-C27A	120.2(5)
Ta1A-Ta2A-C22A-C27A	-141.4(3)	C21A-C22A-C23A-C24A	-0.4(4)
C27A-C22A-C23A-C24A	170.3(3)	Ta2A-C22A-C23A-C24A	-63.9(2)
C21A-C22A-C23A-C28A	-170.0(3)	C27A-C22A-C23A-C28A	0.6(6)
Ta2A-C22A-C23A-C28A	126.5(3)	C21A-C22A-C23A-Ta2A	63.5(2)
C27A-C22A-C23A-Ta2A	-125.9(3)	N2A-Ta2A-C23A-C22A	-55.0(3)
O1A-Ta2A-C23A-C22A	-158.4(2)	N52A-Ta2A-C23A-C22A	107.0(2)
N51A-Ta2A-C23A-C22A	50.0(2)	C20A-Ta2A-C23A-C22A	-78.6(2)
C21A-Ta2A-C23A-C22A	-36.76(19)	C24A-Ta2A-C23A-C22A	-116.5(3)
Ta1A-Ta2A-C23A-C22A	-135.32(18)	N2A-Ta2A-C23A-C24A	61.5(3)
O1A-Ta2A-C23A-C24A	-41.9(2)	N52A-Ta2A-C23A-C24A	-136.5(2)
N51A-Ta2A-C23A-C24A	166.4(2)	C20A-Ta2A-C23A-C24A	37.9(2)
C21A-Ta2A-C23A-C24A	79.7(2)	C22A-Ta2A-C23A-C24A	116.5(3)
Ta1A-Ta2A-C23A-C24A	-18.8(3)	N2A-Ta2A-C23A-C28A	-176.2(3)
O1A-Ta2A-C23A-C28A	80.4(4)	N52A-Ta2A-C23A-C28A	-14.1(4)

N51A-Ta2A-C23A-C28A	-71.2(4)	C20A-Ta2A-C23A-C28A	160.3(4)
C21A-Ta2A-C23A-C28A	-157.9(4)	C24A-Ta2A-C23A-C28A	122.3(5)
C22A-Ta2A-C23A-C28A	-121.2(5)	Ta1A-Ta2A-C23A-C28A	103.5(4)
C22A-C23A-C24A-C20A	0.7(4)	C28A-C23A-C24A-C20A	170.1(3)
Ta2A-C23A-C24A-C20A	-63.6(2)	C22A-C23A-C24A-C29A	-177.3(3)
C28A-C23A-C24A-C29A	-7.8(6)	Ta2A-C23A-C24A-C29A	118.4(3)
C22A-C23A-C24A-Ta2A	64.3(2)	C28A-C23A-C24A-Ta2A	-126.2(4)
C21A-C20A-C24A-C23A	-0.7(4)	C25A-C20A-C24A-C23A	-172.7(3)
Ta2A-C20A-C24A-C23A	67.0(2)	C21A-C20A-C24A-C29A	177.2(3)
C25A-C20A-C24A-C29A	5.2(6)	Ta2A-C20A-C24A-C29A	-115.1(4)
C21A-C20A-C24A-Ta2A	-67.7(2)	C25A-C20A-C24A-Ta2A	120.3(3)
N2A-Ta2A-C24A-C23A	-138.1(2)	O1A-Ta2A-C24A-C23A	138.8(2)
N1A-Ta2A-C24A-C23A	-173.1(2)	N52A-Ta2A-C24A-C23A	45.9(2)
N51A-Ta2A-C24A-C23A	-17.5(3)	C20A-Ta2A-C24A-C23A	-114.8(3)
C21A-Ta2A-C24A-C23A	-76.7(2)	C22A-Ta2A-C24A-C23A	-36.2(2)
Ta1A-Ta2A-C24A-C23A	167.91(19)	N2A-Ta2A-C24A-C20A	-23.3(2)
O1A-Ta2A-C24A-C20A	-106.4(2)	N1A-Ta2A-C24A-C20A	-58.3(3)
N52A-Ta2A-C24A-C20A	160.78(19)	N51A-Ta2A-C24A-C20A	97.4(2)
C21A-Ta2A-C24A-C20A	38.19(19)	C22A-Ta2A-C24A-C20A	78.7(2)
C23A-Ta2A-C24A-C20A	114.8(3)	Ta1A-Ta2A-C24A-C20A	-77.2(2)
N2A-Ta2A-C24A-C29A	99.5(3)	O1A-Ta2A-C24A-C29A	16.4(3)
N1A-Ta2A-C24A-C29A	64.5(4)	N52A-Ta2A-C24A-C29A	-76.4(3)
N51A-Ta2A-C24A-C29A	-139.8(3)	C20A-Ta2A-C24A-C29A	122.8(4)
C21A-Ta2A-C24A-C29A	161.0(4)	C22A-Ta2A-C24A-C29A	-158.5(4)
C23A-Ta2A-C24A-C29A	-122.4(4)	Ta1A-Ta2A-C24A-C29A	45.6(3)
N1A-Ta1A-N31A-C30A	-141.46(19)	O1A-Ta1A-N31A-C30A	-46.1(2)
N2A-Ta1A-N31A-C30A	-103.85(19)	N32A-Ta1A-N31A-C30A	2.85(17)
C10A-Ta1A-N31A-C30A	127.69(19)	C14A-Ta1A-N31A-C30A	136.10(19)
C11A-Ta1A-N31A-C30A	85.6(2)	C13A-Ta1A-N31A-C30A	109.55(19)
C12A-Ta1A-N31A-C30A	81.75(19)	Ta2A-Ta1A-N31A-C30A	-94.75(17)
N1A-Ta1A-N31A-C37A	10.1(3)	O1A-Ta1A-N31A-C37A	105.4(3)
N2A-Ta1A-N31A-C37A	47.7(3)	N32A-Ta1A-N31A-C37A	154.4(3)
C10A-Ta1A-N31A-C37A	-80.8(3)	C14A-Ta1A-N31A-C37A	-72.4(3)
C11A-Ta1A-N31A-C37A	-122.9(3)	C13A-Ta1A-N31A-C37A	-98.9(3)
C12A-Ta1A-N31A-C37A	-126.7(3)	Ta2A-Ta1A-N31A-C37A	56.8(3)
N1A-Ta1A-N32A-C30A	59.0(3)	O1A-Ta1A-N32A-C30A	150.07(19)
N2A-Ta1A-N32A-C30A	68.0(2)	N31A-Ta1A-N32A-C30A	-2.86(17)
C10A-Ta1A-N32A-C30A	-118.1(2)	C14A-Ta1A-N32A-C30A	-72.9(2)
C11A-Ta1A-N32A-C30A	-127.60(19)	C13A-Ta1A-N32A-C30A	-72.8(2)
C12A-Ta1A-N32A-C30A	-101.8(2)	Ta2A-Ta1A-N32A-C30A	109.37(18)
N1A-Ta1A-N32A-C40A	-118.8(4)	O1A-Ta1A-N32A-C40A	-27.7(4)
N2A-Ta1A-N32A-C40A	-109.8(4)	N31A-Ta1A-N32A-C40A	179.3(4)
C10A-Ta1A-N32A-C40A	64.1(4)	C14A-Ta1A-N32A-C40A	109.3(4)
C11A-Ta1A-N32A-C40A	54.6(4)	C13A-Ta1A-N32A-C40A	109.4(4)

C12A-Ta1A-N32A-C40A	80.4(4)	Ta2A-Ta1A-N32A-C40A	-68.4(4)
C40A-N32A-C30A-N31A	-177.2(3)	Ta1A-N32A-C30A-N31A	4.4(3)
C40A-N32A-C30A-C31A	3.2(5)	Ta1A-N32A-C30A-C31A	-175.2(3)
C37A-N31A-C30A-N32A	-162.1(3)	Ta1A-N31A-C30A-N32A	-4.5(3)
C37A-N31A-C30A-C31A	17.5(4)	Ta1A-N31A-C30A-C31A	175.1(3)
N32A-C30A-C31A-C36A	59.6(5)	N31A-C30A-C31A-C36A	-120.0(4)
N32A-C30A-C31A-C32A	-119.9(4)	N31A-C30A-C31A-C32A	60.5(4)
C36A-C31A-C32A-C33A	-0.7(5)	C30A-C31A-C32A-C33A	178.8(3)
C31A-C32A-C33A-C34A	0.1(5)	C32A-C33A-C34A-C35A	0.8(6)
C33A-C34A-C35A-C36A	-1.1(6)	C34A-C35A-C36A-C31A	0.4(6)
C32A-C31A-C36A-C35A	0.5(5)	C30A-C31A-C36A-C35A	-179.0(3)
C30A-N31A-C37A-C38A	179.4(3)	Ta1A-N31A-C37A-C38A	33.3(4)
C30A-N31A-C37A-C39A	57.8(4)	Ta1A-N31A-C37A-C39A	-88.3(4)
C30A-N32A-C40A-C41A	177.6(3)	Ta1A-N32A-C40A-C41A	-5.1(5)
C30A-N32A-C40A-C42A	54.0(4)	Ta1A-N32A-C40A-C42A	-128.6(3)
N2A-Ta2A-N51A-C50A	-138.22(19)	O1A-Ta2A-N51A-C50A	-45.1(3)
N1A-Ta2A-N51A-C50A	-99.20(19)	N52A-Ta2A-N51A-C50A	4.95(17)
C20A-Ta2A-N51A-C50A	134.77(19)	C21A-Ta2A-N51A-C50A	137.32(19)
C24A-Ta2A-N51A-C50A	92.4(2)	C22A-Ta2A-N51A-C50A	107.8(2)
C23A-Ta2A-N51A-C50A	83.0(2)	Ta1A-Ta2A-N51A-C50A	-93.34(18)
N2A-Ta2A-N51A-C57A	11.0(3)	O1A-Ta2A-N51A-C57A	104.1(3)
N1A-Ta2A-N51A-C57A	50.0(3)	N52A-Ta2A-N51A-C57A	154.1(4)
C20A-Ta2A-N51A-C57A	-76.1(4)	C21A-Ta2A-N51A-C57A	-73.5(3)
C24A-Ta2A-N51A-C57A	-118.4(3)	C22A-Ta2A-N51A-C57A	-103.0(4)
C23A-Ta2A-N51A-C57A	-127.8(3)	Ta1A-Ta2A-N51A-C57A	55.8(4)
N2A-Ta2A-N52A-C50A	54.4(2)	O1A-Ta2A-N52A-C50A	148.26(18)
N1A-Ta2A-N52A-C50A	66.65(19)	N51A-Ta2A-N52A-C50A	-4.92(17)
C20A-Ta2A-N52A-C50A	-114.9(2)	C21A-Ta2A-N52A-C50A	-71.5(2)
C24A-Ta2A-N52A-C50A	-130.83(19)	C22A-Ta2A-N52A-C50A	-77.3(2)
C23A-Ta2A-N52A-C50A	-108.1(2)	Ta1A-Ta2A-N52A-C50A	106.90(17)
N2A-Ta2A-N52A-C60A	-118.8(3)	O1A-Ta2A-N52A-C60A	-25.0(3)
N1A-Ta2A-N52A-C60A	-106.6(3)	N51A-Ta2A-N52A-C60A	-178.1(4)
C20A-Ta2A-N52A-C60A	71.8(4)	C21A-Ta2A-N52A-C60A	115.3(3)
C24A-Ta2A-N52A-C60A	56.0(4)	C22A-Ta2A-N52A-C60A	109.5(3)
C23A-Ta2A-N52A-C60A	78.7(3)	Ta1A-Ta2A-N52A-C60A	-66.3(3)
C57A-N51A-C50A-N52A	-166.0(3)	Ta2A-N51A-C50A-N52A	-7.7(3)
C57A-N51A-C50A-C51A	13.7(5)	Ta2A-N51A-C50A-C51A	172.0(3)
C60A-N52A-C50A-N51A	-177.1(3)	Ta2A-N52A-C50A-N51A	8.0(3)
C60A-N52A-C50A-C51A	3.2(5)	Ta2A-N52A-C50A-C51A	-171.7(3)
N51A-C50A-C51A-C52A	69.9(4)	N52A-C50A-C51A-C52A	-110.4(4)
N51A-C50A-C51A-C56A	-112.3(4)	N52A-C50A-C51A-C56A	67.3(4)
C56A-C51A-C52A-C53A	-0.7(5)	C50A-C51A-C52A-C53A	177.0(3)
C51A-C52A-C53A-C54A	-0.2(6)	C52A-C53A-C54A-C55A	0.7(6)
C53A-C54A-C55A-C56A	-0.4(6)	C54A-C55A-C56A-C51A	-0.5(5)

C52A-C51A-C56A-C55A	1.0(5)	C50A-C51A-C56A-C55A	-176.7(3)
C50A-N51A-C57A-C58A	127.6(4)	Ta2A-N51A-C57A-C58A	-16.1(5)
C50A-N51A-C57A-C59A	-108.2(4)	Ta2A-N51A-C57A-C59A	108.1(4)
C50A-N52A-C60A-C61A	-178.4(3)	Ta2A-N52A-C60A-C61A	-6.5(5)
C50A-N52A-C60A-C62A	58.8(4)	Ta2A-N52A-C60A-C62A	-129.3(3)
N1B-Ta1B-Ta2B-N2B	-58.40(14)	O1B-Ta1B-Ta2B-N2B	151.86(13)
N32B-Ta1B-Ta2B-N2B	11.21(13)	N31B-Ta1B-Ta2B-N2B	75.95(13)
C10B-Ta1B-Ta2B-N2B	-135.35(13)	C14B-Ta1B-Ta2B-N2B	-167.73(14)
C11B-Ta1B-Ta2B-N2B	-105.41(14)	C13B-Ta1B-Ta2B-N2B	-175.22(18)
C12B-Ta1B-Ta2B-N2B	-107.5(2)	N1B-Ta1B-Ta2B-O1B	149.74(13)
N2B-Ta1B-Ta2B-O1B	-151.86(13)	N32B-Ta1B-Ta2B-O1B	-140.65(12)
N31B-Ta1B-Ta2B-O1B	-75.91(12)	C10B-Ta1B-Ta2B-O1B	72.78(12)
C14B-Ta1B-Ta2B-O1B	40.40(13)	C11B-Ta1B-Ta2B-O1B	102.73(13)
C13B-Ta1B-Ta2B-O1B	32.92(17)	C12B-Ta1B-Ta2B-O1B	100.64(19)
O1B-Ta1B-Ta2B-N1B	-149.74(13)	N2B-Ta1B-Ta2B-N1B	58.40(14)
N32B-Ta1B-Ta2B-N1B	69.61(13)	N31B-Ta1B-Ta2B-N1B	134.35(12)
C10B-Ta1B-Ta2B-N1B	-76.95(13)	C14B-Ta1B-Ta2B-N1B	-109.33(13)
C11B-Ta1B-Ta2B-N1B	-47.01(14)	C13B-Ta1B-Ta2B-N1B	-116.82(18)
C12B-Ta1B-Ta2B-N1B	-49.1(2)	N1B-Ta1B-Ta2B-N51B	68.12(12)
O1B-Ta1B-Ta2B-N51B	-81.61(11)	N2B-Ta1B-Ta2B-N51B	126.52(13)
N32B-Ta1B-Ta2B-N51B	137.73(11)	N31B-Ta1B-Ta2B-N51B	-157.53(10)
C10B-Ta1B-Ta2B-N51B	-8.83(11)	C14B-Ta1B-Ta2B-N51B	-41.21(12)
C11B-Ta1B-Ta2B-N51B	21.11(12)	C13B-Ta1B-Ta2B-N51B	-48.70(16)
C12B-Ta1B-Ta2B-N51B	19.03(19)	N1B-Ta1B-Ta2B-N52B	3.78(12)
O1B-Ta1B-Ta2B-N52B	-145.96(11)	N2B-Ta1B-Ta2B-N52B	62.18(13)
N32B-Ta1B-Ta2B-N52B	73.39(11)	N31B-Ta1B-Ta2B-N52B	138.13(10)
C10B-Ta1B-Ta2B-N52B	-73.17(11)	C14B-Ta1B-Ta2B-N52B	-105.55(12)
C11B-Ta1B-Ta2B-N52B	-43.23(12)	C13B-Ta1B-Ta2B-N52B	-113.04(16)
C12B-Ta1B-Ta2B-N52B	-45.31(19)	N1B-Ta1B-Ta2B-C20B	-126.44(13)
O1B-Ta1B-Ta2B-C20B	83.82(13)	N2B-Ta1B-Ta2B-C20B	-68.04(14)
N32B-Ta1B-Ta2B-C20B	-56.83(12)	N31B-Ta1B-Ta2B-C20B	7.91(12)
C10B-Ta1B-Ta2B-C20B	156.61(13)	C14B-Ta1B-Ta2B-C20B	124.23(13)
C11B-Ta1B-Ta2B-C20B	-173.45(13)	C13B-Ta1B-Ta2B-C20B	116.74(17)
C12B-Ta1B-Ta2B-C20B	-175.53(19)	N1B-Ta1B-Ta2B-C21B	-99.75(14)
O1B-Ta1B-Ta2B-C21B	110.51(13)	N2B-Ta1B-Ta2B-C21B	-41.35(14)
N32B-Ta1B-Ta2B-C21B	-30.14(13)	N31B-Ta1B-Ta2B-C21B	34.60(12)
C10B-Ta1B-Ta2B-C21B	-176.70(13)	C14B-Ta1B-Ta2B-C21B	150.91(14)
C11B-Ta1B-Ta2B-C21B	-146.76(14)	C13B-Ta1B-Ta2B-C21B	143.43(18)
C12B-Ta1B-Ta2B-C21B	-148.8(2)	N1B-Ta1B-Ta2B-C22B	-119.7(2)
O1B-Ta1B-Ta2B-C22B	90.5(2)	N2B-Ta1B-Ta2B-C22B	-61.3(2)
N32B-Ta1B-Ta2B-C22B	-50.1(2)	N31B-Ta1B-Ta2B-C22B	14.6(2)
C10B-Ta1B-Ta2B-C22B	163.3(2)	C14B-Ta1B-Ta2B-C22B	131.0(2)
C11B-Ta1B-Ta2B-C22B	-166.7(2)	C13B-Ta1B-Ta2B-C22B	123.5(3)
C12B-Ta1B-Ta2B-C22B	-168.8(3)	N1B-Ta1B-Ta2B-C24B	-160.22(13)

O1B-Ta1B-Ta2B-C24B	50.05(13)	N2B-Ta1B-Ta2B-C24B	-101.82(14)
N32B-Ta1B-Ta2B-C24B	-90.61(12)	N31B-Ta1B-Ta2B-C24B	-25.87(12)
C10B-Ta1B-Ta2B-C24B	122.83(13)	C14B-Ta1B-Ta2B-C24B	90.45(13)
C11B-Ta1B-Ta2B-C24B	152.77(13)	C13B-Ta1B-Ta2B-C24B	82.96(17)
C12B-Ta1B-Ta2B-C24B	150.7(2)	N1B-Ta1B-Ta2B-C23B	-176.18(15)
O1B-Ta1B-Ta2B-C23B	34.09(15)	N2B-Ta1B-Ta2B-C23B	-117.78(16)
N32B-Ta1B-Ta2B-C23B	-106.57(14)	N31B-Ta1B-Ta2B-C23B	-41.83(14)
C10B-Ta1B-Ta2B-C23B	106.87(15)	C14B-Ta1B-Ta2B-C23B	74.49(15)
C11B-Ta1B-Ta2B-C23B	136.81(15)	C13B-Ta1B-Ta2B-C23B	67.00(19)
C12B-Ta1B-Ta2B-C23B	134.7(2)	N2B-Ta2B-O1B-Ta1B	-21.00(10)
N1B-Ta2B-O1B-Ta1B	19.93(9)	N51B-Ta2B-O1B-Ta1B	111.03(9)
N52B-Ta2B-O1B-Ta1B	64.45(17)	C20B-Ta2B-O1B-Ta1B	-103.35(10)
C21B-Ta2B-O1B-Ta1B	-105.39(12)	C22B-Ta2B-O1B-Ta1B	-149.30(11)
C24B-Ta2B-O1B-Ta1B	-132.93(11)	C23B-Ta2B-O1B-Ta1B	-158.27(9)
N1B-Ta1B-O1B-Ta2B	-22.64(10)	N2B-Ta1B-O1B-Ta2B	18.70(9)
N32B-Ta1B-O1B-Ta2B	72.93(17)	N31B-Ta1B-O1B-Ta2B	114.21(9)
C10B-Ta1B-O1B-Ta2B	-110.69(10)	C14B-Ta1B-O1B-Ta2B	-143.42(11)
C11B-Ta1B-O1B-Ta2B	-103.22(11)	C13B-Ta1B-O1B-Ta2B	-162.15(9)
C12B-Ta1B-O1B-Ta2B	-139.99(12)	O1B-Ta1B-N1B-N2B	79.51(15)
N32B-Ta1B-N1B-N2B	-65.07(15)	N31B-Ta1B-N1B-N2B	-17.7(2)
C10B-Ta1B-N1B-N2B	167.02(16)	C14B-Ta1B-N1B-N2B	157.92(15)
C11B-Ta1B-N1B-N2B	-160.16(16)	C13B-Ta1B-N1B-N2B	-164.78(15)
C12B-Ta1B-N1B-N2B	-142.21(15)	Ta2B-Ta1B-N1B-N2B	59.53(13)
O1B-Ta1B-N1B-Ta2B	19.98(9)	N2B-Ta1B-N1B-Ta2B	-59.53(13)
N32B-Ta1B-N1B-Ta2B	-124.60(9)	N31B-Ta1B-N1B-Ta2B	-77.25(15)
C10B-Ta1B-N1B-Ta2B	107.49(10)	C14B-Ta1B-N1B-Ta2B	98.39(12)
C11B-Ta1B-N1B-Ta2B	140.31(11)	C13B-Ta1B-N1B-Ta2B	135.69(12)
C12B-Ta1B-N1B-Ta2B	158.26(9)	O1B-Ta2B-N1B-N2B	-98.32(16)
N51B-Ta2B-N1B-N2B	161.77(16)	N52B-Ta2B-N1B-N2B	105.69(16)
C20B-Ta2B-N1B-N2B	-7.5(2)	C21B-Ta2B-N1B-N2B	32.91(19)
C22B-Ta2B-N1B-N2B	68.0(2)	C24B-Ta2B-N1B-N2B	-41.4(3)
Ta1B-Ta2B-N1B-N2B	-77.84(15)	N2B-Ta2B-N1B-Ta1B	77.84(15)
O1B-Ta2B-N1B-Ta1B	-20.47(9)	N51B-Ta2B-N1B-Ta1B	-120.39(10)
N52B-Ta2B-N1B-Ta1B	-176.47(11)	C20B-Ta2B-N1B-Ta1B	70.33(14)
C21B-Ta2B-N1B-Ta1B	110.76(12)	C22B-Ta2B-N1B-Ta1B	145.83(14)
C24B-Ta2B-N1B-Ta1B	36.4(2)	Ta1B-N1B-N2B-Ta2B	-94.62(9)
Ta2B-N1B-N2B-Ta1B	94.62(9)	O1B-Ta2B-N2B-N1B	78.36(15)
N51B-Ta2B-N2B-N1B	-24.6(2)	N52B-Ta2B-N2B-N1B	-67.84(15)
C20B-Ta2B-N2B-N1B	173.70(17)	C21B-Ta2B-N2B-N1B	-152.61(16)
C22B-Ta2B-N2B-N1B	-142.44(15)	C24B-Ta2B-N2B-N1B	157.57(15)
C23B-Ta2B-N2B-N1B	-177.01(16)	Ta1B-Ta2B-N2B-N1B	59.45(13)
O1B-Ta2B-N2B-Ta1B	18.90(9)	N1B-Ta2B-N2B-Ta1B	-59.45(13)
N51B-Ta2B-N2B-Ta1B	-84.07(14)	N52B-Ta2B-N2B-Ta1B	-127.29(10)
C20B-Ta2B-N2B-Ta1B	114.24(11)	C21B-Ta2B-N2B-Ta1B	147.94(11)

