Supplementary Information

Evidence for a Ni^I Active Species in the Catalytic Cross-Coupling of Alkyl Electrophiles

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General Considerations. All manipulations were performed using standard Schlenk techniques or in a nitrogen-filled glove box, unless otherwise noted. Solvents were distilled from Na/benzophenone or CaH₂. All reagents were used as received from commercial vendors unless otherwise noted. Aluminum oxide (activated, neutral, Brockmann I, ~150 mesh) was dried at 200 °C under vacuum for two days prior to use. All gas chromatography was completed using Shimadzu GC-14A with J & W Scientific High Resolution GC column DB-1, 30 meters, I.D. 0.32(mm), Widebore film 0.25 μ m, Serial #US151955414. Initial column temp. 50 °C for 5 min. Ramp at 15 °C/min. Final column temp. 200 °C for 5 min. Injector and detector temperatures were 250 °C. Each injection was 1 μL of a 0.5 mL aliquot filtered through a Whatman[®] Syringe filter (13 mm GD/X disposable filter device, Nylon filter media with polypropylene housing, 150 units, 0.2 μm pore size) that was diluted with excess THF. (TMEDA)Ni(Me)₂ was prepared according to a literature procedure.¹

Preparation of (tpy)NiMe: (TMEDA)Ni(Me)₂ (500 mg, 2.44 mmol) was dissolved in 100 mL diethyl ether. This solution was cooled to -78 °C, and terpyridine (0.5687g, 2.44 mmol) in 25 mL ether was added dropwise to the slurry. After addition was complete, the solution was allowed to warm to room temperature. The solution changed from yellow-green color to a dark violet/black color within 1 hour. The resulting suspension was then allowed to stir overnight. The product was filtered and washed with ether leaving 0.681 g (2.22 mmol) of (tpy)Ni(Me) (91% yield). Compound is paramagnetic. UV-Vis (THF): ε_{576 nm} = 463.07 L mol⁻¹ cm⁻¹. Anal. Calcd for C₁₆H₁₄N₃Ni: C 62.31 (62.60); H 4.37 (4.60).

Representative preparation of a terpyridyl based Ni^I halide complex: (tpy)Ni(I) (4a): Terpyridine (721 mg, 3.1 mmol) was added to a stirred solution of Ni(COD)₂ (850 mg, 3.1 mmol) in 120 mL THF. The resulting green solution was stirred at room temperature for 0.5 h. Methyl iodide (193 μL in 15 mL THF) was then added dropwise to the solution at room temperature. The resulting suspension was stirred for 4 h at room temperature. The olive green solid was then filtered, washed with THF and ether, and dried under vacuum. Yield: 1.19 g (92 %). Compound is paramagnetic. Anal. Calcd for C₁₅H₁₁IN₃Ni: C 42.98 (43.01); H 2.38 (2.65).

¹ Yamamoto, T.; Yamamoto, A.; Ikeda, S. *J. Amer. Chem. Soc.* **1971**, *93*, 3350-9.

Monitoring the transfer of a methyl group from **3 to iodocyclohexane:** Compound **3** (30 mg, 0.1 mmol) and hexamethylbenzene (5 mg, 0.03 mmol) were dissolved in 2.0 mL C₆D₆ and stirred. A solution of iodocyclohexane (12.6 μ L in 0.5 mL C₆D₆) was then added dropwise, and the resulting suspension was stirred in the dark for 24 h at room temperature. The resulting mixture was then filtered over a small plug of alumina packed in a pipette, and the solution was analyzed by ¹H NMR spectroscopy to determine the yield of methylcyclohexane.

Example of catalytic alkane cross-coupling procedure: Preparation of *n*-amyl cyclohexane. A small screw capped vial equipped with a magnetic stir bar was charged with 1-iodocyclohexane (87 μ L, 0.67 mmol) and internal standard (hexadecane, 73 μ L, 0.25 mmol) in THF. (tpy)NiMe (5 mol %) was dissolved in the minimum amount THF and was pipetted into the vial. The total volume of THF at this stage was adjusted to 10 mL. To the stirring vial *n*-pentylzinc bromide (1.35 mL, 0.68 mmol) was syringed into the vial. The vial was capped and stirred in a glove box for 23 hrs at room temperature. Yield was determined by GC (referenced to a calibrated internal standard) to be 64 %.