C22B-Ta2B-N2B-Ta1B	158.10(9)	C24B-Ta2B-N2B-Ta1B	98.11(11)
C23B-Ta2B-N2B-Ta1B	123.53(14)	O1B-Ta1B-N2B-N1B	-96.80(15)
N32B-Ta1B-N2B-N1B	112.08(16)	N31B-Ta1B-N2B-N1B	167.88(15)
C10B-Ta1B-N2B-N1B	-16.6(2)	C14B-Ta1B-N2B-N1B	-50.7(3)
C11B-Ta1B-N2B-N1B	23.29(19)	C13B-Ta1B-N2B-N1B	87.7(6)
C12B-Ta1B-N2B-N1B	60.5(2)	Ta2B-Ta1B-N2B-N1B	-77.97(15)
N1B-Ta1B-N2B-Ta2B	77.97(15)	O1B-Ta1B-N2B-Ta2B	-18.83(9)
N32B-Ta1B-N2B-Ta2B	-169.95(12)	N31B-Ta1B-N2B-Ta2B	-114.15(10)
C10B-Ta1B-N2B-Ta2B	61.33(16)	C14B-Ta1B-N2B-Ta2B	27.3(3)
C11B-Ta1B-N2B-Ta2B	101.26(12)	C13B-Ta1B-N2B-Ta2B	165.6(5)
C12B-Ta1B-N2B-Ta2B	138.42(13)	N1B-Ta1B-C10B-C14B	-165.5(2)
O1B-Ta1B-C10B-C14B	-77.04(19)	N2B-Ta1B-C10B-C14B	-154.53(18)
N32B-Ta1B-C10B-C14B	100.3(2)	N31B-Ta1B-C10B-C14B	19.1(3)
C11B-Ta1B-C10B-C14B	114.9(3)	C13B-Ta1B-C10B-C14B	37.77(18)
C12B-Ta1B-C10B-C14B	77.9(2)	Ta2B-Ta1B-C10B-C14B	-117.42(18)
N1B-Ta1B-C10B-C11B	79.6(2)	O1B-Ta1B-C10B-C11B	168.1(2)
N2B-Ta1B-C10B-C11B	90.6(2)	N32B-Ta1B-C10B-C11B	-14.6(3)
N31B-Ta1B-C10B-C11B	-95.8(2)	C14B-Ta1B-C10B-C11B	-114.9(3)
C13B-Ta1B-C10B-C11B	-77.1(2)	C12B-Ta1B-C10B-C11B	-36.95(19)
Ta2B-Ta1B-C10B-C11B	127.71(18)	N1B-Ta1B-C10B-C15B	-40.7(3)
O1B-Ta1B-C10B-C15B	47.8(3)	N2B-Ta1B-C10B-C15B	-29.7(4)
N32B-Ta1B-C10B-C15B	-134.9(3)	N31B-Ta1B-C10B-C15B	143.9(3)
C14B-Ta1B-C10B-C15B	124.8(4)	C11B-Ta1B-C10B-C15B	-120.3(4)
C13B-Ta1B-C10B-C15B	162.6(4)	C12B-Ta1B-C10B-C15B	-157.3(4)
Ta2B-Ta1B-C10B-C15B	7.4(3)	C14B-C10B-C11B-C12B	0.2(4)
C15B-C10B-C11B-C12B	-173.0(3)	Ta1B-C10B-C11B-C12B	67.2(2)
C14B-C10B-C11B-C16B	173.1(3)	C15B-C10B-C11B-C16B	-0.1(5)
Ta1B-C10B-C11B-C16B	-119.8(3)	C14B-C10B-C11B-Ta1B	-67.1(2)
C15B-C10B-C11B-Ta1B	119.8(3)	N1B-Ta1B-C11B-C10B	-97.6(2)
O1B-Ta1B-C11B-C10B	-13.7(2)	N2B-Ta1B-C11B-C10B	-113.0(2)
N32B-Ta1B-C11B-C10B	168.5(2)	N31B-Ta1B-C11B-C10B	115.0(2)
C14B-Ta1B-C11B-C10B	37.39(19)	C13B-Ta1B-C11B-C10B	78.5(2)
C12B-Ta1B-C11B-C10B	114.9(3)	Ta2B-Ta1B-C11B-C10B	-63.4(2)
N1B-Ta1B-C11B-C12B	147.5(2)	O1B-Ta1B-C11B-C12B	-128.6(2)
N2B-Ta1B-C11B-C12B	132.1(2)	N32B-Ta1B-C11B-C12B	53.6(2)
N31B-Ta1B-C11B-C12B	0.1(3)	C10B-Ta1B-C11B-C12B	-114.9(3)
C14B-Ta1B-C11B-C12B	-77.5(2)	C13B-Ta1B-C11B-C12B	-36.37(19)
Ta2B-Ta1B-C11B-C12B	-178.22(17)	N1B-Ta1B-C11B-C16B	21.7(3)
O1B-Ta1B-C11B-C16B	105.5(3)	N2B-Ta1B-C11B-C16B	6.3(3)
N32B-Ta1B-C11B-C16B	-72.2(3)	N31B-Ta1B-C11B-C16B	-125.7(3)
C10B-Ta1B-C11B-C16B	119.3(4)	C14B-Ta1B-C11B-C16B	156.7(4)
C13B-Ta1B-C11B-C16B	-162.2(4)	C12B-Ta1B-C11B-C16B	-125.9(4)
Ta2B-Ta1B-C11B-C16B	55.9(3)	C10B-C11B-C12B-C13B	-0.5(4)
C16B-C11B-C12B-C13B	-173.1(3)	Ta1B-C11B-C12B-C13B	64.4(2)

C10B-C11B-C12B-C17B	169.9(3)	C16B-C11B-C12B-C17B	-2.7(6)
Ta1B-C11B-C12B-C17B	-125.2(4)	C10B-C11B-C12B-Ta1B	-64.9(2)
C16B-C11B-C12B-Ta1B	122.5(4)	N1B-Ta1B-C12B-C13B	-150.78(18)
O1B-Ta1B-C12B-C13B	-41.7(2)	N2B-Ta1B-C12B-C13B	171.21(17)
N32B-Ta1B-C12B-C13B	119.3(2)	N31B-Ta1B-C12B-C13B	63.88(19)
C10B-Ta1B-C12B-C13B	-78.7(2)	C14B-Ta1B-C12B-C13B	-37.58(18)
C11B-Ta1B-C12B-C13B	-116.2(3)	Ta2B-Ta1B-C12B-C13B	-112.9(2)
N1B-Ta1B-C12B-C11B	-34.6(2)	O1B-Ta1B-C12B-C11B	74.5(2)
N2B-Ta1B-C12B-C11B	-72.6(2)	N32B-Ta1B-C12B-C11B	-124.5(2)
N31B-Ta1B-C12B-C11B	-179.9(2)	C10B-Ta1B-C12B-C11B	37.5(2)
C14B-Ta1B-C12B-C11B	78.6(2)	C13B-Ta1B-C12B-C11B	116.2(3)
Ta2B-Ta1B-C12B-C11B	3.3(3)	N1B-Ta1B-C12B-C17B	90.0(3)
O1B-Ta1B-C12B-C17B	-160.9(3)	N2B-Ta1B-C12B-C17B	52.0(4)
N32B-Ta1B-C12B-C17B	0.1(3)	N31B-Ta1B-C12B-C17B	-55.3(3)
C10B-Ta1B-C12B-C17B	162.1(4)	C14B-Ta1B-C12B-C17B	-156.8(4)
C11B-Ta1B-C12B-C17B	124.6(4)	C13B-Ta1B-C12B-C17B	-119.2(4)
Ta2B-Ta1B-C12B-C17B	127.9(3)	C11B-C12B-C13B-C14B	0.7(4)
C17B-C12B-C13B-C14B	-170.3(3)	Ta1B-C12B-C13B-C14B	64.6(2)
C11B-C12B-C13B-C18B	169.6(3)	C17B-C12B-C13B-C18B	-1.4(5)
Ta1B-C12B-C13B-C18B	-126.5(3)	C11B-C12B-C13B-Ta1B	-63.9(2)
C17B-C12B-C13B-Ta1B	125.1(3)	N1B-Ta1B-C13B-C12B	42.1(2)
O1B-Ta1B-C13B-C12B	150.40(18)	N2B-Ta1B-C13B-C12B	-34.3(6)
N32B-Ta1B-C13B-C12B	-58.08(19)	N31B-Ta1B-C13B-C12B	-115.76(19)
C10B-Ta1B-C13B-C12B	77.4(2)	C14B-Ta1B-C13B-C12B	115.1(3)
C11B-Ta1B-C13B-C12B	36.50(19)	Ta2B-Ta1B-C13B-C12B	127.55(18)
N1B-Ta1B-C13B-C14B	-73.0(3)	O1B-Ta1B-C13B-C14B	35.3(2)
N2B-Ta1B-C13B-C14B	-149.4(5)	N32B-Ta1B-C13B-C14B	-173.2(2)
N31B-Ta1B-C13B-C14B	129.1(2)	C10B-Ta1B-C13B-C14B	-37.7(2)
C11B-Ta1B-C13B-C14B	-78.6(2)	C12B-Ta1B-C13B-C14B	-115.1(3)
Ta2B-Ta1B-C13B-C14B	12.4(3)	N1B-Ta1B-C13B-C18B	164.0(3)
O1B-Ta1B-C13B-C18B	-87.7(3)	N2B-Ta1B-C13B-C18B	87.6(7)
N32B-Ta1B-C13B-C18B	63.8(3)	N31B-Ta1B-C13B-C18B	6.1(3)
C10B-Ta1B-C13B-C18B	-160.7(4)	C14B-Ta1B-C13B-C18B	-123.0(4)
C11B-Ta1B-C13B-C18B	158.4(4)	C12B-Ta1B-C13B-C18B	121.9(4)
Ta2B-Ta1B-C13B-C18B	-110.6(3)	C11B-C10B-C14B-C13B	0.2(4)
C15B-C10B-C14B-C13B	173.0(3)	Ta1B-C10B-C14B-C13B	-67.5(2)
C11B-C10B-C14B-C19B	-175.3(3)	C15B-C10B-C14B-C19B	-2.5(6)
Ta1B-C10B-C14B-C19B	116.9(3)	C11B-C10B-C14B-Ta1B	67.7(2)
C15B-C10B-C14B-Ta1B	-119.5(4)	C12B-C13B-C14B-C10B	-0.6(4)
C18B-C13B-C14B-C10B	-169.1(3)	Ta1B-C13B-C14B-C10B	66.0(2)
C12B-C13B-C14B-C19B	175.0(3)	C18B-C13B-C14B-C19B	6.4(6)
Ta1B-C13B-C14B-C19B	-118.5(3)	C12B-C13B-C14B-Ta1B	-66.5(2)
C18B-C13B-C14B-Ta1B	124.9(3)	N1B-Ta1B-C14B-C10B	16.8(2)
O1B-Ta1B-C14B-C10B	99.5(2)	N2B-Ta1B-C14B-C10B	53.2(3)

N32B-Ta1B-C14B-C10B	-105.8(2)	N31B-Ta1B-C14B-C10B	-166.28(19)
C11B-Ta1B-C14B-C10B	-37.29(19)	C13B-Ta1B-C14B-C10B	-114.2(3)
C12B-Ta1B-C14B-C10B	-77.5(2)	Ta2B-Ta1B-C14B-C10B	73.1(2)
N1B-Ta1B-C14B-C13B	131.0(2)	O1B-Ta1B-C14B-C13B	-146.3(2)
N2B-Ta1B-C14B-C13B	167.4(2)	N32B-Ta1B-C14B-C13B	8.4(3)
N31B-Ta1B-C14B-C13B	-52.1(2)	C10B-Ta1B-C14B-C13B	114.2(3)
C11B-Ta1B-C14B-C13B	76.9(2)	C12B-Ta1B-C14B-C13B	36.67(19)
Ta2B-Ta1B-C14B-C13B	-172.70(17)	N1B-Ta1B-C14B-C19B	-105.3(3)
O1B-Ta1B-C14B-C19B	-22.5(3)	N2B-Ta1B-C14B-C19B	-68.8(4)
N32B-Ta1B-C14B-C19B	132.2(3)	N31B-Ta1B-C14B-C19B	71.7(3)
C10B-Ta1B-C14B-C19B	-122.1(4)	C11B-Ta1B-C14B-C19B	-159.4(3)
C13B-Ta1B-C14B-C19B	123.7(4)	C12B-Ta1B-C14B-C19B	160.4(3)
Ta2B-Ta1B-C14B-C19B	-49.0(3)	N2B-Ta2B-C20B-C24B	-151.7(2)
O1B-Ta2B-C20B-C24B	-63.1(2)	N1B-Ta2B-C20B-C24B	-146.70(19)
N51B-Ta2B-C20B-C24B	51.1(3)	N52B-Ta2B-C20B-C24B	124.6(2)
C21B-Ta2B-C20B-C24B	114.0(3)	C22B-Ta2B-C20B-C24B	76.7(2)
C23B-Ta2B-C20B-C24B	36.1(2)	Ta1B-Ta2B-C20B-C24B	-106.40(19)
N2B-Ta2B-C20B-C21B	94.3(2)	O1B-Ta2B-C20B-C21B	-177.1(2)
N1B-Ta2B-C20B-C21B	99.3(2)	N51B-Ta2B-C20B-C21B	-63.0(3)
N52B-Ta2B-C20B-C21B	10.5(2)	C22B-Ta2B-C20B-C21B	-37.36(19)
C24B-Ta2B-C20B-C21B	-114.0(3)	C23B-Ta2B-C20B-C21B	-77.9(2)
Ta1B-Ta2B-C20B-C21B	139.56(18)	N2B-Ta2B-C20B-C25B	-26.8(3)
O1B-Ta2B-C20B-C25B	61.8(3)	N1B-Ta2B-C20B-C25B	-21.8(3)
N51B-Ta2B-C20B-C25B	176.0(3)	N52B-Ta2B-C20B-C25B	-110.5(3)
C21B-Ta2B-C20B-C25B	-121.1(4)	C22B-Ta2B-C20B-C25B	-158.4(4)
C24B-Ta2B-C20B-C25B	124.9(4)	C23B-Ta2B-C20B-C25B	161.1(4)
Ta1B-Ta2B-C20B-C25B	18.5(3)	C24B-C20B-C21B-C22B	-1.4(4)
C25B-C20B-C21B-C22B	-175.7(3)	Ta2B-C20B-C21B-C22B	67.6(2)
C24B-C20B-C21B-C26B	174.0(3)	C25B-C20B-C21B-C26B	-0.3(5)
Ta2B-C20B-C21B-C26B	-117.0(3)	C24B-C20B-C21B-Ta2B	-69.0(2)
C25B-C20B-C21B-Ta2B	116.7(3)	N2B-Ta2B-C21B-C22B	163.4(2)
O1B-Ta2B-C21B-C22B	-110.68(19)	N1B-Ta2B-C21B-C22B	142.26(18)
N51B-Ta2B-C21B-C22B	26.7(2)	N52B-Ta2B-C21B-C22B	74.99(19)
C20B-Ta2B-C21B-C22B	-114.3(3)	C24B-Ta2B-C21B-C22B	-76.9(2)
C23B-Ta2B-C21B-C22B	-37.02(18)	Ta1B-Ta2B-C21B-C22B	-166.40(15)
N2B-Ta2B-C21B-C20B	-82.3(2)	O1B-Ta2B-C21B-C20B	3.7(2)
N1B-Ta2B-C21B-C20B	-103.4(2)	N51B-Ta2B-C21B-C20B	141.00(19)
N52B-Ta2B-C21B-C20B	-170.7(2)	C22B-Ta2B-C21B-C20B	114.3(3)
C24B-Ta2B-C21B-C20B	37.5(2)	C23B-Ta2B-C21B-C20B	77.3(2)
Ta1B-Ta2B-C21B-C20B	-52.1(2)	N2B-Ta2B-C21B-C26B	37.1(3)
O1B-Ta2B-C21B-C26B	123.1(3)	N1B-Ta2B-C21B-C26B	16.0(3)
N51B-Ta2B-C21B-C26B	-99.6(3)	N52B-Ta2B-C21B-C26B	-51.3(3)
C20B-Ta2B-C21B-C26B	119.4(4)	C22B-Ta2B-C21B-C26B	-126.3(4)
C24B-Ta2B-C21B-C26B	156.9(3)	C23B-Ta2B-C21B-C26B	-163.3(3)

Ta1B-Ta2B-C21B-C26B	67.3(3)	C20B-C21B-C22B-C23B	0.7(4)
C26B-C21B-C22B-C23B	-174.4(3)	Ta2B-C21B-C22B-C23B	66.7(2)
C20B-C21B-C22B-C27B	173.8(3)	C26B-C21B-C22B-C27B	-1.3(6)
Ta2B-C21B-C22B-C27B	-120.2(3)	C20B-C21B-C22B-Ta2B	-66.0(2)
C26B-C21B-C22B-Ta2B	118.9(3)	N2B-Ta2B-C22B-C21B	-18.8(2)
O1B-Ta2B-C22B-C21B	98.8(2)	N1B-Ta2B-C22B-C21B	-62.7(3)
N51B-Ta2B-C22B-C21B	-157.2(2)	N52B-Ta2B-C22B-C21B	-99.7(2)
C20B-Ta2B-C22B-C21B	38.05(19)	C24B-Ta2B-C22B-C21B	78.8(2)
C23B-Ta2B-C22B-C21B	115.2(3)	Ta1B-Ta2B-C22B-C21B	30.1(3)
N2B-Ta2B-C22B-C23B	-133.96(19)	O1B-Ta2B-C22B-C23B	-16.4(2)
N1B-Ta2B-C22B-C23B	-177.85(18)	N51B-Ta2B-C22B-C23B	87.61(19)
N52B-Ta2B-C22B-C23B	145.1(2)	C20B-Ta2B-C22B-C23B	-77.1(2)
C21B-Ta2B-C22B-C23B	-115.2(3)	C24B-Ta2B-C22B-C23B	-36.35(19)
Ta1B-Ta2B-C22B-C23B	-85.1(3)	N2B-Ta2B-C22B-C27B	104.3(3)
O1B-Ta2B-C22B-C27B	-138.1(3)	N1B-Ta2B-C22B-C27B	60.4(4)
N51B-Ta2B-C22B-C27B	-34.1(3)	N52B-Ta2B-C22B-C27B	23.4(3)
C20B-Ta2B-C22B-C27B	161.2(3)	C21B-Ta2B-C22B-C27B	123.1(4)
C24B-Ta2B-C22B-C27B	-158.1(3)	C23B-Ta2B-C22B-C27B	-121.7(4)
Ta1B-Ta2B-C22B-C27B	153.2(2)	C21B-C22B-C23B-C24B	0.3(4)
C27B-C22B-C23B-C24B	-173.1(3)	Ta2B-C22B-C23B-C24B	64.9(2)
C21B-C22B-C23B-C28B	169.0(3)	C27B-C22B-C23B-C28B	-4.4(5)
Ta2B-C22B-C23B-C28B	-126.4(3)	C21B-C22B-C23B-Ta2B	-64.6(2)
C27B-C22B-C23B-Ta2B	122.0(3)	N2B-Ta2B-C23B-C24B	-48.3(3)
O1B-Ta2B-C23B-C24B	52.0(2)	N51B-Ta2B-C23B-C24B	152.1(2)
N52B-Ta2B-C23B-C24B	-151.0(2)	C20B-Ta2B-C23B-C24B	-36.9(2)
C21B-Ta2B-C23B-C24B	-78.6(2)	C22B-Ta2B-C23B-C24B	-115.8(3)
Ta1B-Ta2B-C23B-C24B	28.9(3)	N2B-Ta2B-C23B-C22B	67.6(2)
O1B-Ta2B-C23B-C22B	167.79(18)	N51B-Ta2B-C23B-C22B	-92.09(19)
N52B-Ta2B-C23B-C22B	-35.2(2)	C20B-Ta2B-C23B-C22B	78.9(2)
C21B-Ta2B-C23B-C22B	37.26(18)	C24B-Ta2B-C23B-C22B	115.8(3)
Ta1B-Ta2B-C23B-C22B	144.74(15)	N2B-Ta2B-C23B-C28B	-171.5(3)
O1B-Ta2B-C23B-C28B	-71.2(3)	N51B-Ta2B-C23B-C28B	28.9(3)
N52B-Ta2B-C23B-C28B	85.8(3)	C20B-Ta2B-C23B-C28B	-160.1(4)
C21B-Ta2B-C23B-C28B	158.2(4)	C22B-Ta2B-C23B-C28B	121.0(4)
C24B-Ta2B-C23B-C28B	-123.2(4)	Ta1B-Ta2B-C23B-C28B	-94.3(3)
C22B-C23B-C24B-C20B	-1.2(4)	C28B-C23B-C24B-C20B	-169.7(3)
Ta2B-C23B-C24B-C20B	63.1(2)	C22B-C23B-C24B-C29B	175.2(3)
C28B-C23B-C24B-C29B	6.7(6)	Ta2B-C23B-C24B-C29B	-120.5(3)
C22B-C23B-C24B-Ta2B	-64.3(2)	C28B-C23B-C24B-Ta2B	127.2(3)
C21B-C20B-C24B-C23B	1.6(4)	C25B-C20B-C24B-C23B	175.7(3)
Ta2B-C20B-C24B-C23B	-65.6(2)	C21B-C20B-C24B-C29B	-174.6(3)
C25B-C20B-C24B-C29B	-0.5(6)	Ta2B-C20B-C24B-C29B	118.2(4)
C21B-C20B-C24B-Ta2B	67.2(2)	C25B-C20B-C24B-Ta2B	-118.7(4)
N2B-Ta2B-C24B-C23B	146.4(2)	O1B-Ta2B-C24B-C23B	-128.2(2)

N1B-Ta2B-C24B-C23B	174.52(19)	N51B-Ta2B-C24B-C23B	-31.7(2)
N52B-Ta2B-C24B-C23B	38.9(3)	C20B-Ta2B-C24B-C23B	116.1(3)
C21B-Ta2B-C24B-C23B	77.9(2)	C22B-Ta2B-C24B-C23B	36.99(19)
Ta1B-Ta2B-C24B-C23B	-160.51(18)	N2B-Ta2B-C24B-C20B	30.3(2)
O1B-Ta2B-C24B-C20B	115.7(2)	N1B-Ta2B-C24B-C20B	58.4(3)
N51B-Ta2B-C24B-C20B	-147.84(19)	N52B-Ta2B-C24B-C20B	-77.2(2)
C21B-Ta2B-C24B-C20B	-38.24(19)	C22B-Ta2B-C24B-C20B	-79.1(2)
C23B-Ta2B-C24B-C20B	-116.1(3)	Ta1B-Ta2B-C24B-C20B	83.4(2)
N2B-Ta2B-C24B-C29B	-93.3(3)	O1B-Ta2B-C24B-C29B	-8.0(3)
N1B-Ta2B-C24B-C29B	-65.2(4)	N51B-Ta2B-C24B-C29B	88.5(3)
N52B-Ta2B-C24B-C29B	159.1(3)	C20B-Ta2B-C24B-C29B	-123.6(4)
C21B-Ta2B-C24B-C29B	-161.9(4)	C22B-Ta2B-C24B-C29B	157.2(4)
C23B-Ta2B-C24B-C29B	120.3(4)	Ta1B-Ta2B-C24B-C29B	-40.3(3)
N1B-Ta1B-N31B-C30B	-57.4(3)	O1B-Ta1B-N31B-C30B	-151.5(2)
N2B-Ta1B-N31B-C30B	-69.1(2)	N32B-Ta1B-N31B-C30B	1.80(19)
C10B-Ta1B-N31B-C30B	115.9(2)	C14B-Ta1B-N31B-C30B	126.5(2)
C11B-Ta1B-N31B-C30B	71.4(2)	C13B-Ta1B-N31B-C30B	100.6(2)
C12B-Ta1B-N31B-C30B	71.4(2)	Ta2B-Ta1B-N31B-C30B	-110.17(19)
N1B-Ta1B-N31B-C37B	121.3(4)	O1B-Ta1B-N31B-C37B	27.1(4)
N2B-Ta1B-N31B-C37B	109.5(4)	N32B-Ta1B-N31B-C37B	-179.6(4)
C10B-Ta1B-N31B-C37B	-65.5(4)	C14B-Ta1B-N31B-C37B	-54.9(4)
C11B-Ta1B-N31B-C37B	-110.0(4)	C13B-Ta1B-N31B-C37B	-80.8(4)
C12B-Ta1B-N31B-C37B	-109.9(4)	Ta2B-Ta1B-N31B-C37B	68.5(4)
N1B-Ta1B-N32B-C30B	142.0(2)	O1B-Ta1B-N32B-C30B	48.4(3)
N2B-Ta1B-N32B-C30B	103.8(2)	N31B-Ta1B-N32B-C30B	-1.84(19)
C10B-Ta1B-N32B-C30B	-127.0(2)	C14B-Ta1B-N32B-C30B	-85.1(2)
C11B-Ta1B-N32B-C30B	-135.0(2)	C13B-Ta1B-N32B-C30B	-80.5(2)
C12B-Ta1B-N32B-C30B	-108.5(2)	Ta2B-Ta1B-N32B-C30B	96.1(2)
N1B-Ta1B-N32B-C40B	-10.8(3)	O1B-Ta1B-N32B-C40B	-104.4(3)
N2B-Ta1B-N32B-C40B	-49.0(3)	N31B-Ta1B-N32B-C40B	-154.6(4)
C10B-Ta1B-N32B-C40B	80.2(4)	C14B-Ta1B-N32B-C40B	122.1(3)
C11B-Ta1B-N32B-C40B	72.2(3)	C13B-Ta1B-N32B-C40B	126.8(3)
C12B-Ta1B-N32B-C40B	98.8(3)	Ta2B-Ta1B-N32B-C40B	-56.7(4)
C40B-N32B-C30B-N31B	161.7(3)	Ta1B-N32B-C30B-N31B	2.9(3)
C40B-N32B-C30B-C31B	-21.2(5)	Ta1B-N32B-C30B-C31B	180.0(3)
C37B-N31B-C30B-N32B	178.2(3)	Ta1B-N31B-C30B-N32B	-2.8(3)
C37B-N31B-C30B-C31B	1.1(5)	Ta1B-N31B-C30B-C31B	-179.9(3)
N32B-C30B-C31B-C32B	117.1(4)	N31B-C30B-C31B-C32B	-66.1(5)
N32B-C30B-C31B-C36B	-65.1(5)	N31B-C30B-C31B-C36B	111.7(4)
C36B-C31B-C32B-C33B	-0.4(7)	C30B-C31B-C32B-C33B	177.4(4)
C31B-C32B-C33B-C34B	-0.6(8)	C32B-C33B-C34B-C35B	0.8(8)
C33B-C34B-C35B-C36B	0.1(7)	C32B-C31B-C36B-C35B	1.2(6)
C30B-C31B-C36B-C35B	-176.6(3)	C34B-C35B-C36B-C31B	-1.1(6)
C30B-N31B-C37B-C38B	-172.6(3)	Ta1B-N31B-C37B-C38B	9.0(5)

C30B-N31B-C37B-C39B	-49.4(5)	Ta1B-N31B-C37B-C39B	132.2(3)
C30B-N32B-C40B-C41B	176.5(3)	Ta1B-N32B-C40B-C41B	-35.8(5)
C30B-N32B-C40B-C42B	-61.2(4)	Ta1B-N32B-C40B-C42B	86.5(4)
N2B-Ta2B-N51B-C50B	-46.3(2)	O1B-Ta2B-N51B-C50B	-144.41(19)
N1B-Ta2B-N51B-C50B	-62.3(2)	N52B-Ta2B-N51B-C50B	7.19(18)
C20B-Ta2B-N51B-C50B	103.0(2)	C21B-Ta2B-N51B-C50B	68.0(2)
C22B-Ta2B-N51B-C50B	82.2(2)	C24B-Ta2B-N51B-C50B	131.44(19)
C23B-Ta2B-N51B-C50B	115.1(2)	Ta1B-Ta2B-N51B-C50B	-100.75(18)
N2B-Ta2B-N51B-C57B	131.0(3)	O1B-Ta2B-N51B-C57B	32.9(4)
N1B-Ta2B-N51B-C57B	115.0(4)	N52B-Ta2B-N51B-C57B	-175.5(4)
C20B-Ta2B-N51B-C57B	-79.7(4)	C21B-Ta2B-N51B-C57B	-114.7(3)
C22B-Ta2B-N51B-C57B	-100.5(4)	C24B-Ta2B-N51B-C57B	-51.3(4)
C23B-Ta2B-N51B-C57B	-67.6(4)	Ta1B-Ta2B-N51B-C57B	76.5(4)
N2B-Ta2B-N52B-C50B	135.7(2)	O1B-Ta2B-N52B-C50B	49.8(3)
N1B-Ta2B-N52B-C50B	96.05(19)	N51B-Ta2B-N52B-C50B	-7.23(18)
C20B-Ta2B-N52B-C50B	-143.93(19)	C21B-Ta2B-N52B-C50B	-138.1(2)
C22B-Ta2B-N52B-C50B	-105.3(2)	C24B-Ta2B-N52B-C50B	-106.9(2)
C23B-Ta2B-N52B-C50B	-86.6(2)	Ta1B-Ta2B-N52B-C50B	93.42(18)
N2B-Ta2B-N52B-C60B	-11.8(3)	O1B-Ta2B-N52B-C60B	-97.6(3)
N1B-Ta2B-N52B-C60B	-51.4(3)	N51B-Ta2B-N52B-C60B	-154.7(3)
C20B-Ta2B-N52B-C60B	68.6(3)	C21B-Ta2B-N52B-C60B	74.5(3)
C22B-Ta2B-N52B-C60B	107.2(3)	C24B-Ta2B-N52B-C60B	105.6(3)
C23B-Ta2B-N52B-C60B	126.0(3)	Ta1B-Ta2B-N52B-C60B	-54.0(3)
C60B-N52B-C50B-N51B	160.3(3)	Ta2B-N52B-C50B-N51B	11.1(3)
C60B-N52B-C50B-C51B	-18.4(5)	Ta2B-N52B-C50B-C51B	-167.6(3)
C57B-N51B-C50B-N52B	170.7(3)	Ta2B-N51B-C50B-N52B	-11.3(3)
C57B-N51B-C50B-C51B	-10.6(5)	Ta2B-N51B-C50B-C51B	167.4(3)
N52B-C50B-C51B-C52B	113.7(4)	N51B-C50B-C51B-C52B	-64.9(4)
N52B-C50B-C51B-C56B	-67.0(4)	N51B-C50B-C51B-C56B	114.5(4)
C56B-C51B-C52B-C53B	1.6(5)	C50B-C51B-C52B-C53B	-179.0(3)
C51B-C52B-C53B-C54B	-0.2(5)	C52B-C53B-C54B-C55B	-1.1(6)
C53B-C54B-C55B-C56B	1.1(6)	C54B-C55B-C56B-C51B	0.3(6)
C52B-C51B-C56B-C55B	-1.6(5)	C50B-C51B-C56B-C55B	179.0(3)
C50B-N51B-C57B-C58B	174.4(3)	Ta2B-N51B-C57B-C58B	-2.4(5)
C50B-N51B-C57B-C59B	-62.3(4)	Ta2B-N51B-C57B-C59B	121.0(3)
C50B-N52B-C60B-C61B	-37.6(4)	Ta2B-N52B-C60B-C61B	100.3(3)
C50B-N52B-C60B-C62B	90.0(4)	Ta2B-N52B-C60B-C62B	-132.0(3)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 9b.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1A	0.01602(6)	0.01449(6)	0.01395(6)	0.00278(5)	-0.00171(5)	-0.00096(5)
Ta2A	0.01850(6)	0.01380(6)	0.01406(6)	0.00160(5)	0.00012(5)	-0.00006(5)
O1A	0.0175(11)	0.0158(11)	0.0184(12)	0.0021(9)	0.0009(9)	-0.0009(9)
N1A	0.0206(14)	0.0182(14)	0.0155(14)	-0.0003(11)	-0.0006(10)	0.0007(11)
N2A	0.0194(14)	0.0165(14)	0.0203(15)	0.0026(11)	0.0004(11)	-0.0004(11)
C10A	0.0316(19)	0.0146(16)	0.0170(17)	0.0004(13)	-0.0023(13)	-0.0059(14)
C11A	0.0265(18)	0.0196(17)	0.0228(18)	-0.0017(14)	0.0003(14)	-0.0081(14)
C12A	0.0258(18)	0.0205(17)	0.0217(18)	-0.0014(14)	-0.0085(14)	-0.0078(14)
C13A	0.0306(19)	0.0168(17)	0.0190(17)	-0.0007(14)	-0.0017(14)	-0.0040(14)
C14A	0.0316(19)	0.0122(16)	0.0189(17)	-0.0033(13)	-0.0028(14)	-0.0014(14)
C15A	0.052(2)	0.0153(17)	0.025(2)	0.0033(15)	-0.0024(16)	-0.0043(16)
C16A	0.0250(19)	0.041(2)	0.035(2)	0.0023(18)	0.0001(16)	-0.0112(17)
C17A	0.037(2)	0.043(2)	0.031(2)	0.0029(19)	-0.0152(17)	-0.0039(18)
C18A	0.048(2)	0.036(2)	0.0192(19)	-0.0011(17)	-0.0010(16)	-0.0054(18)
C19A	0.041(2)	0.0206(19)	0.036(2)	-0.0002(16)	-0.0017(17)	0.0052(16)
C20A	0.0337(19)	0.0121(16)	0.0245(19)	-0.0012(14)	-0.0055(15)	-0.0014(14)
C21A	0.0338(19)	0.0140(16)	0.0221(18)	-0.0043(14)	-0.0001(14)	-0.0033(14)
C22A	0.043(2)	0.0155(17)	0.0234(19)	-0.0039(14)	-0.0058(15)	0.0062(15)
C23A	0.049(2)	0.0143(17)	0.029(2)	-0.0021(15)	0.0141(17)	0.0029(16)
C24A	0.032(2)	0.0140(17)	0.041(2)	-0.0062(16)	0.0053(16)	0.0061(15)
C25A	0.063(3)	0.0187(19)	0.032(2)	0.0055(17)	-0.0164(19)	-0.0018(18)
C26A	0.037(2)	0.029(2)	0.047(3)	-0.0040(19)	0.0038(18)	-0.0147(17)
C27A	0.077(3)	0.034(2)	0.028(2)	-0.0088(18)	-0.018(2)	0.017(2)
C28A	0.098(4)	0.028(2)	0.037(3)	-0.0072(19)	0.034(2)	-0.005(2)
C29A	0.033(2)	0.033(2)	0.073(3)	-0.014(2)	0.007(2)	0.0092(18)
N31A	0.0183(14)	0.0233(15)	0.0161(14)	0.0045(12)	0.0001(10)	-0.0027(11)
N32A	0.0177(14)	0.0247(15)	0.0251(16)	0.0086(13)	-0.0052(11)	0.0016(12)
C30A	0.0210(16)	0.0189(16)	0.0150(16)	0.0021(13)	-0.0057(12)	-0.0061(13)
C31A	0.0269(18)	0.0242(18)	0.0217(18)	0.0069(15)	-0.0074(14)	-0.0054(14)
C32A	0.032(2)	0.031(2)	0.0229(19)	0.0095(16)	-0.0065(15)	-0.0042(16)
C33A	0.039(2)	0.048(3)	0.021(2)	0.0138(18)	-0.0041(16)	-0.0053(19)
C34A	0.043(2)	0.041(2)	0.033(2)	0.0259(19)	-0.0046(18)	-0.0092(19)
C35A	0.043(2)	0.024(2)	0.040(2)	0.0149(18)	-0.0053(18)	-0.0055(17)
C36A	0.035(2)	0.029(2)	0.026(2)	0.0089(16)	-0.0043(15)	-0.0047(16)
C37A	0.0222(17)	0.0289(19)	0.0161(17)	0.0049(14)	0.0003(13)	-0.0019(14)
C38A	0.0264(19)	0.034(2)	0.0231(19)	0.0049(16)	0.0054(14)	0.0040(15)
C39A	0.0205(18)	0.037(2)	0.033(2)	0.0044(17)	0.0023(15)	-0.0058(15)
C40A	0.0241(18)	0.0250(19)	0.037(2)	0.0094(16)	-0.0069(15)	0.0024(15)
C41A	0.0218(19)	0.052(3)	0.052(3)	0.018(2)	0.0001(17)	0.0108(18)
C42A	0.031(2)	0.050(3)	0.048(3)	0.021(2)	-0.0184(18)	0.0032(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N51A	0.0196(14)	0.0190(14)	0.0168(14)	0.0034(11)	-0.0010(11)	-0.0024(11)
N52A	0.0184(14)	0.0184(14)	0.0167(14)	0.0050(11)	0.0022(10)	-0.0019(11)
C50A	0.0259(17)	0.0175(16)	0.0119(16)	-0.0018(13)	-0.0015(12)	0.0016(13)
C51A	0.0206(16)	0.0213(17)	0.0198(17)	0.0035(14)	0.0024(13)	0.0023(13)
C52A	0.0301(19)	0.0236(18)	0.0229(19)	-0.0003(15)	-0.0020(14)	-0.0010(15)
C53A	0.030(2)	0.039(2)	0.0229(19)	0.0103(17)	-0.0044(15)	0.0018(17)
C54A	0.0259(19)	0.032(2)	0.034(2)	0.0167(17)	-0.0004(15)	0.0075(16)
C55A	0.0265(19)	0.0225(18)	0.036(2)	0.0038(16)	0.0029(15)	0.0045(15)
C56A	0.0234(17)	0.0239(18)	0.0216(18)	-0.0014(14)	0.0001(13)	0.0038(14)
C57A	0.0200(17)	0.035(2)	0.0260(19)	0.0061(16)	-0.0030(14)	0.0022(15)
C58A	0.022(2)	0.091(4)	0.034(2)	0.007(2)	0.0026(17)	0.003(2)
C59A	0.030(2)	0.064(3)	0.035(2)	0.000(2)	-0.0072(17)	-0.003(2)
C60A	0.0226(17)	0.0219(18)	0.0212(18)	0.0057(14)	0.0038(13)	-0.0022(14)
C61A	0.0249(18)	0.032(2)	0.030(2)	0.0090(17)	0.0054(15)	-0.0045(15)
C62A	0.036(2)	0.046(2)	0.024(2)	0.0102(18)	0.0082(16)	-0.0018(18)
Ta1B	0.01403(6)	0.01880(7)	0.01504(7)	-0.00014(5)	-0.00089(5)	-0.00010(5)
Ta2B	0.01429(6)	0.01641(7)	0.01469(6)	0.00088(5)	-0.00009(5)	0.00037(5)
O1B	0.0182(11)	0.0185(12)	0.0188(12)	0.0017(9)	0.0016(9)	-0.0011(9)
N1B	0.0183(14)	0.0168(14)	0.0222(15)	-0.0019(11)	0.0006(11)	0.0013(11)
N2B	0.0175(14)	0.0236(15)	0.0208(15)	0.0003(12)	0.0007(11)	0.0013(11)
C10B	0.0108(15)	0.039(2)	0.0194(17)	0.0002(15)	0.0014(12)	0.0030(14)
C11B	0.0203(17)	0.0300(19)	0.0238(19)	0.0010(15)	0.0076(13)	0.0076(14)
C12B	0.0211(17)	0.032(2)	0.0175(17)	-0.0054(15)	0.0059(13)	0.0006(14)
C13B	0.0168(16)	0.033(2)	0.0150(16)	0.0012(14)	0.0040(12)	-0.0014(14)
C14B	0.0187(16)	0.0317(19)	0.0177(17)	-0.0052(15)	0.0076(13)	-0.0058(14)
C15B	0.0178(18)	0.075(3)	0.025(2)	0.003(2)	-0.0008(15)	0.0089(19)
C16B	0.042(2)	0.038(2)	0.045(3)	0.009(2)	0.0066(19)	0.0185(19)
C17B	0.033(2)	0.044(2)	0.028(2)	-0.0134(18)	0.0046(16)	-0.0037(18)
C18B	0.038(2)	0.047(2)	0.022(2)	0.0094(18)	0.0075(16)	0.0096(18)
C19B	0.038(2)	0.035(2)	0.029(2)	-0.0041(17)	0.0060(16)	-0.0102(17)
C20B	0.0225(18)	0.032(2)	0.0220(18)	0.0000(15)	0.0039(14)	0.0117(15)
C21B	0.0164(16)	0.0256(18)	0.0248(18)	0.0016(15)	0.0056(13)	0.0059(13)
C22B	0.0221(17)	0.0202(17)	0.0203(17)	0.0015(14)	0.0048(13)	0.0048(13)
C23B	0.0233(17)	0.0198(17)	0.0265(19)	0.0001(15)	0.0066(14)	0.0020(14)
C24B	0.0300(19)	0.0261(19)	0.030(2)	0.0064(16)	0.0150(15)	0.0133(15)
C25B	0.029(2)	0.064(3)	0.029(2)	0.002(2)	-0.0023(16)	0.020(2)
C26B	0.0216(18)	0.037(2)	0.039(2)	0.0004(18)	0.0085(16)	-0.0045(16)
C27B	0.037(2)	0.036(2)	0.0192(19)	0.0018(16)	0.0042(15)	0.0095(17)
C28B	0.035(2)	0.029(2)	0.053(3)	-0.0145(19)	0.0103(19)	-0.0038(17)
C29B	0.069(3)	0.030(2)	0.048(3)	0.014(2)	0.023(2)	0.018(2)
N31B	0.0204(14)	0.0231(15)	0.0218(15)	0.0026(12)	-0.0014(11)	0.0034(12)
N32B	0.0189(14)	0.0249(15)	0.0227(15)	-0.0004(12)	-0.0027(11)	-0.0038(12)
C30B	0.0151(16)	0.037(2)	0.0134(16)	0.0003(15)	0.0021(12)	-0.0002(14)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C31B	0.0182(17)	0.036(2)	0.0200(18)	0.0009(15)	-0.0023(13)	-0.0017(15)
C32B	0.024(2)	0.085(4)	0.022(2)	-0.005(2)	0.0010(15)	0.005(2)
C33B	0.020(2)	0.130(5)	0.034(3)	-0.003(3)	-0.0009(17)	0.015(3)
C34B	0.025(2)	0.088(4)	0.027(2)	0.006(2)	-0.0142(16)	-0.005(2)
C35B	0.034(2)	0.050(3)	0.0181(19)	-0.0014(17)	-0.0036(15)	-0.0044(18)
C36B	0.0280(19)	0.036(2)	0.0198(18)	0.0016(16)	0.0025(14)	-0.0004(16)
C37B	0.0293(19)	0.032(2)	0.027(2)	0.0048(16)	0.0013(15)	0.0091(16)
C38B	0.056(3)	0.024(2)	0.034(2)	0.0028(17)	-0.0050(19)	0.0079(19)
C39B	0.052(3)	0.041(2)	0.033(2)	0.0092(19)	-0.0066(19)	0.014(2)
C40B	0.035(2)	0.028(2)	0.027(2)	0.0010(16)	-0.0072(16)	-0.0139(16)
C41B	0.058(3)	0.024(2)	0.042(3)	0.0020(18)	-0.010(2)	-0.0103(19)
C42B	0.041(2)	0.047(3)	0.038(2)	0.002(2)	0.0029(18)	-0.022(2)
N51B	0.0168(13)	0.0182(14)	0.0193(14)	0.0034(11)	-0.0035(10)	-0.0009(11)
N52B	0.0199(14)	0.0165(14)	0.0173(14)	0.0018(11)	-0.0016(11)	-0.0010(11)
C50B	0.0230(17)	0.0179(16)	0.0133(16)	-0.0017(13)	0.0012(12)	0.0029(13)
C51B	0.0213(17)	0.0154(16)	0.0254(18)	0.0018(14)	-0.0053(13)	-0.0001(13)
C52B	0.0296(19)	0.0200(18)	0.031(2)	-0.0025(15)	-0.0032(15)	0.0020(15)
C53B	0.029(2)	0.023(2)	0.057(3)	-0.0076(19)	-0.0070(18)	0.0082(16)
C54B	0.042(2)	0.020(2)	0.066(3)	0.009(2)	-0.027(2)	0.0011(17)
C55B	0.044(2)	0.035(2)	0.038(2)	0.0172(19)	-0.0157(19)	-0.0031(19)
C56B	0.0269(19)	0.0276(19)	0.029(2)	0.0078(16)	-0.0022(15)	0.0004(15)
C57B	0.0178(16)	0.0220(17)	0.0244(18)	0.0036(14)	-0.0019(13)	-0.0017(13)
C58B	0.0242(18)	0.0259(19)	0.035(2)	0.0093(16)	-0.0033(15)	-0.0059(15)
C59B	0.036(2)	0.029(2)	0.030(2)	0.0038(17)	-0.0119(16)	-0.0080(16)
C60B	0.0261(18)	0.0185(17)	0.0235(18)	0.0010(14)	-0.0037(14)	-0.0064(14)
C61B	0.034(2)	0.0203(18)	0.034(2)	-0.0003(16)	0.0002(16)	-0.0030(15)
C62B	0.038(2)	0.026(2)	0.032(2)	0.0054(17)	0.0049(16)	-0.0104(16)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 9b.