Magnetic Properties of **3**:

Calculation of diamagnetic susceptibilities for (**3**):

15 x C (aromatic ring)=	15(-6.24e-6)	=	-93.6 e-6 emu
11 x H	=	11(-2.93e-6)	= -32.23 e-6 emu
3 x N (aromatic ring) =	3(-4.6e-6)	=	-13.8e-6 emu
1 x C	=	1(-6.0e-6)	= -6.0 e-6 emu
3 x H	=	3(-2.93e-6)	= -8.79 e-6 emu
1 x Ni*	=	1(-12.8e-6)	= -12.8 e-6 emu
			-167.22 e-6 emu

(*) A diamagnetic correction for Ni(I) is not reported.

Solution magnetic susceptibilities were calculated using the Evans NMR method with a superconducting NMR spectrometer according to eq 1:² Diamagnetic correction for THF solvent: -0.735 e-6 cm³g⁻¹

$$\chi_g = 3\Delta\nu/4\pi\nu c + \chi_o \quad (1)$$

where

χ_g = gram susceptibility

c = concentration in g/mL

$\Delta\nu$ = observed shift difference in Hz

ν = spectrometer frequency in Hz

χ_o = mass susceptibility of solvent

² (a) Sur, S. K. *J. Magnetic Resonance* **1989**, 82, 169-173. (b) Schubert, E. M. *J. Chem. Ed.* **1992**, 68, p.62.

X-ray Structure Report

for **4b**

Experimental

Data Collection

A green crystal of $C_{27}H_{35}IN_3Ni$ was grown from slow vapor diffusion of pentane into a THF solution of **4b**. The crystal was then covered in Paratone-N oil and mounted on a glass fiber. All measurements were made on a Rigaku Mercury CCD area detector with graphite monochromated Mo- $K\alpha$ radiation.

Indexing was performed from 480 images that were exposed for 10 seconds. The crystal-to-detector distance was 32.77 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

$$\begin{aligned}a &= 10.429(12) \text{ \AA} \\b &= 12.149(8) \text{ \AA} \quad \beta = 99.985(6)^\circ \\c &= 21.08(2) \text{ \AA} \\V &= 2630.5(40) \text{ \AA}^3\end{aligned}$$

For $Z = 4$ and F.W. = 587.20, the calculated density is 1.48 g/cm^3 . The systematic absences of:

$$\begin{aligned}h0l: & l \neq 2n \\0k0: & k \neq 2n\end{aligned}$$

uniquely determine the space group to be:

$$P2_1/c \text{ (\#14)}$$

The data were collected at a temperature of $-100 \pm 1^\circ\text{C}$ to a maximum 2θ value of 55.7° . A total of 480 oscillation images were collected. The crystal-to-detector distance was 32.77 mm. Readout was performed in the 0.068 mm pixel mode.

Data Reduction

A total of 15442 reflections was collected. Data were collected and processed using CrystalClear (Rigaku). Net intensities and sigmas were derived as follows:

$$F^2 = [\Sigma(P_i - mB_{ave})] \cdot L_p^{-1}$$

where P_i is the value in counts of the i^{th} pixel
 m is the number of pixels in the integration area
 B_{ave} is the background average
 L_p is the Lorentz and polarization factor

$$B_{ave} = \Sigma(B_j)/n$$

where n is the number of pixels in the background area
 B_j is the value of the j^{th} pixel in counts

$$\sigma^2(F^2_{hkl}) = [(\Sigma P_i) + m((\Sigma(B_{ave} - B_j)^2)/(n-1))] \cdot L_p \cdot \text{errmul} + (\text{erradd} \cdot F^2)^2$$

where $\text{erradd} = 0.00$
 $\text{errmul} = 1.00$

The linear absorption coefficient, μ , for Mo-K α radiation is 19.3 cm⁻¹. was applied which resulted in transmission factors ranging from 0.6655 to 1.0000. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods² and expanded using Fourier techniques³. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement⁴ on F^2 was based on 6135 observed reflections and 299 variable parameters and converged (largest parameter shift was less than 0.01 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.040$$

$$wR2 = [\Sigma (w (F_o^2 - F_c^2)^2) / \Sigma w(F_o^2)^2]^{1/2} = 0.113$$

The standard deviation of an observation of unit weight⁵ was 1.13. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 2.45 and -0.72 e⁻/Å³, respectively.