	x/a	y/b	z/c	U(eq)
H15A	0.2395	0.5859	0.7603	0.046
H15B	0.1203	0.6341	0.7810	0.046
H15C	0.2645	0.6729	0.7879	0.046
H16A	-0.0481	0.7572	0.7367	0.051
H16B	-0.0715	0.6650	0.7352	0.051
H16C	-0.1241	0.7094	0.6858	0.051
H17A	-0.0307	0.6836	0.5699	0.057
H17B	0.0430	0.7668	0.5689	0.057
H17C	-0.0716	0.7562	0.6084	0.057
H18A	0.2310	0.6476	0.5460	0.052
H18B	0.3720	0.6717	0.5739	0.052

	x/a	y/b	z/c	U(eq)
H18C	0.2780	0.7374	0.5569	0.052
H19A	0.4629	0.6584	0.7079	0.049
H19B	0.4522	0.6222	0.6467	0.049
H19C	0.3936	0.5742	0.6921	0.049
H25A	0.1527	1.0269	0.7359	0.058
H25B	0.2993	1.0110	0.7223	0.058
H25C	0.2657	1.0922	0.7531	0.058
H26A	0.5170	1.0913	0.8145	0.057
H26B	0.5173	1.0167	0.7717	0.057
H26C	0.5864	1.0151	0.8303	0.057
H27A	0.4342	1.0131	0.9569	0.071
H27B	0.5484	0.9953	0.9176	0.071
H27C	0.4662	0.9251	0.9390	0.071
H28A	0.2234	0.9070	0.9522	0.081
H28B	0.0840	0.9142	0.9224	0.081
H28C	0.1572	0.9890	0.9549	0.081
H29A	0.0006	1.0028	0.7943	0.07
H29B	-0.0197	0.9837	0.8546	0.07
H29C	-0.0012	0.9147	0.8090	0.07
H32A	0.3067	0.8752	0.5157	0.034
H33A	0.3334	0.9641	0.4518	0.043
H34A	0.3309	1.0967	0.4768	0.046
H35A	0.3072	1.1420	0.5659	0.043
H36A	0.2790	1.0540	0.6297	0.036
H37A	0.4945	0.8541	0.5782	0.027
H38A	0.5651	0.7905	0.6763	0.041
H38B	0.6596	0.7969	0.6283	0.041
H38C	0.5314	0.7407	0.6198	0.041
H39A	0.5145	0.9771	0.6285	0.045
H39B	0.6502	0.9361	0.6321	0.045
H39C	0.5580	0.9374	0.6813	0.045
H40A	0.0787	0.9965	0.6527	0.034
H41A	-0.0922	0.8668	0.6639	0.061
H41B	-0.1164	0.9562	0.6809	0.061
H41C	-0.0094	0.9126	0.7138	0.061
H42A	0.0556	0.9508	0.5592	0.064
H42B	-0.0792	0.9757	0.5824	0.064
H42C	-0.0493	0.8857	0.5728	0.064
H52A	0.5390	0.7810	0.9719	0.031
H53A	0.6130	0.6846	1.0233	0.036
H54A	0.5854	0.5544	0.9895	0.036
H55A	0.4886	0.5206	0.9045	0.034
H56A	0.4158	0.6165	0.8522	0.028

	x/a	y/b	z/c	U(eq)
H57A	0.6469	0.7599	0.8599	0.032
H58A	0.6355	0.7755	0.7704	0.073
H58B	0.7688	0.8183	0.7953	0.073
H58C	0.6466	0.8682	0.7816	0.073
H59A	0.7018	0.9235	0.8796	0.066
H59B	0.8030	0.8579	0.8885	0.066
H59C	0.6831	0.8671	0.9259	0.066
H60A	0.1984	0.6730	0.8716	0.026
H61A	0.0369	0.8027	0.8812	0.043
H61B	-0.0125	0.7132	0.8734	0.043
H61C	0.0545	0.7520	0.8257	0.043
H62A	0.2730	0.7149	0.9609	0.052
H62B	0.1198	0.6947	0.9571	0.052
H62C	0.1737	0.7834	0.9620	0.052
H15D	1.2037	0.3911	0.7466	0.059
H15E	1.2378	0.3029	0.7307	0.059
H15F	1.1198	0.3215	0.7678	0.059
H16D	1.0069	0.1460	0.6511	0.061
H16E	1.0149	0.1800	0.7128	0.061
H16F	1.1430	0.1792	0.6797	0.061
H17D	0.9047	0.1751	0.5768	0.054
H17E	0.9473	0.2359	0.5359	0.054
H17F	0.8074	0.2394	0.5602	0.054
H18D	0.9850	0.3936	0.5355	0.052
H18E	0.9326	0.4626	0.5742	0.052
H18F	0.8375	0.3898	0.5519	0.052
H19D	1.0558	0.5009	0.7059	0.052
H19E	1.0568	0.5113	0.6432	0.052
H19F	1.1840	0.4847	0.6746	0.052
H25D	0.5016	0.3798	0.7486	0.061
H25E	0.5406	0.4657	0.7344	0.061
H25F	0.4268	0.4522	0.7738	0.061
H26D	0.4321	0.3470	0.8628	0.049
H26E	0.5475	0.2978	0.8851	0.049
H26F	0.5130	0.2947	0.8219	0.049
H27D	0.8358	0.3910	0.9489	0.046
H27E	0.6927	0.3514	0.9486	0.046
H27F	0.7208	0.4397	0.9730	0.046
H28D	0.9138	0.5801	0.8810	0.06
H28E	0.9131	0.5265	0.9297	0.06
H28F	0.8088	0.5916	0.9253	0.06
H29D	0.7186	0.6231	0.8163	0.071
H29E	0.6645	0.5742	0.7617	0.071

	x/a	y/b	z/c	U(eq)
H29F	0.8155	0.5749	0.7800	0.071
H32B	0.3798	0.3726	0.6442	0.053
H33B	0.1949	0.3596	0.5853	0.074
H34B	0.2070	0.3019	0.4984	0.057
H35B	0.4002	0.2549	0.4705	0.042
H36B	0.5836	0.2647	0.5296	0.034
H37B	0.5600	0.4864	0.6508	0.035
H38D	0.7777	0.5274	0.6866	0.058
H38E	0.7054	0.5884	0.6528	0.058
H38F	0.8134	0.5364	0.6262	0.058
H39D	0.6777	0.4668	0.5501	0.063
H39E	0.5876	0.5371	0.5664	0.063
H39F	0.5276	0.4496	0.5593	0.063
H40B	0.5830	0.1756	0.6092	0.037
H41D	0.7814	0.1308	0.6392	0.063
H41E	0.6679	0.0856	0.6665	0.063
H41F	0.7524	0.1550	0.7004	0.063
H42D	0.5343	0.2131	0.7199	0.064
H42E	0.4617	0.1432	0.6818	0.064
H42F	0.4392	0.2312	0.6705	0.064
H52B	1.1772	0.2326	0.8312	0.033
H53B	1.3225	0.1535	0.8712	0.045
H54B	1.3001	0.1242	0.9587	0.052
H55B	1.1355	0.1772	1.0080	0.047
H56B	0.9891	0.2568	0.9684	0.033
H57B	1.1981	0.3766	0.8550	0.026
H58D	1.1049	0.4744	0.8027	0.043
H58E	1.2317	0.5032	0.8400	0.043
H58F	1.0912	0.5256	0.8584	0.043
H59D	1.0874	0.4615	0.9431	0.048
H59E	1.2401	0.4616	0.9350	0.048
H59F	1.1628	0.3830	0.9460	0.048
H60B	0.7032	0.2048	0.8308	0.028
H61D	0.9002	0.1568	0.7974	0.045
H61E	0.8054	0.0928	0.8193	0.045
H61F	0.9315	0.1272	0.8551	0.045
H62D	0.8115	0.1696	0.9320	0.048
H62E	0.6771	0.1349	0.9026	0.048
H62F	0.6915	0.2242	0.9262	0.048

Table 9. Data collection details for 9b.

Axis	dx/mm	2θ/°	ω/°	φ/°	χ/°	Width/°	Frames	Time/s
Omega	50.830	-31.50	328.50	90.00	54.71	-0.30	610	35.00
Omega	50.830	-31.50	328.50	210.00	54.71	-0.30	610	35.00
Omega	50.830	-31.50	328.50	330.00	54.71	-0.30	610	35.00
Phi	50.830	-31.50	148.50	0.00	54.71	-0.30	300	35.00

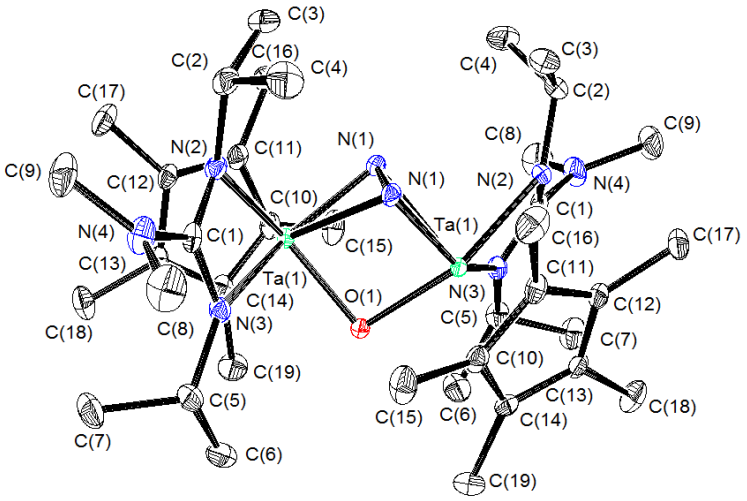
Table 10. Platon CheckCIF for 9b.

```
#===============================================================================
# PLATON/CHECK-(160910) versus check.def version of 160910  for entry: 2068
# Data From: 2068.cif - Data Type: CIF          Bond Precision   C-C = 0.0051 A
# Refl Data: 2068.fcf - Data Type: SHELXL                          Temp = 150 K
#
# UCL 10.3290(13)   17.301(2)   25.090(3)  95.3168(19)    93.183(2)   92.545(2)
# WaveLength 0.71073    Volume Reported    4452.1(10)  Calculated     4451.9(9)
# SpaceGroup from Symmetry P -1          Hall: -P 1
#                 Reported P-1                -P 1
# MoietyFormula C46 H68 N6 O Ta2
#      Reported C46 H68 N6 O Ta2
#    SumFormula C46 H68 N6 O Ta2
#      Reported C46 H68 N6 O Ta2
# Mr        =   1082.97[Calc],   1082.96[Rep]
# Dx,gcm-3  =     1.616[Calc],     1.616[Rep]
# Z         =         4[Calc],         4[Rep]
# Mu (mm-1) =     4.953[Calc],     4.952[Rep]
# F000      =    2160.0[Calc],    2160.0[Rep]  or F000' =   2155.13[Calc]
# Reported   T Limits: Tmin=0.479             Tmax=0.906  AbsCorr=MULTI-SCAN
# Calculated T Limits: Tmin=0.510 Tmin'=0.287  Tmax=0.906
# Reported   Hmax= 13, Kmax= 22, Lmax= 32, Nref= 20406        , Th(max)= 27.500
# Obs in FCF Hmax= 13, Kmax= 22, Lmax= 32, Nref= 20406        , Th(max)= 27.499
# Calculated Hmax= 13, Kmax= 22, Lmax= 32, Nref= 20478        , Ratio  =  0.996
# Reported   Rho(min) = -0.97, Rho(max) =  1.00 e/Ang**3 (From CIF)
# Calculated Rho(min) = -0.93, Rho(max) =  0.99 e/Ang**3 (From CIF+FCF data)
# w=1/[sigma**2(Fo**2)+(0.0100P)**2+  5.8180P], P=(Fo**2+2*Fc**2)/3
# R= 0.0246( 17028), wR2= 0.0462( 20406), S = 1.000      (From CIF+FCF data)
# R= 0.0246( 17028), wR2= 0.0462( 20406), S = 1.000      (From FCF data only)
# R= 0.0246( 17028), wR2= 0.0462( 20406), S = 1.001, Npar=1027
#===============================================================================

>>> The Following Model and Quality ALERTS were generated     - (Acta-Mode) <<<
================================================================================
374_ALERT_2_A Long   N - N         Bond  N1A    -   N2A    ...       1.50 Ang.
374_ALERT_2_A Long   N - N         Bond  N1B    -   N2B    ...       1.49 Ang.
#===============================================================================
220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...       3.41 Ratio
241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       C33B
324_ALERT_2_C Check for Possibly Missing H on Coordinating....        N1A
324_ALERT_2_C Check for Possibly Missing H on Coordinating....        N2A
324_ALERT_2_C Check for Possibly Missing H on Coordinating....        N1B
324_ALERT_2_C Check for Possibly Missing H on Coordinating....        N2B
601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .      34.00 A**3
910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) .....         5
911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600         32
#===============================================================================
083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.       5.82
#===============================================================================

>>> The Following Improvement and Query ALERTS were generated - (Acta-Mode) <<<
================================================================================
912_ALERT_4_C Missing # of FCF Reflections Above STh/L=  0.600         35
#===============================================================================
380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety       C27B
#===============================================================================
```

{Cp*Ta[N(iPr)C(NMe$_2$)N(iPr]}$_2$(μ-η^2:η^2-N$_2$)(μ-O) (9c)



A red prism of $(C_{10}H_{15})_2(C_9H_{20}N_3)_2Ta_2N_2O{\cdot}C_6D_6$, approximate dimensions 0.165×0.27×0.275 mm^3, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured at 220(2) K on a three-circle diffractometer system equipped with Bruker Smart Apex II CCD area detector using a graphite monochromator and a MoKα fine-focus sealed tube (λ= 0.71073 Å) . The detector was placed at a distance of 5.000 cm from the crystal.

A total of 1818 frames were collected with a scan width of -0.5° an exposure time of 20 sec/frame using Apex2 (Bruker, 2005). The total data collection time was 13.1 hours. The frames were integrated with Apex2 software package using a narrow-frame integration algorithm. The integration of the data using a Orthorhombic unit cell yielded a total of 29807 reflections to a maximum θ angle of 30.00°, of which 6702 were independent (completeness = 100.0%, R_{int} = 3.60%, R_{sig} = 2.55%) and 6617 were greater than 2σ(I). The final cell dimensions of a = 15.4459(12) Å, b = 15.9426(13) Å, c = 18.6329(15) Å, α = 90°, β = 90°, γ = 90°, V = 4588.3(6) Å^3, are based upon the refinement of the XYZ-centroids of 24924 reflections with 2.6 < θ < 32.2° using Apex2 software. Analysis of the data showed 0 % decay during data collection. Data were corrected for absorption effects with the Semi-empirical from equivalents method using SADABS (Sheldrick, 1996). The minimum and maximum transmission coefficients were 0.287 and 0.452.

The structure was solved and refined using the SHELXS-97 (Sheldrick, 1990) and SHELXL-97 (Sheldrick, 1997) software in the space group C222$_1$ with Z = 4 for the formula unit $(C_{10}H_{15})_2(C_9H_{20}N_3)_2Ta_2N_2O{\cdot}C_6D_6$. The final anisotropic full-matrix least-squares refinement on F^2 with 262 variables converged at R_1 = 1.71 % for the observed data and wR_2 = 4.13 % for all data. The goodness-of-fit was 1.002. The largest peak on the final difference map was 1.486 e$^-$/Å^3 and the largest hole was -1.199 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.585 g/cm^3 and F(000), 2200 e$^-$.

Comments:

- Data quality:	very good
- Twinning:	merohedral twinning refined to a 3:2 ratio
- Disorder:	none
- H-atoms:	constrained geometry as riding on attached atom (A) U_{iso}(H)=1.5U_{iso}(A) for CH_3 and 1.2U_{iso}(A) for other groups
- Residual density:	near heavy atoms
- Structure quality:	excellent

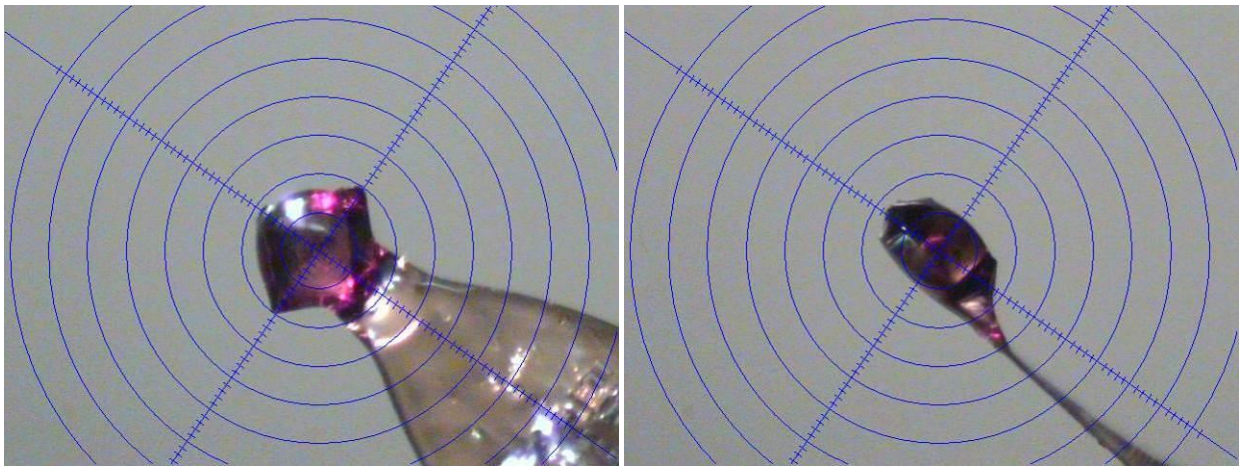


Table 1. Crystal data and structure refinement for **9c**.

X-ray lab book No.	**9c**
Crystal ID	**9c**
Empirical formula	$(C_{10}H_{15})_2(C_9H_{20}N_3)_2Ta_2N_2O\cdot C_6D_6$
Formula weight	1095.03
Temperature	220(2) K
Wavelength	0.71073 Å
Crystal size	0.275×0.27×0.165 mm^3
Crystal habit	red prism
Crystal system	Orthorhombic
Space group	$C222_1$
Unit cell dimensions	a = 15.4459(12) Å α = 90°
	b = 15.9426(13) Å β = 90°
	c = 18.6329(15) Å γ = 90°
Volume	4588.3(6) $Å^3$
Z	4
Density, ρ_{calc}	1.585 g/cm^3
Absorption coefficient, μ	4.807 mm^{-1}
F(000)	2200 ē
Diffractometer	Bruker Smart Apex II CCD area detector
Radiation source	fine-focus sealed tube, MoKα
Detector distance	5.000 cm
Data collection method	ω and φ scans
Total frames	1818
Frame size	512 pixels
Frame width	-0.5°
Exposure per frame	20 sec
Total measurement time	13.1 hours
θ range for data collection	2.14 to 30.00°
Index ranges	$-21 \le h \le 21$, $-22 \le k \le 21$, $-26 \le l \le 26$
Reflections collected	29807
Independent reflections	6702
Observed reflection, I>2σ(I)	6617
Coverage of independent reflections	100.0 %
Variation in check reflections	0 %
Absorption correction	Semi-empirical from equivalents
	SADABS (Sheldrick, 1996)
Max. and min. transmission	0.452 and 0.287
Structure solution technique	direct
Structure solution program	SHELXS-97 (Sheldrick, 1990)

Refinement technique		Full-matrix least-squares on F^2
Refinement program		SHELXL-97 (Sheldrick, 1997)
Function minimized		$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters		6702 / 0 / 262
Goodness-of-fit on F^2		1.002
Δ/σ_{max}		0.003
Final R indices:	R_1, $I>2\sigma(I)$	0.0171
	wR_2, all data	0.0413
	R_{int}	0.0360
	R_{sig}	0.0255
Weighting scheme		$w = 1/[\sigma^2(F_o^2)+ (0.01P)^2 + 9.32P]$, $P = [\max(F_o^2 ,0) + 2F_o^2]/3$
Absolute structure parameter		0.390(7)
Largest diff. peak and hole		1.486 and -1.199 $\bar{e}/Å^3$

$R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table 2. Atomic coordinates and equivalent* isotropic atomic displacement parameters (Å^2) for **9c**.

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Ta1	0.255082(5)	0.490693(5)	0.077216(4)	0.01675(3)
O1	0.16786(13)	0.5000	0.0000	0.0192(4)
N1	0.33738(13)	0.45577(15)	-0.01365(10)	0.0214(4)
N2	0.34687(14)	0.40201(14)	0.13046(12)	0.0235(4)
N3	0.21501(15)	0.35703(13)	0.10328(12)	0.0236(4)
C1	0.29264(18)	0.33668(17)	0.13030(14)	0.0257(5)
N4	0.3144(2)	0.25772(15)	0.15503(15)	0.0378(6)
C2	0.44159(19)	0.3894(2)	0.12877(17)	0.0350(6)
C3	0.48801(18)	0.4726(2)	0.11874(19)	0.0435(8)
C4	0.4708(2)	0.3281(2)	0.0698(2)	0.0493(9)
C5	0.1383(2)	0.30315(19)	0.10870(17)	0.0333(6)
C6	0.05907(19)	0.3525(2)	0.0847(2)	0.0422(7)
C7	0.1201(3)	0.2647(2)	0.18253(19)	0.0465(8)
C8	0.2972(3)	0.1826(2)	0.1142(2)	0.0545(10)
C9	0.3626(3)	0.2463(3)	0.2205(2)	0.0529(10)
C10	0.21480(19)	0.63276(16)	0.11610(15)	0.0272(5)
C11	0.2939(2)	0.61577(17)	0.15261(14)	0.0281(5)
C12	0.27658(18)	0.55160(17)	0.20315(13)	0.0269(5)
C13	0.18753(18)	0.52901(18)	0.19705(13)	0.0265(5)
C14	0.14939(19)	0.58008(18)	0.14451(15)	0.0272(5)
C15	0.2025(3)	0.70444(19)	0.06522(17)	0.0434(8)
C16	0.3747(2)	0.6654(2)	0.14250(19)	0.0439(8)
C17	0.3368(2)	0.5196(2)	0.26045(15)	0.0417(7)
C18	0.1429(2)	0.4721(2)	0.24963(16)	0.0428(8)
C19	0.0550(2)	0.5836(2)	0.1252(2)	0.0429(8)
C21	0.1983(3)	0.0000	0.0000	0.0598(14)
C22	0.2403(4)	-0.0522(3)	0.0459(2)	0.0658(11)
C23	0.3298(4)	-0.0516(4)	0.0457(3)	0.0843(19)
C24	0.3736(4)	0.0000	0.0000	0.091(3)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic atomic displacement parameters* (Å^2) for **9c**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ta1	0.01823(4)	0.01785(4)	0.01416(4)	0.00069(3)	0.00043(3)	0.00103(3)
O1	0.0186(9)	0.0220(12)	0.0169(10)	0.0001(10)	0.000	0.000
N1	0.0227(9)	0.0255(11)	0.0161(10)	-0.0032(8)	0.0008(7)	0.0021(7)
N2	0.0228(10)	0.0279(10)	0.0197(10)	0.0028(8)	-0.0021(8)	0.0057(8)
N3	0.0283(10)	0.0207(9)	0.0218(10)	0.0045(8)	-0.0002(8)	-0.0021(7)
C1	0.0355(13)	0.0251(12)	0.0164(11)	0.0048(9)	0.0004(9)	0.0046(10)
N4	0.0522(17)	0.0268(12)	0.0343(13)	0.0102(10)	-0.0048(12)	0.0096(11)
C2	0.0268(13)	0.0491(17)	0.0290(15)	0.0058(13)	-0.0036(11)	0.0111(12)
C3	0.0236(12)	0.064(2)	0.0428(17)	-0.0003(16)	-0.0044(11)	-0.0025(13)
C4	0.0391(16)	0.055(2)	0.054(2)	0.0001(18)	0.0076(16)	0.0219(14)
C5	0.0375(15)	0.0301(13)	0.0323(15)	0.0062(11)	0.0013(12)	-0.0111(11)
C6	0.0314(14)	0.0484(18)	0.047(2)	0.0108(17)	-0.0029(14)	-0.0121(12)
C7	0.056(2)	0.0435(18)	0.0398(19)	0.0161(15)	0.0089(15)	-0.0116(16)
C8	0.080(3)	0.0237(14)	0.060(2)	0.0043(15)	-0.003(2)	0.0087(15)
C9	0.068(3)	0.054(2)	0.037(2)	0.0201(16)	-0.0061(17)	0.0156(18)

C10	0.0386(14)	0.0230(11)	0.0200(12)	-0.0042(9)	0.0028(10)	0.0043(9)
C11	0.0379(15)	0.0281(13)	0.0182(12)	-0.0081(10)	-0.0002(10)	-0.0031(11)
C12	0.0324(13)	0.0325(13)	0.0159(10)	-0.0041(9)	-0.0003(9)	0.0047(10)
C13	0.0347(13)	0.0289(13)	0.0159(10)	-0.0004(9)	0.0061(9)	0.0062(10)
C14	0.0293(13)	0.0302(13)	0.0220(12)	-0.0041(10)	0.0042(10)	0.0089(10)
C15	0.073(2)	0.0266(13)	0.0308(16)	0.0033(11)	-0.0001(14)	0.0099(13)
C16	0.0471(19)	0.0456(18)	0.0390(18)	-0.0154(15)	0.0046(14)	-0.0179(15)
C17	0.0474(16)	0.057(2)	0.0210(13)	-0.0043(14)	-0.0089(11)	0.0145(15)
C18	0.0556(19)	0.0448(18)	0.0280(15)	0.0039(13)	0.0143(13)	-0.0040(14)
C19	0.0290(14)	0.0528(19)	0.0469(19)	-0.0004(15)	0.0013(13)	0.0137(13)
C21	0.044(2)	0.071(4)	0.064(3)	-0.011(3)	0.000	0.000
C22	0.089(3)	0.056(2)	0.053(2)	0.0001(17)	0.014(2)	0.007(3)
C23	0.091(4)	0.106(4)	0.057(3)	-0.035(3)	-0.023(3)	0.054(3)
C24	0.041(3)	0.157(9)	0.075(5)	-0.072(6)	0.000	0.000

* The anisotropic atomic displacement factor exponent takes the form:$-2\pi^2$ [$h^2a^{*2}U_{11}$ +... + 2hka*b*U_{12}]

Table 4. Hydrogen atom coordinates and isotropic atomic displacement parameters (Å^2) for **9c**.

Atom	*x/a*	*y/b*	*z/c*	U_{iso}
H2	0.4594	0.3659	0.1757	0.042
H3A	0.4717	0.5107	0.1570	0.065
H3B	0.4719	0.4967	0.0729	0.065
H3C	0.5501	0.4635	0.1199	0.065
H4A	0.4534	0.3496	0.0232	0.074
H4B	0.4440	0.2739	0.0777	0.074
H4C	0.5333	0.3223	0.0712	0.074
H5	0.1462	0.2563	0.0745	0.040
H6A	0.0699	0.3770	0.0379	0.063
H6B	0.0472	0.3967	0.1190	0.063
H6C	0.0096	0.3152	0.0818	0.063
H7A	0.1007	0.3082	0.2152	0.070
H7B	0.1727	0.2394	0.2011	0.070
H7C	0.0755	0.2222	0.1781	0.070
H8A	0.2784	0.1978	0.0663	0.082
H8B	0.2522	0.1503	0.1377	0.082
H8C	0.3496	0.1492	0.1111	0.082
H9A	0.3626	0.2982	0.2477	0.079
H9B	0.4217	0.2307	0.2092	0.079
H9C	0.3359	0.2023	0.2489	0.079
H15A	0.2465	0.7022	0.0282	0.065
H15B	0.2073	0.7570	0.0912	0.065
H15C	0.1457	0.7006	0.0433	0.065
H16A	0.4173	0.6483	0.1778	0.066
H16B	0.3620	0.7246	0.1484	0.066
H16C	0.3973	0.6557	0.0947	0.066
H17A	0.3945	0.5419	0.2524	0.063
H17B	0.3386	0.4589	0.2588	0.063
H17C	0.3162	0.5376	0.3072	0.063
H18A	0.0876	0.4546	0.2301	0.064
H18B	0.1337	0.5018	0.2944	0.064
H18C	0.1787	0.4231	0.2583	0.064
H19A	0.0228	0.5459	0.1561	0.064
H19B	0.0475	0.5667	0.0756	0.064

H19C	0.0338	0.6404	0.1315	0.064
D21	0.1374	0.0000	0.0000	0.072
D22	0.2094	-0.0877	0.0770	0.079
D23	0.3605	-0.0869	0.0770	0.101
D24	0.4345	0.0000	0.0000	0.109

Table 5. Bond lengths (Å) and angles (°) for **9c**.

Ta1-N1#1	1.936(2)	Ta1-O1	1.9766(14)	Ta1-N1	2.1893(19)
Ta1-N2	2.235(2)	Ta1-N3	2.272(2)	Ta1-C10	2.458(3)
Ta1-C14	2.504(3)	Ta1-C11	2.512(3)	Ta1-C13	2.539(2)
Ta1-C12	2.561(2)	Ta1-Ta1#1	2.8928(3)	O1-Ta1#1	1.9766(14)
N1-N1#1	1.499(4)	N1-Ta1#1	1.936(2)	N2-C1	1.337(4)
N2-C2	1.477(3)	N3-C1	1.340(3)	N3-C5	1.467(3)
C1-N4	1.382(3)	N4-C9	1.441(4)	N4-C8	1.444(4)
C2-C3	1.519(5)	C2-C4	1.539(5)	C5-C6	1.522(4)
C5-C7	1.532(4)	C10-C14	1.416(4)	C10-C11	1.424(4)
C10-C15	1.497(4)	C11-C12	1.416(4)	C11-C16	1.490(4)
C12-C13	1.426(4)	C12-C17	1.505(4)	C13-C14	1.403(4)
C13-C18	1.503(4)	C14-C19	1.502(4)	C21-C22#2	1.358(5)
C21-C22	1.358(5)	C22-C23	1.383(7)	C23-C24	1.364(7)
C24-C23#2	1.364(7)				
N1#1-Ta1-O1	88.23(7)	N1#1-Ta1-N1	42.07(12)	O1-Ta1-N1	81.48(7)
N1#1-Ta1-N2	97.70(9)	O1-Ta1-N2	143.43(6)	N1-Ta1-N2	79.28(8)
N1#1-Ta1-N3	136.34(9)	O1-Ta1-N3	92.31(6)	N1-Ta1-N3	94.87(8)
N2-Ta1-N3	58.96(8)	N1#1-Ta1-C10	86.57(9)	O1-Ta1-C10	88.45(7)
N1-Ta1-C10	127.54(9)	N2-Ta1-C10	127.79(9)	N3-Ta1-C10	137.09(8)
N1#1-Ta1-C14	118.92(9)	O1-Ta1-C14	82.96(8)	N1-Ta1-C14	155.61(9)
N2-Ta1-C14	123.47(9)	N3-Ta1-C14	104.43(9)	C10-Ta1-C14	33.16(9)
N1#1-Ta1-C11	80.53(9)	O1-Ta1-C11	120.67(7)	N1-Ta1-C11	119.74(9)
N2-Ta1-C11	95.90(9)	N3-Ta1-C11	133.64(9)	C10-Ta1-C11	33.27(9)
C14-Ta1-C11	54.79(10)	N1#1-Ta1-C13	134.57(9)	O1-Ta1-C13	110.00(8)
N1-Ta1-C13	168.49(9)	N2-Ta1-C13	91.29(8)	N3-Ta1-C13	85.74(9)
C10-Ta1-C13	54.20(9)	C14-Ta1-C13	32.30(9)	C11-Ta1-C13	54.21(9)
N1#1-Ta1-C12	107.95(9)	O1-Ta1-C12	136.62(7)	N1-Ta1-C12	136.87(8)
N2-Ta1-C12	75.58(8)	N3-Ta1-C12	101.25(9)	C10-Ta1-C12	54.08(9)
C14-Ta1-C12	53.83(9)	C11-Ta1-C12	32.39(9)	C13-Ta1-C12	32.48(9)
N1#1-Ta1-Ta1#1	49.17(6)	O1-Ta1-Ta1#1	42.96(4)	N1-Ta1-Ta1#1	41.99(6)
N2-Ta1-Ta1#1	120.43(6)	N3-Ta1-Ta1#1	107.99(6)	C10-Ta1-Ta1#1	101.46(7)
C14-Ta1-Ta1#1	116.09(7)	C11-Ta1-Ta1#1	118.35(7)	C13-Ta1-Ta1#1	148.21(6)
C12-Ta1-Ta1#1	150.75(6)	Ta1#1-O1-Ta1	94.07(9)	N1#1-N1-Ta1#1	78.04(13)
N1#1-N1-Ta1	59.88(10)	Ta1#1-N1-Ta1	88.84(8)	C1-N2-C2	121.0(2)
C1-N2-Ta1	95.42(16)	C2-N2-Ta1	134.82(19)	C1-N3-C5	123.7(2)
C1-N3-Ta1	93.65(16)	C5-N3-Ta1	141.64(18)	N2-C1-N3	111.9(2)
N2-C1-N4	123.8(3)	N3-C1-N4	124.3(3)	C1-N4-C9	121.5(3)
C1-N4-C8	122.3(3)	C9-N4-C8	115.9(3)	N2-C2-C3	110.6(2)
N2-C2-C4	113.1(3)	C3-C2-C4	109.2(3)	N3-C5-C6	109.1(2)
N3-C5-C7	116.4(3)	C6-C5-C7	108.9(3)	C14-C10-C11	108.7(2)
C14-C10-C15	126.8(3)	C11-C10-C15	123.8(3)	C14-C10-Ta1	75.19(15)
C11-C10-Ta1	75.43(15)	C15-C10-Ta1	123.29(19)	C12-C11-C10	107.1(3)
C12-C11-C16	128.7(3)	C10-C11-C16	123.8(3)	C12-C11-Ta1	75.72(15)
C10-C11-Ta1	71.30(15)	C16-C11-Ta1	123.42(19)	C11-C12-C13	108.1(2)
C11-C12-C17	126.9(3)	C13-C12-C17	124.6(3)	C11-C12-Ta1	71.88(14)
C13-C12-Ta1	72.92(14)	C17-C12-Ta1	126.99(19)	C14-C13-C12	108.3(2)
C14-C13-C18	127.8(3)	C12-C13-C18	122.9(3)	C14-C13-Ta1	72.46(14)
C12-C13-Ta1	74.61(14)	C18-C13-Ta1	128.0(2)	C13-C14-C10	107.8(3)
C13-C14-C19	126.6(3)	C10-C14-C19	125.5(3)	C13-C14-Ta1	75.25(15)
C10-C14-Ta1	71.66(14)	C19-C14-Ta1	122.3(2)	C22#2-C21-C22	122.9(6)

C21-C22-C23	118.1(5)	C24-C23-C22	120.2(5)	C23-C24-C23#2	120.4(6)

Symmetry transformation codes:#1 x,-y+1,-z #2 x,-y,-z

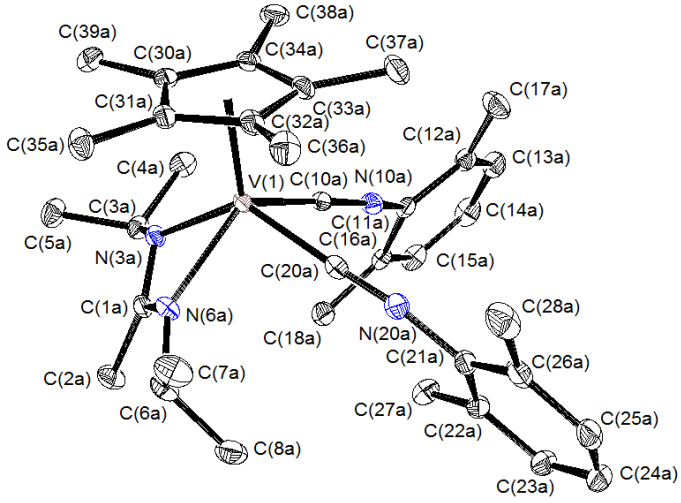
Table 6. Torsion angles (°) for **9c**.

N1#1-Ta1-O1-Ta1#1	22.09(7)	N1-Ta1-O1-Ta1#1	-19.64(6)	N2-Ta1-O1-Ta1#1	-78.47(11)
N3-Ta1-O1-Ta1#1	-114.22(6)	C10-Ta1-O1-Ta1#1	108.71(7)	C14-Ta1-O1-Ta1#1	141.52(7)
C11-Ta1-O1-Ta1#1	99.99(8)	C13-Ta1-O1-Ta1#1	159.47(7)	C12-Ta1-O1-Ta1#1	136.69(10)
O1-Ta1-N1-N1#1	96.85(11)	N2-Ta1-N1-N1#1	-114.41(12)	N3-Ta1-N1-N1#1	-171.53(12)
C10-Ta1-N1-N1#1	15.46(15)	C14-Ta1-N1-N1#1	45.9(2)	C11-Ta1-N1-N1#1	-23.70(15)
C13-Ta1-N1-N1#1	-78.9(5)	C12-Ta1-N1-N1#1	-59.36(18)	Ta1#1-Ta1-N1-N1#1	76.84(14)
N1#1-Ta1-N1-Ta1#1	-76.84(14)	O1-Ta1-N1-Ta1#1	20.02(6)	N2-Ta1-N1-Ta1#1	168.76(10)
N3-Ta1-N1-Ta1#1	111.63(9)	C10-Ta1-N1-Ta1#1	-61.37(12)	C14-Ta1-N1-Ta1#1	-30.9(2)
C11-Ta1-N1-Ta1#1	-100.54(10)	C13-Ta1-N1-Ta1#1	-155.8(4)	C12-Ta1-N1-Ta1#1	-136.19(10)
N1#1-Ta1-N2-C1	-138.70(16)	O1-Ta1-N2-C1	-41.2(2)	N1-Ta1-N2-C1	-100.70(17)
N3-Ta1-N2-C1	1.71(15)	C10-Ta1-N2-C1	129.66(17)	C14-Ta1-N2-C1	88.89(18)
C11-Ta1-N2-C1	140.09(17)	C13-Ta1-N2-C1	85.95(17)	C12-Ta1-N2-C1	114.66(17)
Ta1#1-Ta1-N2-C1	-92.00(16)	N1#1-Ta1-N2-C2	6.7(3)	O1-Ta1-N2-C2	104.2(3)
N1-Ta1-N2-C2	44.7(3)	N3-Ta1-N2-C2	147.1(3)	C10-Ta1-N2-C2	-84.9(3)
C14-Ta1-N2-C2	-125.7(3)	C11-Ta1-N2-C2	-74.5(3)	C13-Ta1-N2-C2	-128.6(3)
C12-Ta1-N2-C2	-99.9(3)	Ta1#1-Ta1-N2-C2	53.4(3)	N1#1-Ta1-N3-C1	64.5(2)
O1-Ta1-N3-C1	154.33(16)	N1-Ta1-N3-C1	72.69(16)	N2-Ta1-N3-C1	-1.70(15)
C10-Ta1-N3-C1	-115.46(18)	C14-Ta1-N3-C1	-122.35(16)	C11-Ta1-N3-C1	-67.6(2)
C13-Ta1-N3-C1	-95.78(17)	C12-Ta1-N3-C1	-67.11(17)	Ta1#1-Ta1-N3-C1	113.53(15)
N1#1-Ta1-N3-C5	-127.9(3)	O1-Ta1-N3-C5	-38.1(3)	N1-Ta1-N3-C5	-119.7(3)
N2-Ta1-N3-C5	165.9(3)	C10-Ta1-N3-C5	52.1(3)	C14-Ta1-N3-C5	45.2(3)
C11-Ta1-N3-C5	100.0(3)	C13-Ta1-N3-C5	71.8(3)	C12-Ta1-N3-C5	100.5(3)
Ta1#1-Ta1-N3-C5	-78.9(3)	C2-N2-C1-N3	-154.7(2)	Ta1-N2-C1-N3	-2.7(2)
C2-N2-C1-N4	25.2(4)	Ta1-N2-C1-N4	177.2(2)	C5-N3-C1-N2	-168.1(2)
Ta1-N3-C1-N2	2.6(2)	C5-N3-C1-N4	11.9(4)	Ta1-N3-C1-N4	-177.3(3)
N2-C1-N4-C9	43.0(5)	N3-C1-N4-C9	-137.1(3)	N2-C1-N4-C8	-131.5(4)
N3-C1-N4-C8	48.4(5)	C1-N2-C2-C3	172.0(3)	Ta1-N2-C2-C3	33.2(4)
C1-N2-C2-C4	49.3(4)	Ta1-N2-C2-C4	-89.5(3)	C1-N3-C5-C6	169.7(3)
Ta1-N3-C5-C6	4.7(4)	C1-N3-C5-C7	46.1(4)	Ta1-N3-C5-C7	-118.9(3)
N1#1-Ta1-C10-C14	167.79(17)	O1-Ta1-C10-C14	79.47(16)	N1-Ta1-C10-C14	157.48(15)
N2-Ta1-C10-C14	-95.12(19)	N3-Ta1-C10-C14	-12.3(2)	C11-Ta1-C10-C14	-114.3(2)
C13-Ta1-C10-C14	-36.71(16)	C12-Ta1-C10-C14	-77.08(18)	Ta1#1-Ta1-C10-C14	120.67(15)
N1#1-Ta1-C10-C11	-77.93(16)	O1-Ta1-C10-C11	-166.25(16)	N1-Ta1-C10-C11	-88.24(17)
N2-Ta1-C10-C11	19.2(2)	N3-Ta1-C10-C11	102.03(18)	C14-Ta1-C10-C11	114.3(2)
C13-Ta1-C10-C11	77.56(17)	C12-Ta1-C10-C11	37.20(15)	Ta1#1-Ta1-C10-C11	-125.05(15)
N1#1-Ta1-C10-C15	43.2(3)	O1-Ta1-C10-C15	-45.1(3)	N1-Ta1-C10-C15	32.9(3)
N2-Ta1-C10-C15	140.3(2)	N3-Ta1-C10-C15	-136.8(3)	C14-Ta1-C10-C15	-124.6(3)
C11-Ta1-C10-C15	121.2(3)	C13-Ta1-C10-C15	-161.3(3)	C12-Ta1-C10-C15	158.4(3)
Ta1#1-Ta1-C10-C15	-3.9(3)	C14-C10-C11-C12	0.6(3)	C15-C10-C11-C12	171.5(2)
Ta1-C10-C11-C12	-67.89(18)	C14-C10-C11-C16	-173.3(3)	C15-C10-C11-C16	-2.3(4)
Ta1-C10-C11-C16	118.2(3)	C14-C10-C11-Ta1	68.48(18)	C15-C10-C11-Ta1	-120.6(3)
N1#1-Ta1-C11-C12	-147.79(18)	O1-Ta1-C11-C12	129.99(15)	N1-Ta1-C11-C12	-131.94(16)
N2-Ta1-C11-C12	-50.93(17)	N3-Ta1-C11-C12	0.9(2)	C10-Ta1-C11-C12	114.0(2)
C14-Ta1-C11-C12	76.35(18)	C13-Ta1-C11-C12	36.40(15)	Ta1#1-Ta1-C11-C12	179.69(13)
N1#1-Ta1-C11-C10	98.26(16)	O1-Ta1-C11-C10	16.03(18)	N1-Ta1-C11-C10	114.11(17)
N2-Ta1-C11-C10	-164.89(16)	N3-Ta1-C11-C10	-113.04(16)	C14-Ta1-C11-C10	-37.61(16)
C13-Ta1-C11-C10	-77.55(18)	C12-Ta1-C11-C10	-114.0(2)	Ta1#1-Ta1-C11-C10	65.74(17)
N1#1-Ta1-C11-C16	-20.5(3)	O1-Ta1-C11-C16	-102.7(3)	N1-Ta1-C11-C16	-4.6(3)
N2-Ta1-C11-C16	76.4(3)	N3-Ta1-C11-C16	128.2(3)	C10-Ta1-C11-C16	-118.8(3)
C14-Ta1-C11-C16	-156.4(3)	C13-Ta1-C11-C16	163.7(3)	C12-Ta1-C11-C16	127.3(3)
Ta1#1-Ta1-C11-C16	-53.0(3)	C10-C11-C12-C13	0.5(3)	C16-C11-C12-C13	174.0(3)
Ta1-C11-C12-C13	-64.38(18)	C10-C11-C12-C17	-172.0(3)	C16-C11-C12-C17	1.5(5)
Ta1-C11-C12-C17	123.1(3)	C10-C11-C12-Ta1	64.89(17)	C16-C11-C12-Ta1	-121.6(3)
N1#1-Ta1-C12-C11	33.56(18)	O1-Ta1-C12-C11	-73.64(19)	N1-Ta1-C12-C11	70.9(2)
N2-Ta1-C12-C11	127.11(18)	N3-Ta1-C12-C11	-179.33(16)	C10-Ta1-C12-C11	-38.25(17)