Neutral atom scattering factors were taken from Cromer and Waber⁶. Anomalous dispersion effects were included in F_{calc}⁷; the values for Δf' and Δf'' were those of Creagh and McAuley⁸. The values for the mass attenuation coefficients are those of Creagh and Hubbell⁹. All calculations were performed using the CrystalStructure^{10,11} crystallographic software package except for refinement, which was performed using SHELXL-97¹².

References

(1) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000. J.W. Pflugrath (1999) Acta Cryst. D55, 1718-1725.

(2) SHELX97: Sheldrick, G.M. (1997).

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized: (SHELXL97)

$$\sum w(F_o^2 - F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.}$$

(5) Standard deviation of an observation of unit weight:

$$[\sum w(F_o^2 - F_c^2)^2 / (N_o - N_v)]^{1/2}$$

where: N_o = number of observations

N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J. ; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

- (9) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (10) CrystalStructure 3.6.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSO (2000-2004). 9009 New Trails Dr. The Woodlands TX 77381 USA.
- (11) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)
- (12) SHELX97: Sheldrick, G.M. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data for **4b**

Empirical Formula	C ₂₇ H ₃₅ IN ₃ Ni
Formula Weight	587.20
Crystal Color, Habit	green, prism
Crystal Dimensions	0.50 X 0.45 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
Detector Position	32.77 mm
Pixel Size	0.068 mm
Lattice Parameters	a = 10.429(12) Å b = 12.149(8) Å c = 21.08(2) Å β = 99.985(6) ° V = 2630.5(40) Å ³
Space Group	P2 ₁ /c (#14)
Z value	4
D _{calc}	1.483 g/cm ³
F ₀₀₀	1196.00
μ(MoKα)	19.30 cm ⁻¹

B. Intensity Measurements for **4b**

Detector	Rigaku Mercury
Radiation	MoK α ($\lambda = 0.71070 \text{ \AA}$) graphite monochromated
scan:	
Number of images: 360	
Slice: -70.0000 - 110.0000	
Image width: 0.5000	
Exp time: 10.0000	
Rotation axis: Omega	
Omega: 0.0000	
Chi: 45.0000	
Phi: 0.0000	
scan:	
Number of images: 120	
Slice: -30.0000 - 30.0000	
Image width: 0.5000	
Exp time: 10.0000	
Rotation axis: Omega	
Omega: 0.0000	
Chi: 45.0000	
Detector Aperture	70 mm x 70 mm
Data Images	480 exposures
Detector Position	32.77 mm
Pixel Size	0.068 mm
$2\theta_{\text{max}}$	55.7 $^{\circ}$
No. of Reflections Measured	Total: 15442
Corrections	Lorentz-polarization Absorption (trans. factors: 0.6655 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (F_o^2 - F_c^2)^2$
Least Squares Weights	$w = 1 / [\sigma^2(F_o^2) + (0.0910 \cdot P)^2 + 4.5864 \cdot P]$ where $P = (\text{Max}(F_o^2, 0) + 2F_c^2)/3$
$2\theta_{\text{max}}$ cutoff	55.7°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	6135
No. Variables	299
Reflection/Parameter Ratio	20.52
Residuals: R (All reflections)	0.056
Residuals: R1 ($I > 2.00\sigma(I)$)	0.040
Residuals: wR2 (All reflections)	0.113
Goodness of Fit Indicator	1.125
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	2.45 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.72 e ⁻ /Å ³

Table S1. Atomic coordinates and B_{iso}/B_{eq} for **4b**.