C14-Ta1-C12-C11	-79.58(18)	C13-Ta1-C12-C11	-116.3(2)	Ta1#1-Ta1-C12-C11	-0.6(2)
N1#1-Ta1-C12-C13	149.86(16)	O1-Ta1-C12-C13	42.7(2)	N1-Ta1-C12-C13	-172.84(15)
N2-Ta1-C12-C13	-116.58(17)	N3-Ta1-C12-C13	-63.02(17)	C10-Ta1-C12-C13	78.05(17)
C14-Ta1-C12-C13	36.73(15)	C11-Ta1-C12-C13	116.3(2)	Ta1#1-Ta1-C12-C13	115.75(17)
N1#1-Ta1-C12-C17	-89.4(3)	O1-Ta1-C12-C17	163.4(2)	N1-Ta1-C12-C17	-52.1(3)
N2-Ta1-C12-C17	4.2(3)	N3-Ta1-C12-C17	57.7(3)	C10-Ta1-C12-C17	-161.2(3)
C14-Ta1-C12-C17	157.5(3)	C11-Ta1-C12-C17	-122.9(3)	C13-Ta1-C12-C17	120.8(3)
Ta1#1-Ta1-C12-C17	-123.5(2)	C11-C12-C13-C14	-1.4(3)	C17-C12-C13-C14	171.3(3)
Ta1-C12-C13-C14	-65.14(18)	C11-C12-C13-C18	-170.6(3)	C17-C12-C13-C18	2.1(4)
Ta1-C12-C13-C18	125.7(3)	C11-C12-C13-Ta1	63.71(18)	C17-C12-C13-Ta1	-123.6(3)
N1#1-Ta1-C13-C14	73.3(2)	O1-Ta1-C13-C14	-34.93(18)	N1-Ta1-C13-C14	140.6(4)
N2-Ta1-C13-C14	175.41(17)	N3-Ta1-C13-C14	-125.85(18)	C10-Ta1-C13-C14	37.73(17)
C11-Ta1-C13-C14	79.07(19)	C12-Ta1-C13-C14	115.4(2)	Ta1#1-Ta1-C13-C14	-7.9(2)
N1#1-Ta1-C13-C12	-42.1(2)	O1-Ta1-C13-C12	-150.31(14)	N1-Ta1-C13-C12	25.3(5)
N2-Ta1-C13-C12	60.03(16)	N3-Ta1-C13-C12	118.78(17)	C10-Ta1-C13-C12	-77.64(17)
C14-Ta1-C13-C12	-115.4(2)	C11-Ta1-C13-C12	-36.31(15)	Ta1#1-Ta1-C13-C12	-123.33(16)
N1#1-Ta1-C13-C18	-162.0(2)	O1-Ta1-C13-C18	89.8(3)	N1-Ta1-C13-C18	-94.7(5)
N2-Ta1-C13-C18	-59.9(3)	N3-Ta1-C13-C18	-1.2(3)	C10-Ta1-C13-C18	162.4(3)
C14-Ta1-C13-C18	124.7(3)	C11-Ta1-C13-C18	-156.2(3)	C12-Ta1-C13-C18	-119.9(3)
Ta1#1-Ta1-C13-C18	116.7(2)	C12-C13-C14-C10	1.8(3)	C18-C13-C14-C10	170.3(3)
Ta1-C13-C14-C10	-64.77(18)	C12-C13-C14-C19	-173.9(3)	C18-C13-C14-C19	-5.5(5)
Ta1-C13-C14-C19	119.5(3)	C12-C13-C14-Ta1	66.56(18)	C18-C13-C14-Ta1	-124.9(3)
C11-C10-C14-C13	-1.5(3)	C15-C10-C14-C13	-172.1(3)	Ta1-C10-C14-C13	67.17(18)
C11-C10-C14-C19	174.3(3)	C15-C10-C14-C19	3.7(4)	Ta1-C10-C14-C19	-117.0(3)
C11-C10-C14-Ta1	-68.65(18)	C15-C10-C14-Ta1	120.7(3)	N1#1-Ta1-C14-C13	-128.79(17)
O1-Ta1-C14-C13	147.17(17)	N1-Ta1-C14-C13	-162.16(19)	N2-Ta1-C14-C13	-5.5(2)
N3-Ta1-C14-C13	56.59(18)	C10-Ta1-C14-C13	-114.8(3)	C11-Ta1-C14-C13	-77.10(19)
C12-Ta1-C14-C13	-36.94(16)	Ta1#1-Ta1-C14-C13	175.35(15)	N1#1-Ta1-C14-C10	-14.0(2)
O1-Ta1-C14-C10	-98.00(16)	N1-Ta1-C14-C10	-47.3(3)	N2-Ta1-C14-C10	109.33(17)
N3-Ta1-C14-C10	171.42(15)	C11-Ta1-C14-C10	37.74(15)	C13-Ta1-C14-C10	114.8(3)
C12-Ta1-C14-C10	77.90(18)	Ta1#1-Ta1-C14-C10	-69.82(17)	N1#1-Ta1-C14-C19	107.0(3)
O1-Ta1-C14-C19	22.9(2)	N1-Ta1-C14-C19	73.6(3)	N2-Ta1-C14-C19	-129.7(2)
N3-Ta1-C14-C19	-67.6(3)	C10-Ta1-C14-C19	120.9(3)	C11-Ta1-C14-C19	158.7(3)
C13-Ta1-C14-C19	-124.2(3)	C12-Ta1-C14-C19	-161.2(3)	Ta1#1-Ta1-C14-C19	51.1(3)
C22#2-C21-C22-C23	0.1(3)	C21-C22-C23-C24	-0.3(6)	C22-C23-C24-C23#2	0.1(3)

Symmetry transformation codes:#1 x,-y+1,-z #2 x,-y,-z

Cp*V[N(iPr)C(Me)N(iPr][CN(2,6-$Me_2C_6H_3$)]$_2$ (10)



A dark brown prism-like specimen of $C_{36}H_{50}N_4V$, approximate dimensions 0.19 mm × 0.19 mm × 0.41 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX-II CCD system equipped with a graphite monochromator and a MoKα sealed tube (λ = 0.71073 Å). Data collection temperature was 150 K.

The total exposure time was 25.25 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 71077 reflections to a maximum θ angle of27.50° (0.77 Å resolution), of which 15274 were independent (average redundancy 4.653, completeness = 100.0%, R_{int} = 2.98%) and 12613 (82.58%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.9991(5) Å, b = 36.8188(16) Å, c =15.0590(7) Å, β = 93.1035(7)°, V = 6643.2(5) Å^3, are based upon the refinement of the XYZ-centroids of 9959 reflections above 20 σ(I) with 4.372° < 2θ < 60.91°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8680 and 0.9400. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group $P2_1/n$, with Z = 8 for the formula unit, $C_{36}H_{50}N_4V$. The final anisotropic full-matrix least-squares refinement on F^2 with 811 variables converged at R_1 =3.69%, for the observed data and wR_2 = 7.60% for all data. The goodness-of-fit was 1.000. The largest peak in the final difference electron density synthesis was 0.305 e$^-$/Å^3 and the largest hole was -0.385 e$^-$/Å^3 with an RMS deviation of 0.043 e$^-$/Å^3. On the basis of the final model, the calculated density was 1.179 g/cm^3 and F(000), 2536 e$^-$.

APEX2 Version 2010.11-3 (Bruker AXS Inc.)
SAINT Version 7.68A (Bruker AXS Inc., 2009)

SADABS Version 2008/1 (G. M. Sheldrick, Bruker AXS Inc.)
XPREP Version 2008/2 (G. M. Sheldrick, Bruker AXS Inc.)
XS Version 2008/1 (G. M. Sheldrick, *Acta Cryst.* (2008). A**64**, 112-122)
XL Version 2012/4 (G. M. Sheldrick, (2012) University of Gottingen, Germany)
Platon (A. L. Spek, *Acta Cryst.* (1990). A**46**, C-34)

Table 1. Sample and crystal data for 10.

Identification code	**10**
Chemical formula	$C_{36}H_{50}N_4V$
Formula weight	589.74
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal size	0.19 × 0.19 × 0.41 mm
Crystal habit	dark brown prism
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.9991(5) Å α = 90°
	b = 36.8188(16) Å β = 93.1035(7)°
	c = 15.0590(7) Å γ = 90°
Volume	6643.2(5) $Å^3$
Z	8
Density (calculated)	1.179 Mg/cm^3
Absorption coefficient	0.328 mm^{-1}
F(000)	2536

Table 2. Data collection and structure refinement for 10.

Diffractometer	Bruker APEX-II CCD
Radiation source	sealed tube, MoKα
Theta range for data collection	1.75 to 27.50°
Index ranges	$-15 \le h \le 15$, $-47 \le k \le 47$, $-19 \le l \le 19$
Reflections collected	71077
Independent reflections	15274 [R(int) = 0.0298]
Coverage of	100.0%

independent reflections		
Absorption correction	multi-scan	
Max. and min. transmission	0.9400 and 0.8680	
Structure solution technique	direct methods	
Structure solution program	ShelXS-97 (Sheldrick, 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	ShelXL-2014 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	15274 / 0 / 811	
Goodness-of-fit on F^2	1.000	
Δ/σ_{max}	0.003	
Final R indices	12613 data; $I>2\sigma(I)$	$R_1 = 0.0369$, $wR_2 = 0.0715$
	all data	$R_1 = 0.0479$, $wR_2 = 0.0760$
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0100P)^2+5.3300P]$, $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.305 and -0.385 eÅ^{-3}	
R.M.S. deviation from mean	0.043 eÅ^{-3}	

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})| / \Sigma[F_o^2]$
$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$
$\text{GOOF} = S = \{\Sigma[w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 10.

U(eq) is defined as one third of the trace of the orthogonalized

U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
V1	0.57299(2)	0.28206(2)	0.21444(2)	0.01844(6)
C1A	0.45958(12)	0.32929(4)	0.29317(10)	0.0237(3)
C2A	0.42435(15)	0.36527(4)	0.33212(12)	0.0351(4)
N3A	0.52314(10)	0.30507(3)	0.33761(8)	0.0224(3)
C3A	0.56193(13)	0.31228(4)	0.43007(10)	0.0268(3)
C4A	0.66687(15)	0.29059(5)	0.45620(11)	0.0340(4)
C5A	0.47157(16)	0.30329(5)	0.49512(12)	0.0392(4)
N6A	0.43743(10)	0.31951(3)	0.20915(9)	0.0248(3)
C6A	0.37513(14)	0.34356(5)	0.14620(11)	0.0325(4)
C7A	0.33310(16)	0.32202(5)	0.06486(13)	0.0435(5)
C8A	0.44165(16)	0.37657(5)	0.11654(12)	0.0386(4)
C10A	0.72693(12)	0.29653(4)	0.24691(10)	0.0212(3)
N10A	0.82153(10)	0.30601(3)	0.25675(9)	0.0276(3)
C11A	0.91980(12)	0.31936(4)	0.29766(10)	0.0238(3)
C12A	0.02048(13)	0.30131(4)	0.28219(11)	0.0286(3)
C13A	0.11790(14)	0.31454(5)	0.32468(12)	0.0368(4)
C14A	0.11610(15)	0.34455(5)	0.37939(12)	0.0407(4)
C15A	0.01670(15)	0.36257(5)	0.39126(11)	0.0355(4)
C16A	0.91649(13)	0.35081(4)	0.35018(10)	0.0267(3)
C17A	0.02043(15)	0.26931(5)	0.22033(14)	0.0434(5)
C18A	0.81029(15)	0.37183(5)	0.35988(12)	0.0341(4)
C20A	0.61975(12)	0.30594(4)	0.10500(10)	0.0228(3)
N20A	0.65364(12)	0.32047(4)	0.04198(9)	0.0294(3)
C21A	0.70416(13)	0.34491(4)	0.98617(10)	0.0274(3)
C22A	0.75793(13)	0.37554(4)	0.02353(11)	0.0288(3)
C23A	0.80457(15)	0.40007(5)	0.96589(12)	0.0372(4)
C24A	0.79824(16)	0.39430(6)	0.87509(13)	0.0434(5)
C25A	0.74524(16)	0.36389(6)	0.83987(12)	0.0421(5)
C26A	0.69613(14)	0.33848(5)	0.89402(11)	0.0340(4)
C27A	0.76687(15)	0.38128(5)	0.12236(11)	0.0333(4)
C28A	0.63598(18)	0.30581(6)	0.85702(12)	0.0466(5)
C30A	0.51748(13)	0.22541(4)	0.27079(11)	0.0260(3)

	x/a	y/b	z/c	U(eq)
C31A	0.45171(13)	0.23257(4)	0.19192(11)	0.0257(3)
C32A	0.52322(13)	0.23516(4)	0.12010(11)	0.0273(3)
C33A	0.63511(13)	0.23021(4)	0.15607(11)	0.0281(3)
C34A	0.63132(13)	0.22392(4)	0.24945(11)	0.0277(3)
C35A	0.32661(13)	0.23510(5)	0.18758(12)	0.0338(4)
C36A	0.48834(15)	0.23647(5)	0.02265(11)	0.0368(4)
C37A	0.73621(14)	0.22567(5)	0.10218(13)	0.0392(4)
C38A	0.72911(14)	0.21231(5)	0.30984(13)	0.0380(4)
C39A	0.46879(15)	0.21903(4)	0.35906(12)	0.0337(4)
V2	0.73940(2)	0.53088(2)	0.25929(2)	0.01856(6)
C1B	0.61857(12)	0.57679(4)	0.33723(10)	0.0229(3)
C2B	0.57469(14)	0.61208(4)	0.37383(11)	0.0318(4)
N3B	0.69163(10)	0.55563(3)	0.38209(8)	0.0235(3)
C3B	0.73195(13)	0.56580(4)	0.47246(10)	0.0274(3)
C4B	0.84650(14)	0.54956(5)	0.49622(11)	0.0335(4)
C5B	0.65014(15)	0.55370(5)	0.54149(11)	0.0371(4)
N6B	0.59473(10)	0.56459(3)	0.25544(8)	0.0229(3)
C6B	0.52396(13)	0.58588(4)	0.19185(10)	0.0268(3)
C7B	0.48083(15)	0.56195(5)	0.11517(11)	0.0366(4)
C8B	0.58325(15)	0.61908(5)	0.15569(12)	0.0357(4)
C10B	0.88940(12)	0.55054(4)	0.28502(10)	0.0217(3)
N10B	0.98149(11)	0.56258(3)	0.29520(9)	0.0272(3)
C11B	0.07047(12)	0.58207(4)	0.33389(9)	0.0222(3)
C12B	0.17734(13)	0.56629(4)	0.33895(10)	0.0250(3)
C13B	0.26572(13)	0.58693(5)	0.37511(10)	0.0294(3)
C14B	0.24915(14)	0.62192(5)	0.40506(11)	0.0334(4)
C15B	0.14332(14)	0.63697(5)	0.39941(10)	0.0307(4)
C16B	0.05152(13)	0.61772(4)	0.36385(10)	0.0251(3)
C17B	0.19584(14)	0.52859(5)	0.30452(13)	0.0358(4)
C18B	0.93714(14)	0.63464(4)	0.35710(12)	0.0331(4)
C20B	0.76948(12)	0.55060(4)	0.13998(10)	0.0220(3)
N20B	0.79124(11)	0.56056(3)	0.06813(9)	0.0265(3)
C21B	0.83664(13)	0.57906(4)	0.99787(11)	0.0278(3)

	x/a	y/b	z/c	U(eq)
C22B	0.89766(14)	0.61083(5)	0.01665(13)	0.0357(4)
C23B	0.93958(16)	0.62938(6)	0.94500(16)	0.0500(5)
C24B	0.92087(17)	0.61704(7)	0.85903(15)	0.0566(6)
C25B	0.86051(16)	0.58582(7)	0.84228(13)	0.0488(5)
C26B	0.81653(14)	0.56590(5)	0.91072(11)	0.0358(4)
C27B	0.91609(16)	0.62382(5)	0.11061(14)	0.0447(5)
C28B	0.75076(17)	0.53204(6)	0.89327(13)	0.0487(5)
C30B	0.71190(13)	0.47395(4)	0.32923(11)	0.0272(3)
C31B	0.63388(13)	0.47737(4)	0.25589(11)	0.0255(3)
C32B	0.69364(13)	0.48025(4)	0.17736(11)	0.0252(3)
C33B	0.81056(13)	0.47980(4)	0.20337(11)	0.0265(3)
C34B	0.82078(13)	0.47566(4)	0.29756(11)	0.0281(3)
C35B	0.68047(16)	0.46632(5)	0.42224(12)	0.0389(4)
C36B	0.50924(13)	0.47607(5)	0.26128(12)	0.0352(4)
C37B	0.64346(15)	0.47718(5)	0.08412(11)	0.0344(4)
C38B	0.90618(14)	0.47859(5)	0.14247(13)	0.0365(4)
C39B	0.92852(14)	0.46853(5)	0.35073(13)	0.0394(4)

Table 4. Bond lengths (Å) for 10.

V1-C10A	1.9589(15)	V1-C20A	1.9758(16)
V1-N6A	2.1305(12)	V1-N3A	2.1532(12)
V1-C33A	2.2458(15)	V1-C32A	2.2945(15)
V1-C34A	2.3043(15)	V1-C31A	2.3451(15)
V1-C30A	2.3614(15)	C1A-N6A	1.328(2)
C1A-N3A	1.3302(19)	C1A-C2A	1.518(2)
C2A-H2A1	0.98	C2A-H2A2	0.98
C2A-H2A3	0.98	N3A-C3A	1.4682(19)
C3A-C4A	1.524(2)	C3A-C5A	1.536(2)
C3A-H3A	1.0	C4A-H4A1	0.98
C4A-H4A2	0.98	C4A-H4A3	0.98
C5A-H5A1	0.98	C5A-H5A2	0.98
C5A-H5A3	0.98	N6A-C6A	1.471(2)
C6A-C7A	1.522(2)	C6A-C8A	1.534(2)

C6A-H6A	1.0	C7A-H7A1	0.98
C7A-H7A2	0.98	C7A-H7A3	0.98
C8A-H8A1	0.98	C8A-H8A2	0.98
C8A-H8A3	0.98	C10A-N10A	1.1891(19)
N10A-C11A	1.3904(19)	C11A-C16A	1.404(2)
C11A-C12A	1.409(2)	C12A-C13A	1.390(2)
C12A-C17A	1.502(2)	C13A-C14A	1.379(3)
C13A-H13A	0.95	C14A-C15A	1.385(3)
C14A-H14A	0.95	C15A-C16A	1.391(2)
C15A-H15A	0.95	C16A-C18A	1.505(2)
C17A-H17A	0.98	C17A-H17B	0.98
C17A-H17C	0.98	C18A-H18A	0.98
C18A-H18B	0.98	C18A-H18C	0.98
C20A-N20A	1.181(2)	N20A-C21A	1.392(2)
C21A-C22A	1.402(2)	C21A-C26A	1.406(2)
C22A-C23A	1.391(2)	C22A-C27A	1.501(2)
C23A-C24A	1.382(3)	C23A-H23A	0.95
C24A-C25A	1.379(3)	C24A-H24A	0.95
C25A-C26A	1.393(3)	C25A-H25A	0.95
C26A-C28A	1.495(3)	C27A-H27A	0.98
C27A-H27B	0.98	C27A-H27C	0.98
C28A-H28A	0.98	C28A-H28B	0.98
C28A-H28C	0.98	C30A-C31A	1.415(2)
C30A-C34A	1.421(2)	C30A-C39A	1.499(2)
C31A-C32A	1.420(2)	C31A-C35A	1.502(2)
C32A-C33A	1.432(2)	C32A-C36A	1.505(2)
C33A-C34A	1.428(2)	C33A-C37A	1.505(2)
C34A-C38A	1.507(2)	C35A-H35A	0.98
C35A-H35B	0.98	C35A-H35C	0.98
C36A-H36A	0.98	C36A-H36B	0.98
C36A-H36C	0.98	C37A-H37A	0.98
C37A-H37B	0.98	C37A-H37C	0.98
C38A-H38A	0.98	C38A-H38B	0.98
C38A-H38C	0.98	C39A-H39A	0.98

C39A-H39B	0.98	C39A-H39C	0.98
V2-C10B	1.9591(15)	V2-C20B	1.9890(16)
V2-N6B	2.1323(12)	V2-N3B	2.1665(12)
V2-C33B	2.2478(15)	V2-C32B	2.2856(15)
V2-C34B	2.3148(15)	V2-C31B	2.3410(15)
V2-C30B	2.3767(15)	C1B-N6B	1.3275(19)
C1B-N3B	1.3295(19)	C1B-C2B	1.517(2)
C2B-H2B1	0.98	C2B-H2B2	0.98
C2B-H2B3	0.98	N3B-C3B	1.4680(19)
C3B-C4B	1.524(2)	C3B-C5B	1.534(2)
C3B-H3B	1.0	C4B-H4B1	0.98
C4B-H4B2	0.98	C4B-H4B3	0.98
C5B-H5B1	0.98	C5B-H5B2	0.98
C5B-H5B3	0.98	N6B-C6B	1.4713(18)
C6B-C7B	1.521(2)	C6B-C8B	1.529(2)
C6B-H6B	1.0	C7B-H7B1	0.98
C7B-H7B2	0.98	C7B-H7B3	0.98
C8B-H8B1	0.98	C8B-H8B2	0.98
C8B-H8B3	0.98	C10B-N10B	1.1929(19)
N10B-C11B	1.3881(19)	C11B-C12B	1.406(2)
C11B-C16B	1.411(2)	C12B-C13B	1.392(2)
C12B-C17B	1.502(2)	C13B-C14B	1.383(2)
C13B-H13B	0.95	C14B-C15B	1.384(2)
C14B-H14B	0.95	C15B-C16B	1.392(2)
C15B-H15B	0.95	C16B-C18B	1.506(2)
C17B-H17D	0.98	C17B-H17E	0.98
C17B-H17F	0.98	C18B-H18D	0.98
C18B-H18E	0.98	C18B-H18F	0.98
C20B-N20B	1.1849(19)	N20B-C21B	1.394(2)
C21B-C22B	1.401(2)	C21B-C26B	1.408(2)
C22B-C23B	1.394(3)	C22B-C27B	1.498(3)
C23B-C24B	1.379(3)	C23B-H23B	0.95
C24B-C25B	1.375(3)	C24B-H24B	0.95
C25B-C26B	1.392(3)	C25B-H25B	0.95

C26B-C28B	1.491(3)	C27B-H27D	0.98
C27B-H27E	0.98	C27B-H27F	0.98
C28B-H28D	0.98	C28B-H28E	0.98
C28B-H28F	0.98	C30B-C31B	1.414(2)
C30B-C34B	1.416(2)	C30B-C35B	1.497(2)
C31B-C32B	1.420(2)	C31B-C36B	1.503(2)
C32B-C33B	1.436(2)	C32B-C37B	1.502(2)
C33B-C34B	1.425(2)	C33B-C38B	1.508(2)
C34B-C39B	1.506(2)	C35B-H35D	0.98
C35B-H35E	0.98	C35B-H35F	0.98
C36B-H36D	0.98	C36B-H36E	0.98
C36B-H36F	0.98	C37B-H37D	0.98
C37B-H37E	0.98	C37B-H37F	0.98
C38B-H38D	0.98	C38B-H38E	0.98
C38B-H38F	0.98	C39B-H39D	0.98
C39B-H39E	0.98	C39B-H39F	0.98

Table 5. Bond angles (°) for 10.

C10A-V1-C20A	77.33(6)	C10A-V1-N6A	122.75(5)
C20A-V1-N6A	86.08(6)	C10A-V1-N3A	88.86(5)
C20A-V1-N3A	130.40(5)	N6A-V1-N3A	61.99(5)
C10A-V1-C33A	90.02(6)	C20A-V1-C33A	86.36(6)
N6A-V1-C33A	143.55(6)	N3A-V1-C33A	141.74(6)
C10A-V1-C32A	124.72(6)	C20A-V1-C32A	83.95(6)
N6A-V1-C32A	106.94(5)	N3A-V1-C32A	138.97(5)
C33A-V1-C32A	36.75(6)	C10A-V1-C34A	85.69(6)
C20A-V1-C34A	120.51(6)	N6A-V1-C34A	146.26(5)
N3A-V1-C34A	105.28(5)	C33A-V1-C34A	36.56(6)
C32A-V1-C34A	60.54(6)	C10A-V1-C31A	144.77(6)
C20A-V1-C31A	115.29(6)	N6A-V1-C31A	91.77(5)
N3A-V1-C31A	103.36(5)	C33A-V1-C31A	59.96(5)
C32A-V1-C31A	35.62(5)	C34A-V1-C31A	59.32(5)
C10A-V1-C30A	115.53(6)	C20A-V1-C30A	142.30(6)
N6A-V1-C30A	110.82(5)	N3A-V1-C30A	86.62(5)

C33A-V1-C30A	59.72(6)	C32A-V1-C30A	59.25(6)
C34A-V1-C30A	35.44(5)	C31A-V1-C30A	34.99(6)
N6A-C1A-N3A	112.15(13)	N6A-C1A-C2A	124.00(14)
N3A-C1A-C2A	123.68(14)	C1A-C2A-H2A1	109.5
C1A-C2A-H2A2	109.5	H2A1-C2A-H2A2	109.5
C1A-C2A-H2A3	109.5	H2A1-C2A-H2A3	109.5
H2A2-C2A-H2A3	109.5	C1A-N3A-C3A	119.98(12)
C1A-N3A-V1	90.51(9)	C3A-N3A-V1	143.08(10)
N3A-C3A-C4A	111.42(13)	N3A-C3A-C5A	111.55(13)
C4A-C3A-C5A	108.92(14)	N3A-C3A-H3A	108.3
C4A-C3A-H3A	108.3	C5A-C3A-H3A	108.3
C3A-C4A-H4A1	109.5	C3A-C4A-H4A2	109.5
H4A1-C4A-H4A2	109.5	C3A-C4A-H4A3	109.5
H4A1-C4A-H4A3	109.5	H4A2-C4A-H4A3	109.5
C3A-C5A-H5A1	109.5	C3A-C5A-H5A2	109.5
H5A1-C5A-H5A2	109.5	C3A-C5A-H5A3	109.5
H5A1-C5A-H5A3	109.5	H5A2-C5A-H5A3	109.5
C1A-N6A-C6A	121.26(13)	C1A-N6A-V1	91.54(9)
C6A-N6A-V1	140.70(10)	N6A-C6A-C7A	109.85(14)
N6A-C6A-C8A	114.22(14)	C7A-C6A-C8A	109.48(15)
N6A-C6A-H6A	107.7	C7A-C6A-H6A	107.7
C8A-C6A-H6A	107.7	C6A-C7A-H7A1	109.5
C6A-C7A-H7A2	109.5	H7A1-C7A-H7A2	109.5
C6A-C7A-H7A3	109.5	H7A1-C7A-H7A3	109.5
H7A2-C7A-H7A3	109.5	C6A-C8A-H8A1	109.5
C6A-C8A-H8A2	109.5	H8A1-C8A-H8A2	109.5
C6A-C8A-H8A3	109.5	H8A1-C8A-H8A3	109.5
H8A2-C8A-H8A3	109.5	N10A-C10A-V1	172.66(13)
C10A-N10A-C11A	160.04(16)	N10A-C11A-C16A	119.48(14)
N10A-C11A-C12A	118.29(14)	C16A-C11A-C12A	122.19(14)
C13A-C12A-C11A	117.76(16)	C13A-C12A-C17A	122.18(15)
C11A-C12A-C17A	120.06(14)	C14A-C13A-C12A	121.05(17)
C14A-C13A-H13A	119.5	C12A-C13A-H13A	119.5
C13A-C14A-C15A	120.16(16)	C13A-C14A-H14A	119.9

C15A-C14A-H14A	119.9	C14A-C15A-C16A	121.54(17)
C14A-C15A-H15A	119.2	C16A-C15A-H15A	119.2
C15A-C16A-C11A	117.19(15)	C15A-C16A-C18A	120.85(15)
C11A-C16A-C18A	121.93(14)	C12A-C17A-H17A	109.5
C12A-C17A-H17B	109.5	H17A-C17A-H17B	109.5
C12A-C17A-H17C	109.5	H17A-C17A-H17C	109.5
H17B-C17A-H17C	109.5	C16A-C18A-H18A	109.5
C16A-C18A-H18B	109.5	H18A-C18A-H18B	109.5
C16A-C18A-H18C	109.5	H18A-C18A-H18C	109.5
H18B-C18A-H18C	109.5	N20A-C20A-V1	176.18(13)
C20A-N20A-C21A	163.37(16)	N20A-C21A-C22A	118.92(14)
N20A-C21A-C26A	118.57(16)	C22A-C21A-C26A	122.48(15)
C23A-C22A-C21A	117.64(16)	C23A-C22A-C27A	121.16(16)
C21A-C22A-C27A	121.19(14)	C24A-C23A-C22A	121.02(19)
C24A-C23A-H23A	119.5	C22A-C23A-H23A	119.5
C25A-C24A-C23A	120.31(17)	C25A-C24A-H24A	119.8
C23A-C24A-H24A	119.8	C24A-C25A-C26A	121.40(17)
C24A-C25A-H25A	119.3	C26A-C25A-H25A	119.3
C25A-C26A-C21A	117.14(17)	C25A-C26A-C28A	122.23(17)
C21A-C26A-C28A	120.62(16)	C22A-C27A-H27A	109.5
C22A-C27A-H27B	109.5	H27A-C27A-H27B	109.5
C22A-C27A-H27C	109.5	H27A-C27A-H27C	109.5
H27B-C27A-H27C	109.5	C26A-C28A-H28A	109.5
C26A-C28A-H28B	109.5	H28A-C28A-H28B	109.5
C26A-C28A-H28C	109.5	H28A-C28A-H28C	109.5
H28B-C28A-H28C	109.5	C31A-C30A-C34A	108.46(14)
C31A-C30A-C39A	123.17(14)	C34A-C30A-C39A	128.32(15)
C31A-C30A-V1	71.87(9)	C34A-C30A-V1	70.09(8)
C39A-C30A-V1	126.02(10)	C30A-C31A-C32A	108.63(14)
C30A-C31A-C35A	123.98(15)	C32A-C31A-C35A	127.34(15)
C30A-C31A-V1	73.14(8)	C32A-C31A-V1	70.25(8)
C35A-C31A-V1	124.70(11)	C31A-C32A-C33A	107.23(14)
C31A-C32A-C36A	126.69(15)	C33A-C32A-C36A	125.35(15)
C31A-C32A-V1	74.14(9)	C33A-C32A-V1	69.78(8)

C36A-C32A-V1	128.98(11)	C34A-C33A-C32A	108.29(14)
C34A-C33A-C37A	125.62(15)	C32A-C33A-C37A	125.23(16)
C34A-C33A-V1	73.95(9)	C32A-C33A-V1	73.48(8)
C37A-C33A-V1	126.86(11)	C30A-C34A-C33A	107.38(14)
C30A-C34A-C38A	126.93(16)	C33A-C34A-C38A	125.09(15)
C30A-C34A-V1	74.47(9)	C33A-C34A-V1	69.49(9)
C38A-C34A-V1	128.21(11)	C31A-C35A-H35A	109.5
C31A-C35A-H35B	109.5	H35A-C35A-H35B	109.5
C31A-C35A-H35C	109.5	H35A-C35A-H35C	109.5
H35B-C35A-H35C	109.5	C32A-C36A-H36A	109.5
C32A-C36A-H36B	109.5	H36A-C36A-H36B	109.5
C32A-C36A-H36C	109.5	H36A-C36A-H36C	109.5
H36B-C36A-H36C	109.5	C33A-C37A-H37A	109.5
C33A-C37A-H37B	109.5	H37A-C37A-H37B	109.5
C33A-C37A-H37C	109.5	H37A-C37A-H37C	109.5
H37B-C37A-H37C	109.5	C34A-C38A-H38A	109.5
C34A-C38A-H38B	109.5	H38A-C38A-H38B	109.5
C34A-C38A-H38C	109.5	H38A-C38A-H38C	109.5
H38B-C38A-H38C	109.5	C30A-C39A-H39A	109.5
C30A-C39A-H39B	109.5	H39A-C39A-H39B	109.5
C30A-C39A-H39C	109.5	H39A-C39A-H39C	109.5
H39B-C39A-H39C	109.5	C10B-V2-C20B	80.44(6)
C10B-V2-N6B	121.87(5)	C20B-V2-N6B	87.14(5)
C10B-V2-N3B	87.62(5)	C20B-V2-N3B	133.38(5)
N6B-V2-N3B	61.68(5)	C10B-V2-C33B	91.13(6)
C20B-V2-C33B	82.87(6)	N6B-V2-C33B	143.33(5)
N3B-V2-C33B	142.67(5)	C10B-V2-C32B	126.83(6)
C20B-V2-C32B	81.96(6)	N6B-V2-C32B	106.77(5)
N3B-V2-C32B	137.46(5)	C33B-V2-C32B	36.93(5)
C10B-V2-C34B	84.54(6)	C20B-V2-C34B	116.80(6)
N6B-V2-C34B	148.20(5)	N3B-V2-C34B	106.53(5)
C33B-V2-C34B	36.37(6)	C32B-V2-C34B	60.26(5)
C10B-V2-C31B	143.65(6)	C20B-V2-C31B	114.33(6)
N6B-V2-C31B	92.91(5)	N3B-V2-C31B	101.82(5)

C33B-V2-C31B	60.24(6)	C32B-V2-C31B	35.71(6)
C34B-V2-C31B	59.11(5)	C10B-V2-C30B	112.73(6)
C20B-V2-C30B	139.34(6)	N6B-V2-C30B	113.14(5)
N3B-V2-C30B	86.74(5)	C33B-V2-C30B	59.53(6)
C32B-V2-C30B	59.00(6)	C34B-V2-C30B	35.11(6)
C31B-V2-C30B	34.88(5)	N6B-C1B-N3B	112.10(13)
N6B-C1B-C2B	124.42(14)	N3B-C1B-C2B	123.35(14)
C1B-C2B-H2B1	109.5	C1B-C2B-H2B2	109.5
H2B1-C2B-H2B2	109.5	C1B-C2B-H2B3	109.5
H2B1-C2B-H2B3	109.5	H2B2-C2B-H2B3	109.5
C1B-N3B-C3B	119.77(13)	C1B-N3B-V2	90.60(9)
C3B-N3B-V2	144.05(10)	N3B-C3B-C4B	111.43(13)
N3B-C3B-C5B	111.30(13)	C4B-C3B-C5B	109.21(14)
N3B-C3B-H3B	108.3	C4B-C3B-H3B	108.3
C5B-C3B-H3B	108.3	C3B-C4B-H4B1	109.5
C3B-C4B-H4B2	109.5	H4B1-C4B-H4B2	109.5
C3B-C4B-H4B3	109.5	H4B1-C4B-H4B3	109.5
H4B2-C4B-H4B3	109.5	C3B-C5B-H5B1	109.5
C3B-C5B-H5B2	109.5	H5B1-C5B-H5B2	109.5
C3B-C5B-H5B3	109.5	H5B1-C5B-H5B3	109.5
H5B2-C5B-H5B3	109.5	C1B-N6B-C6B	120.76(13)
C1B-N6B-V2	92.15(9)	C6B-N6B-V2	140.19(10)
N6B-C6B-C7B	110.25(13)	N6B-C6B-C8B	113.22(13)
C7B-C6B-C8B	109.78(14)	N6B-C6B-H6B	107.8
C7B-C6B-H6B	107.8	C8B-C6B-H6B	107.8
C6B-C7B-H7B1	109.5	C6B-C7B-H7B2	109.5
H7B1-C7B-H7B2	109.5	C6B-C7B-H7B3	109.5
H7B1-C7B-H7B3	109.5	H7B2-C7B-H7B3	109.5
C6B-C8B-H8B1	109.5	C6B-C8B-H8B2	109.5
H8B1-C8B-H8B2	109.5	C6B-C8B-H8B3	109.5
H8B1-C8B-H8B3	109.5	H8B2-C8B-H8B3	109.5
N10B-C10B-V2	175.98(13)	C10B-N10B-C11B	158.78(15)
N10B-C11B-C12B	119.19(14)	N10B-C11B-C16B	118.79(13)
C12B-C11B-C16B	121.97(14)	C13B-C12B-C11B	117.97(15)

C13B-C12B-C17B	121.07(15)	C11B-C12B-C17B	120.95(14)
C14B-C13B-C12B	121.10(15)	C14B-C13B-H13B	119.4
C12B-C13B-H13B	119.4	C13B-C14B-C15B	120.03(15)
C13B-C14B-H14B	120.0	C15B-C14B-H14B	120.0
C14B-C15B-C16B	121.63(15)	C14B-C15B-H15B	119.2
C16B-C15B-H15B	119.2	C15B-C16B-C11B	117.30(15)
C15B-C16B-C18B	120.99(15)	C11B-C16B-C18B	121.71(14)
C12B-C17B-H17D	109.5	C12B-C17B-H17E	109.5
H17D-C17B-H17E	109.5	C12B-C17B-H17F	109.5
H17D-C17B-H17F	109.5	H17E-C17B-H17F	109.5
C16B-C18B-H18D	109.5	C16B-C18B-H18E	109.5
H18D-C18B-H18E	109.5	C16B-C18B-H18F	109.5
H18D-C18B-H18F	109.5	H18E-C18B-H18F	109.5
N20B-C20B-V2	176.05(13)	C20B-N20B-C21B	163.52(16)
N20B-C21B-C22B	118.45(15)	N20B-C21B-C26B	119.02(15)
C22B-C21B-C26B	122.49(16)	C23B-C22B-C21B	117.36(19)
C23B-C22B-C27B	122.25(18)	C21B-C22B-C27B	120.40(16)
C24B-C23B-C22B	121.2(2)	C24B-C23B-H23B	119.4
C22B-C23B-H23B	119.4	C25B-C24B-C23B	120.35(19)
C25B-C24B-H24B	119.8	C23B-C24B-H24B	119.8
C24B-C25B-C26B	121.5(2)	C24B-C25B-H25B	119.3
C26B-C25B-H25B	119.3	C25B-C26B-C21B	117.15(19)
C25B-C26B-C28B	121.89(18)	C21B-C26B-C28B	120.96(16)
C22B-C27B-H27D	109.5	C22B-C27B-H27E	109.5
H27D-C27B-H27E	109.5	C22B-C27B-H27F	109.5
H27D-C27B-H27F	109.5	H27E-C27B-H27F	109.5
C26B-C28B-H28D	109.5	C26B-C28B-H28E	109.5
H28D-C28B-H28E	109.5	C26B-C28B-H28F	109.5
H28D-C28B-H28F	109.5	H28E-C28B-H28F	109.5
C31B-C30B-C34B	108.47(14)	C31B-C30B-C35B	123.91(15)
C34B-C30B-C35B	127.39(15)	C31B-C30B-V2	71.18(8)
C34B-C30B-V2	70.06(8)	C35B-C30B-V2	128.92(11)
C30B-C31B-C32B	108.32(14)	C30B-C31B-C36B	125.00(15)
C32B-C31B-C36B	126.60(15)	C30B-C31B-V2	73.94(9)

C32B-C31B-V2	70.02(8)	C36B-C31B-V2	124.34(11)
C31B-C32B-C33B	107.57(14)	C31B-C32B-C37B	125.32(14)
C33B-C32B-C37B	126.19(15)	C31B-C32B-V2	74.27(9)
C33B-C32B-V2	70.10(8)	C37B-C32B-V2	129.68(11)
C34B-C33B-C32B	107.62(14)	C34B-C33B-C38B	125.09(15)
C32B-C33B-C38B	126.78(15)	C34B-C33B-V2	74.38(9)
C32B-C33B-V2	72.97(8)	C38B-C33B-V2	124.72(11)
C30B-C34B-C33B	107.98(14)	C30B-C34B-C39B	126.44(16)
C33B-C34B-C39B	124.94(16)	C30B-C34B-V2	74.84(9)
C33B-C34B-V2	69.26(8)	C39B-C34B-V2	128.58(11)
C30B-C35B-H35D	109.5	C30B-C35B-H35E	109.5
H35D-C35B-H35E	109.5	C30B-C35B-H35F	109.5
H35D-C35B-H35F	109.5	H35E-C35B-H35F	109.5
C31B-C36B-H36D	109.5	C31B-C36B-H36E	109.5
H36D-C36B-H36E	109.5	C31B-C36B-H36F	109.5
H36D-C36B-H36F	109.5	H36E-C36B-H36F	109.5
C32B-C37B-H37D	109.5	C32B-C37B-H37E	109.5
H37D-C37B-H37E	109.5	C32B-C37B-H37F	109.5
H37D-C37B-H37F	109.5	H37E-C37B-H37F	109.5
C33B-C38B-H38D	109.5	C33B-C38B-H38E	109.5
H38D-C38B-H38E	109.5	C33B-C38B-H38F	109.5
H38D-C38B-H38F	109.5	H38E-C38B-H38F	109.5
C34B-C39B-H39D	109.5	C34B-C39B-H39E	109.5
H39D-C39B-H39E	109.5	C34B-C39B-H39F	109.5
H39D-C39B-H39F	109.5	H39E-C39B-H39F	109.5

Table 6. Torsion angles (°) for 10.

N6A-C1A-N3A-C3A	176.32(13)	C2A-C1A-N3A-C3A	0.8(2)
N6A-C1A-N3A-V1	18.19(13)	C2A-C1A-N3A-V1	-157.29(14)
C1A-N3A-C3A-C4A	-156.86(14)	V1-N3A-C3A-C4A	-15.2(2)
C1A-N3A-C3A-C5A	81.17(18)	V1-N3A-C3A-C5A	-137.13(15)
N3A-C1A-N6A-C6A	-175.60(13)	C2A-C1A-N6A-C6A	-0.1(2)
N3A-C1A-N6A-V1	-18.39(13)	C2A-C1A-N6A-V1	157.07(14)
C1A-N6A-C6A-C7A	-163.77(15)	V1-N6A-C6A-C7A	53.9(2)

C1A-N6A-C6A-C8A	72.77(19)	V1-N6A-C6A-C8A	-69.5(2)
C10A-N10A-C11A-C16A	-46.0(5)	C10A-N10A-C11A-C12A	136.1(4)
N10A-C11A-C12A-C13A	-178.92(14)	C16A-C11A-C12A-C13A	3.3(2)
N10A-C11A-C12A-C17A	2.1(2)	C16A-C11A-C12A-C17A	-175.69(15)
C11A-C12A-C13A-C14A	-0.6(3)	C17A-C12A-C13A-C14A	178.31(17)
C12A-C13A-C14A-C15A	-1.5(3)	C13A-C14A-C15A-C16A	1.1(3)
C14A-C15A-C16A-C11A	1.4(2)	C14A-C15A-C16A-C18A	-176.74(16)
N10A-C11A-C16A-C15A	178.58(14)	C12A-C11A-C16A-C15A	-3.6(2)
N10A-C11A-C16A-C18A	-3.3(2)	C12A-C11A-C16A-C18A	174.49(14)
C20A-N20A-C21A-C22A	2.1(6)	C20A-N20A-C21A-C26A	-175.9(5)
N20A-C21A-C22A-C23A	-178.01(14)	C26A-C21A-C22A-C23A	-0.1(2)
N20A-C21A-C22A-C27A	3.2(2)	C26A-C21A-C22A-C27A	-178.89(15)
C21A-C22A-C23A-C24A	-0.2(2)	C27A-C22A-C23A-C24A	178.62(16)
C22A-C23A-C24A-C25A	0.0(3)	C23A-C24A-C25A-C26A	0.6(3)
C24A-C25A-C26A-C21A	-0.8(3)	C24A-C25A-C26A-C28A	178.52(17)
N20A-C21A-C26A-C25A	178.49(15)	C22A-C21A-C26A-C25A	0.6(2)
N20A-C21A-C26A-C28A	-0.8(2)	C22A-C21A-C26A-C28A	-178.76(16)
C34A-C30A-C31A-C32A	0.80(17)	C39A-C30A-C31A-C32A	-176.66(14)
V1-C30A-C31A-C32A	61.65(10)	C34A-C30A-C31A-C35A	178.28(14)
C39A-C30A-C31A-C35A	0.8(2)	V1-C30A-C31A-C35A	-120.86(15)
C34A-C30A-C31A-V1	-60.85(10)	C39A-C30A-C31A-V1	121.68(14)
C30A-C31A-C32A-C33A	-1.17(17)	C35A-C31A-C32A-C33A	-178.54(15)
V1-C31A-C32A-C33A	62.33(10)	C30A-C31A-C32A-C36A	169.37(15)
C35A-C31A-C32A-C36A	-8.0(3)	V1-C31A-C32A-C36A	-127.14(16)
C30A-C31A-C32A-V1	-63.50(10)	C35A-C31A-C32A-V1	119.13(16)
C31A-C32A-C33A-C34A	1.10(17)	C36A-C32A-C33A-C34A	-169.60(15)
V1-C32A-C33A-C34A	66.31(10)	C31A-C32A-C33A-C37A	170.97(15)
C36A-C32A-C33A-C37A	0.3(3)	V1-C32A-C33A-C37A	-123.82(16)
C31A-C32A-C33A-V1	-65.21(10)	C36A-C32A-C33A-V1	124.09(16)
C31A-C30A-C34A-C33A	-0.11(17)	C39A-C30A-C34A-C33A	177.18(15)
V1-C30A-C34A-C33A	-62.09(10)	C31A-C30A-C34A-C38A	-171.56(15)
C39A-C30A-C34A-C38A	5.7(3)	V1-C30A-C34A-C38A	126.46(16)
C31A-C30A-C34A-V1	61.98(10)	C39A-C30A-C34A-V1	-120.72(16)
C32A-C33A-C34A-C30A	-0.61(17)	C37A-C33A-C34A-C30A	-170.44(15)

V1-C33A-C34A-C30A	65.38(10)	C32A-C33A-C34A-C38A	171.03(14)
C37A-C33A-C34A-C38A	1.2(2)	V1-C33A-C34A-C38A	-122.97(15)
C32A-C33A-C34A-V1	-66.00(10)	C37A-C33A-C34A-V1	124.18(16)
N6B-C1B-N3B-C3B	177.14(13)	C2B-C1B-N3B-C3B	1.2(2)
N6B-C1B-N3B-V2	17.32(13)	C2B-C1B-N3B-V2	-158.61(14)
C1B-N3B-C3B-C4B	-154.54(14)	V2-N3B-C3B-C4B	-10.5(2)
C1B-N3B-C3B-C5B	83.30(18)	V2-N3B-C3B-C5B	-132.68(16)
N3B-C1B-N6B-C6B	-174.10(13)	C2B-C1B-N6B-C6B	1.8(2)
N3B-C1B-N6B-V2	-17.62(13)	C2B-C1B-N6B-V2	158.26(14)
C1B-N6B-C6B-C7B	-162.95(14)	V2-N6B-C6B-C7B	55.6(2)
C1B-N6B-C6B-C8B	73.62(18)	V2-N6B-C6B-C8B	-67.9(2)
C10B-N10B-C11B-C12B	137.9(4)	C10B-N10B-C11B-C16B	-44.5(5)
N10B-C11B-C12B-C13B	177.70(14)	C16B-C11B-C12B-C13B	0.2(2)
N10B-C11B-C12B-C17B	-1.0(2)	C16B-C11B-C12B-C17B	-178.48(14)
C11B-C12B-C13B-C14B	-0.1(2)	C17B-C12B-C13B-C14B	178.59(15)
C12B-C13B-C14B-C15B	0.0(2)	C13B-C14B-C15B-C16B	-0.1(2)
C14B-C15B-C16B-C11B	0.2(2)	C14B-C15B-C16B-C18B	-179.23(15)
N10B-C11B-C16B-C15B	-177.76(14)	C12B-C11B-C16B-C15B	-0.3(2)
N10B-C11B-C16B-C18B	1.7(2)	C12B-C11B-C16B-C18B	179.16(14)
C20B-N20B-C21B-C22B	-11.7(6)	C20B-N20B-C21B-C26B	170.4(5)
N20B-C21B-C22B-C23B	-178.27(15)	C26B-C21B-C22B-C23B	-0.4(2)
N20B-C21B-C22B-C27B	1.8(2)	C26B-C21B-C22B-C27B	179.60(16)
C21B-C22B-C23B-C24B	0.5(3)	C27B-C22B-C23B-C24B	-179.54(18)
C22B-C23B-C24B-C25B	-0.4(3)	C23B-C24B-C25B-C26B	0.2(3)
C24B-C25B-C26B-C21B	-0.1(3)	C24B-C25B-C26B-C28B	179.88(18)
N20B-C21B-C26B-C25B	178.07(14)	C22B-C21B-C26B-C25B	0.2(2)
N20B-C21B-C26B-C28B	-1.9(2)	C22B-C21B-C26B-C28B	-179.74(16)
C34B-C30B-C31B-C32B	1.56(17)	C35B-C30B-C31B-C32B	-173.24(14)
V2-C30B-C31B-C32B	61.97(10)	C34B-C30B-C31B-C36B	178.58(14)
C35B-C30B-C31B-C36B	3.8(2)	V2-C30B-C31B-C36B	-121.01(15)
C34B-C30B-C31B-V2	-60.41(11)	C35B-C30B-C31B-V2	124.79(15)
C30B-C31B-C32B-C33B	-1.90(17)	C36B-C31B-C32B-C33B	-178.86(15)
V2-C31B-C32B-C33B	62.61(10)	C30B-C31B-C32B-C37B	167.66(14)
C36B-C31B-C32B-C37B	-9.3(2)	V2-C31B-C32B-C37B	-127.84(15)

C30B-C31B-C32B-V2	-64.51(11)	C36B-C31B-C32B-V2	118.53(15)
C31B-C32B-C33B-C34B	1.52(16)	C37B-C32B-C33B-C34B	-167.92(15)
V2-C32B-C33B-C34B	66.87(10)	C31B-C32B-C33B-C38B	173.67(14)
C37B-C32B-C33B-C38B	4.2(2)	V2-C32B-C33B-C38B	-120.99(16)
C31B-C32B-C33B-V2	-65.35(10)	C37B-C32B-C33B-V2	125.21(15)
C31B-C30B-C34B-C33B	-0.60(17)	C35B-C30B-C34B-C33B	173.96(15)
V2-C30B-C34B-C33B	-61.72(10)	C31B-C30B-C34B-C39B	-171.79(15)
C35B-C30B-C34B-C39B	2.8(3)	V2-C30B-C34B-C39B	127.09(16)
C31B-C30B-C34B-V2	61.12(11)	C35B-C30B-C34B-V2	-124.32(16)
C32B-C33B-C34B-C30B	-0.57(17)	C38B-C33B-C34B-C30B	-172.88(14)
V2-C33B-C34B-C30B	65.36(11)	C32B-C33B-C34B-C39B	170.78(14)
C38B-C33B-C34B-C39B	-1.5(2)	V2-C33B-C34B-C39B	-123.29(15)
C32B-C33B-C34B-V2	-65.93(10)	C38B-C33B-C34B-V2	121.76(15)

Table 7. Anisotropic atomic displacement parameters ($Å^2$) for 10.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V1	0.01624(11)	0.01711(11)	0.02203(12)	-0.00249(9)	0.00164(9)	0.00087(9)
C1A	0.0184(7)	0.0232(7)	0.0299(8)	-0.0028(6)	0.0063(6)	0.0013(6)
C2A	0.0397(10)	0.0276(8)	0.0383(10)	-0.0070(7)	0.0050(8)	0.0084(7)
N3A	0.0219(6)	0.0231(6)	0.0223(6)	-0.0023(5)	0.0031(5)	0.0006(5)
C3A	0.0311(8)	0.0268(8)	0.0227(8)	-0.0028(6)	0.0044(6)	-0.0028(6)
C4A	0.0393(10)	0.0374(9)	0.0248(8)	0.0025(7)	-0.0034(7)	-0.0010(8)
C5A	0.0473(11)	0.0421(10)	0.0294(9)	-0.0024(8)	0.0134(8)	-0.0067(8)
N6A	0.0213(6)	0.0254(6)	0.0276(7)	-0.0027(5)	-0.0003(5)	0.0059(5)
C6A	0.0264(8)	0.0346(9)	0.0360(9)	-0.0001(7)	-0.0025(7)	0.0118(7)
C7A	0.0393(10)	0.0482(11)	0.0411(11)	-0.0006(9)	-0.0155(8)	0.0106(9)
C8A	0.0416(10)	0.0338(9)	0.0402(10)	0.0055(8)	-0.0011(8)	0.0132(8)
C10A	0.0230(7)	0.0188(7)	0.0220(7)	0.0013(6)	0.0030(6)	0.0029(6)
N10A	0.0201(6)	0.0242(6)	0.0384(8)	0.0020(6)	0.0003(6)	0.0006(5)
C11A	0.0196(7)	0.0269(7)	0.0249(8)	0.0081(6)	0.0010(6)	-0.0039(6)
C12A	0.0218(8)	0.0316(8)	0.0324(9)	0.0072(7)	0.0019(6)	0.0000(6)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C13A	0.0198(8)	0.0464(10)	0.0439(10)	0.0106(8)	-0.0016(7)	-0.0008(7)
C14A	0.0282(9)	0.0540(12)	0.0388(10)	0.0057(9)	-0.0090(8)	-0.0133(8)
C15A	0.0403(10)	0.0379(9)	0.0279(9)	0.0014(7)	-0.0016(7)	-0.0119(8)
C16A	0.0297(8)	0.0282(8)	0.0227(8)	0.0065(6)	0.0041(6)	-0.0044(6)
C17A	0.0274(9)	0.0413(10)	0.0615(13)	-0.0073(9)	0.0038(9)	0.0076(8)
C18A	0.0376(9)	0.0314(9)	0.0338(9)	-0.0015(7)	0.0080(7)	0.0003(7)
C20A	0.0203(7)	0.0246(7)	0.0233(8)	-0.0048(6)	-0.0005(6)	0.0027(6)
N20A	0.0346(8)	0.0279(7)	0.0262(7)	-0.0016(6)	0.0072(6)	0.0031(6)
C21A	0.0257(8)	0.0339(8)	0.0230(8)	0.0065(6)	0.0055(6)	0.0092(7)
C22A	0.0254(8)	0.0338(9)	0.0275(8)	0.0091(7)	0.0034(6)	0.0064(7)
C23A	0.0324(9)	0.0390(10)	0.0406(10)	0.0150(8)	0.0065(8)	0.0051(8)
C24A	0.0412(11)	0.0505(12)	0.0400(10)	0.0224(9)	0.0152(8)	0.0135(9)
C25A	0.0465(11)	0.0582(12)	0.0225(9)	0.0113(8)	0.0115(8)	0.0244(10)
C26A	0.0332(9)	0.0436(10)	0.0257(8)	0.0008(7)	0.0056(7)	0.0170(8)
C27A	0.0369(9)	0.0329(9)	0.0298(9)	0.0052(7)	-0.0011(7)	-0.0048(7)
C28A	0.0565(13)	0.0548(12)	0.0286(9)	-0.0098(9)	0.0039(9)	0.0150(10)
C30A	0.0262(8)	0.0163(7)	0.0359(9)	-0.0031(6)	0.0045(7)	-0.0023(6)
C31A	0.0234(8)	0.0197(7)	0.0343(9)	-0.0079(6)	0.0052(6)	-0.0031(6)
C32A	0.0265(8)	0.0212(7)	0.0345(9)	-0.0102(6)	0.0057(7)	-0.0024(6)
C33A	0.0233(8)	0.0203(7)	0.0415(9)	-0.0083(7)	0.0083(7)	0.0002(6)
C34A	0.0246(8)	0.0170(7)	0.0416(9)	-0.0021(6)	0.0028(7)	0.0011(6)
C35A	0.0227(8)	0.0374(9)	0.0414(10)	-0.0095(8)	0.0034(7)	-0.0052(7)
C36A	0.0394(10)	0.0371(9)	0.0340(9)	-0.0141(8)	0.0039(8)	-0.0066(8)
C37A	0.0294(9)	0.0334(9)	0.0561(12)	-0.0133(8)	0.0155(8)	0.0023(7)
C38A	0.0298(9)	0.0258(8)	0.0579(12)	0.0071(8)	-0.0013(8)	0.0051(7)
C39A	0.0366(9)	0.0253(8)	0.0397(10)	0.0025(7)	0.0067(8)	-0.0061(7)
V2	0.01771(12)	0.01773(11)	0.01991(12)	-0.00079(9)	-0.00209(9)	0.00046(9)
C1B	0.0194(7)	0.0244(7)	0.0251(8)	-0.0021(6)	0.0023(6)	-0.0004(6)
C2B	0.0320(9)	0.0315(9)	0.0315(9)	-0.0078(7)	-0.0012(7)	0.0061(7)
N3B	0.0225(6)	0.0278(7)	0.0198(6)	-0.0019(5)	-0.0014(5)	0.0016(5)
C3B	0.0310(8)	0.0303(8)	0.0207(7)	-0.0013(6)	-0.0019(6)	-0.0013(7)
C4B	0.0340(9)	0.0418(10)	0.0238(8)	0.0010(7)	-0.0070(7)	-0.0006(8)
C5B	0.0430(10)	0.0440(10)	0.0247(8)	-0.0018(7)	0.0050(7)	0.0005(8)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N6B	0.0204(6)	0.0248(6)	0.0233(6)	-0.0007(5)	-0.0021(5)	0.0033(5)
C6B	0.0224(7)	0.0309(8)	0.0265(8)	-0.0011(6)	-0.0047(6)	0.0071(6)
C7B	0.0331(9)	0.0424(10)	0.0328(9)	-0.0043(8)	-0.0117(7)	0.0090(8)
C8B	0.0363(9)	0.0327(9)	0.0380(10)	0.0069(8)	-0.0003(8)	0.0090(7)
C10B	0.0243(7)	0.0192(7)	0.0212(7)	-0.0002(6)	-0.0006(6)	0.0037(6)
N10B	0.0220(7)	0.0219(6)	0.0373(8)	-0.0003(6)	-0.0025(6)	-0.0002(5)
C11B	0.0216(7)	0.0253(7)	0.0196(7)	0.0030(6)	-0.0003(6)	-0.0047(6)
C12B	0.0234(7)	0.0306(8)	0.0211(7)	0.0049(6)	0.0014(6)	-0.0020(6)
C13B	0.0220(8)	0.0430(9)	0.0229(8)	0.0061(7)	-0.0017(6)	-0.0044(7)
C14B	0.0308(9)	0.0455(10)	0.0236(8)	-0.0012(7)	-0.0021(7)	-0.0153(8)
C15B	0.0399(9)	0.0295(8)	0.0229(8)	-0.0041(6)	0.0032(7)	-0.0084(7)
C16B	0.0287(8)	0.0260(8)	0.0208(7)	0.0028(6)	0.0027(6)	-0.0028(6)
C17B	0.0269(8)	0.0320(9)	0.0483(11)	0.0008(8)	0.0010(8)	0.0039(7)
C18B	0.0346(9)	0.0264(8)	0.0381(10)	-0.0019(7)	0.0013(7)	0.0038(7)
C20B	0.0190(7)	0.0207(7)	0.0258(8)	-0.0038(6)	-0.0027(6)	0.0014(6)
N20B	0.0287(7)	0.0258(7)	0.0251(7)	-0.0005(5)	0.0031(5)	0.0031(5)
C21B	0.0216(7)	0.0333(8)	0.0289(8)	0.0091(7)	0.0053(6)	0.0089(6)
C22B	0.0248(8)	0.0346(9)	0.0479(11)	0.0122(8)	0.0052(7)	0.0069(7)
C23B	0.0322(10)	0.0461(12)	0.0727(15)	0.0282(11)	0.0120(10)	0.0056(9)
C24B	0.0380(11)	0.0764(16)	0.0570(14)	0.0427(12)	0.0187(10)	0.0209(11)
C25B	0.0372(10)	0.0790(15)	0.0309(10)	0.0184(10)	0.0102(8)	0.0266(11)
C26B	0.0272(8)	0.0517(11)	0.0287(9)	0.0046(8)	0.0043(7)	0.0161(8)
C27B	0.0379(10)	0.0332(10)	0.0630(13)	-0.0019(9)	0.0024(9)	-0.0068(8)
C28B	0.0491(12)	0.0661(14)	0.0308(10)	-0.0131(9)	0.0003(8)	0.0071(10)
C30B	0.0312(8)	0.0176(7)	0.0323(8)	0.0028(6)	-0.0032(7)	-0.0030(6)
C31B	0.0244(8)	0.0188(7)	0.0329(8)	-0.0003(6)	-0.0020(6)	-0.0023(6)
C32B	0.0260(8)	0.0181(7)	0.0311(8)	-0.0051(6)	-0.0015(6)	-0.0004(6)
C33B	0.0247(8)	0.0175(7)	0.0372(9)	-0.0038(6)	0.0002(7)	0.0015(6)
C34B	0.0264(8)	0.0171(7)	0.0398(9)	0.0020(6)	-0.0073(7)	0.0005(6)
C35B	0.0475(11)	0.0325(9)	0.0363(10)	0.0096(8)	-0.0018(8)	-0.0085(8)
C36B	0.0251(8)	0.0350(9)	0.0455(10)	0.0026(8)	0.0011(7)	-0.0054(7)
C37B	0.0388(10)	0.0313(9)	0.0324(9)	-0.0093(7)	-0.0042(7)	-0.0031(7)
C38B	0.0288(9)	0.0281(8)	0.0532(11)	-0.0094(8)	0.0080(8)	0.0040(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C39B	0.0315(9)	0.0269(9)	0.0579(12)	0.0073(8)	-0.0141(8)	0.0024(7)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 10.

	x/a	y/b	z/c	U(eq)
H2A1	0.4862	0.3826	0.3307	0.054(4)
H2A2	0.4044	0.3616	0.3937	0.054(4)
H2A3	0.3597	0.3748	0.2970	0.054(4)
H3A	0.5802	0.3387	0.4358	0.024(4)
H4A1	0.6513	0.2646	0.4490	0.043(3)
H4A2	0.6899	0.2956	0.5184	0.043(3)
H4A3	0.7269	0.2976	0.4180	0.043(3)
H5A1	0.4017	0.3154	0.4757	0.046(3)
H5A2	0.4956	0.3118	0.5548	0.046(3)
H5A3	0.4598	0.2770	0.4964	0.046(3)
H6A	0.3085	0.3528	0.1763	0.029(4)
H7A1	0.3967	0.3115	0.0358	0.049(3)
H7A2	0.2918	0.3382	0.0232	0.049(3)
H7A3	0.2838	0.3025	0.0832	0.049(3)
H8A1	0.4732	0.3895	0.1690	0.049(3)
H8A2	0.3921	0.3929	0.0815	0.049(3)
H8A3	0.5022	0.3684	0.0802	0.049(3)
H13A	1.1868	0.3027	0.3159	0.041(5)
H14A	1.1832	0.3529	0.4090	0.046(6)
H15A	1.0170	0.3835	0.4283	0.042(5)
H17A	1.0975	0.2619	0.2115	0.058(4)
H17B	0.9837	0.2760	0.1630	0.058(4)
H17C	0.9800	0.2491	0.2461	0.058(4)
H18A	0.8161	0.3859	0.4151	0.068(4)
H18B	0.7474	0.3549	0.3616	0.068(4)
H18C	0.7983	0.3883	0.3092	0.068(4)
H23A	0.8413	0.4211	-0.0107	0.047(6)
H24A	0.8305	0.4114	-0.1633	0.058(6)

	x/a	y/b	z/c	U(eq)
H25A	0.7422	0.3602	-0.2227	0.046(6)
H27A	0.7959	0.4057	0.1354	0.060(4)
H27B	0.8176	0.3632	0.1499	0.060(4)
H27C	0.6929	0.3787	0.1463	0.060(4)
H28A	0.6302	0.3073	-0.2080	0.055(4)
H28B	0.5610	0.3048	-0.1203	0.055(4)
H28C	0.6773	0.2838	-0.1248	0.055(4)
H35A	0.2949	0.2113	0.2006	0.046(3)
H35B	0.3000	0.2429	0.1279	0.046(3)
H35C	0.3033	0.2528	0.2315	0.046(3)
H36A	0.4890	0.2119	-0.0021	0.053(3)
H36B	0.5404	0.2518	-0.0084	0.053(3)
H36C	0.4129	0.2466	0.0150	0.053(3)
H37A	0.8032	0.2328	0.1381	0.071(4)
H37B	0.7285	0.2410	0.0490	0.071(4)
H37C	0.7428	0.2002	0.0843	0.071(4)
H38A	0.7074	0.2124	0.3716	0.065(4)
H38B	0.7913	0.2292	0.3035	0.065(4)
H38C	0.7522	0.1878	0.2937	0.065(4)
H39A	0.4211	0.2396	0.3733	0.042(3)
H39B	0.5292	0.2166	0.4051	0.042(3)
H39C	0.4243	0.1967	0.3564	0.042(3)
H2B1	0.6334	0.6306	0.3740	0.048(3)
H2B2	0.5522	0.6082	0.4347	0.048(3)
H2B3	0.5101	0.6203	0.3364	0.048(3)
H3B	0.7385	0.5929	0.4752	0.026(4)
H4B1	0.8436	0.5232	0.4878	0.040(3)
H4B2	0.8682	0.5550	0.5585	0.040(3)
H4B3	0.9014	0.5600	0.4577	0.040(3)
H5B1	0.5753	0.5628	0.5244	0.047(3)
H5B2	0.6743	0.5634	0.6000	0.047(3)
H5B3	0.6485	0.5271	0.5442	0.047(3)
H6B	0.4581	0.5947	0.2236	0.024(4)

	x/a	y/b	z/c	U(eq)
H7B1	0.5440	0.5528	0.0831	0.043(3)
H7B2	0.4314	0.5762	0.0746	0.043(3)
H7B3	0.4393	0.5414	0.1385	0.043(3)
H8B1	0.6111	0.6344	0.2053	0.049(3)
H8B2	0.5307	0.6330	0.1171	0.049(3)
H8B3	0.6460	0.6111	0.1214	0.049(3)
H13B	1.3387	0.5768	0.3793	0.034(5)
H14B	1.3105	0.6356	0.4295	0.037(5)
H15B	1.1331	0.6610	0.4203	0.032(5)
H17D	1.2760	0.5243	0.3009	0.058(4)
H17E	1.1587	0.5261	0.2453	0.058(4)
H17F	1.1648	0.5108	0.3449	0.058(4)
H18D	0.9385	0.6576	0.3899	0.090(5)
H18E	0.8834	0.6181	0.3825	0.090(5)
H18F	0.9151	0.6392	0.2945	0.090(5)
H23B	0.9818	0.6509	-0.0444	0.054(6)
H24B	0.9498	0.6302	-0.1889	0.066(7)
H25B	0.8486	0.5777	-0.2173	0.054(6)
H27D	0.9634	0.6455	0.1118	0.066(4)
H27E	0.9528	0.6047	0.1467	0.066(4)
H27F	0.8441	0.6297	0.1348	0.066(4)
H28D	0.7368	0.5289	-0.1710	0.059(4)
H28E	0.6794	0.5338	-0.0783	0.059(4)
H28F	0.7928	0.5112	-0.0824	0.059(4)
H35D	0.6191	0.4824	0.4373	0.052(3)
H35E	0.7450	0.4707	0.4636	0.052(3)
H35F	0.6567	0.4410	0.4268	0.052(3)
H36D	0.4868	0.4517	0.2790	0.076(4)
H36E	0.4735	0.4820	0.2030	0.076(4)
H36F	0.4862	0.4938	0.3053	0.076(4)
H37D	0.6326	0.4515	0.0689	0.067(4)
H37E	0.6937	0.4883	0.0428	0.067(4)
H37F	0.5713	0.4897	0.0799	0.067(4)

	x/a	y/b	z/c	U(eq)
H38D	0.9678	0.4935	0.1675	0.055(4)
H38E	0.8814	0.4880	0.0838	0.055(4)
H38F	0.9315	0.4534	0.1365	0.055(4)
H39D	0.9156	0.4699	0.4143	0.077(5)
H39E	0.9840	0.4868	0.3359	0.077(5)
H39F	0.9561	0.4443	0.3366	0.077(5)

References

S1) Decker, J. M.; Geib, S. J.; Meyer, T. Y. *Organometallics* **1999**, *18*, 4417.

S2) Yonke, B. L.; Keane, A. J.; Zavalij, P. Y.; Sita, L. R. *Organometallics* **2011**, *31*, 345.

S3) Hirotsu, M.; Fontaine, P. P.; Epshteyn, A.; Zavalij, P. Y.; Sita, L. R. *J. Am. Chem. Soc.* **2007**, *129*, 9284.

S4) Mata, J. D. L.; Fandos, R.; Gómez, M.; Gómez-Sal, P.; Martinez-Carrera, S.; Royo, P. *Organometallics* **1990**, *8*, 2846.

S5) Abernethy, C. D.; Bottomley, F.; Decken, A. *Organometallics* **1997**, *16*, 1865.

S6) Methylcyclohexane was purified by Na/K alloy and isolated by vacuum transfer.

S7) Error at the 95% confidence interval was calculated using the student's *t* distribution, see: Wilson, E. B., Jr. *An Introduction to Scientific Research*; Dover: New York, 1990.