atom	x	y	z	B _{eq}
I(1)	0.30363(2)	0.65043(2)	0.368128(10)	2.343(5)
Ni(1)	0.14194(3)	0.48988(3)	0.36730(2)	1.676(8)
N(1)	0.1807(2)	0.4327(2)	0.45895(11)	1.78(5)
N(2)	-0.0157(2)	0.4120(2)	0.37213(11)	1.62(5)
N(3)	0.0565(3)	0.4917(2)	0.27272(12)	2.04(5)
C(1)	0.0969(3)	0.5425(3)	0.2231(2)	2.64(7)
C(2)	0.0218(3)	0.5520(3)	0.1631(1)	2.44(6)
C(3)	-0.1032(3)	0.5076(2)	0.1505(1)	1.92(6)
C(4)	-0.1449(3)	0.4536(2)	0.20141(13)	1.78(5)
C(5)	-0.0640(3)	0.4482(2)	0.26112(13)	1.67(5)
C(6)	-0.1054(3)	0.3986(2)	0.31862(13)	1.60(5)
C(7)	-0.2235(3)	0.3481(2)	0.32065(13)	1.71(5)
C(8)	-0.2546(3)	0.3154(2)	0.37991(13)	1.60(5)
C(9)	-0.1592(3)	0.3293(2)	0.43520(13)	1.64(5)
C(10)	-0.0393(3)	0.3748(2)	0.42927(12)	1.53(5)
C(11)	0.0781(3)	0.3850(2)	0.48020(12)	1.49(5)
C(12)	0.0884(3)	0.3411(2)	0.5419(1)	1.66(5)
C(13)	0.2090(3)	0.3391(2)	0.5831(1)	1.70(5)
C(14)	0.3137(3)	0.3865(3)	0.5600(1)	2.12(6)
C(15)	0.2952(3)	0.4339(3)	0.4995(2)	2.15(6)
C(16)	0.2304(3)	0.2800(2)	0.6486(1)	1.98(5)
C(17)	0.3209(3)	0.3489(3)	0.6992(2)	2.69(7)
C(18)	0.2968(4)	0.1699(3)	0.6402(2)	3.18(7)
C(19)	0.1026(3)	0.2606(3)	0.6731(2)	2.68(7)
C(20)	-0.3892(3)	0.2659(2)	0.3809(1)	1.78(5)
C(21)	-0.4948(3)	0.3446(3)	0.3465(2)	2.84(7)
C(22)	-0.4145(3)	0.2479(3)	0.4492(2)	2.90(7)
C(23)	-0.3979(4)	0.1557(3)	0.3445(2)	2.85(7)
C(24)	-0.1882(3)	0.5161(3)	0.0835(1)	2.41(6)
C(25)	-0.1829(6)	0.6332(4)	0.0578(2)	4.80(11)
C(26)	-0.3297(3)	0.4849(3)	0.0840(2)	2.70(7)
C(27)	-0.1318(3)	0.4348(4)	0.0393(2)	3.17(7)

$$B_{eq} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

Table S2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} for **4b**.

atom	x	y	z	B _{eq}
H(1A1)	0.1818	0.5735	0.2299	3.158
H(2A1)	0.0553	0.5893	0.1299	2.921
H(4A1)	-0.2286	0.4204	0.1954	2.132
H(7A1)	-0.2834	0.3355	0.2819	2.053
H(9A1)	-0.1764	0.3080	0.4763	1.974
H(12A1)	0.0134	0.3124	0.5560	1.974
H(14A1)	0.3979	0.3861	0.5859	2.526
H(15A1)	0.3672	0.4691	0.4859	2.605
H(17A1)	0.2852	0.4233	0.7007	4.027
H(17B1)	0.4076	0.3531	0.6874	4.027
H(17C1)	0.3273	0.3142	0.7416	4.027
H(18A1)	0.2426	0.1270	0.6064	4.737
H(18B1)	0.3084	0.1288	0.6808	4.737
H(18C1)	0.3820	0.1833	0.6281	4.737
H(19A1)	0.0488	0.2085	0.6445	4.027
H(19B1)	0.0559	0.3305	0.6735	4.027
H(19C1)	0.1212	0.2303	0.7168	4.027
H(21A1)	-0.4862	0.4164	0.3680	4.263
H(21B1)	-0.5811	0.3139	0.3481	4.263
H(21C1)	-0.4842	0.3536	0.3015	4.263
H(22A1)	-0.3514	0.1948	0.4713	4.342
H(22B1)	-0.5029	0.2194	0.4475	4.342
H(22C1)	-0.4054	0.3179	0.4726	4.342
H(23A1)	-0.3334	0.1044	0.3674	4.263
H(23B1)	-0.3804	0.1678	0.3009	4.263
H(23C1)	-0.4853	0.1248	0.3422	4.263
H(25A1)	-0.2040	0.6855	0.0898	7.185
H(25B1)	-0.2461	0.6408	0.0178	7.185
H(25C1)	-0.0952	0.6483	0.0492	7.185
H(26A1)	-0.3645	0.5313	0.1151	4.027
H(26B1)	-0.3344	0.4075	0.0964	4.027
H(26C1)	-0.3811	0.4960	0.0410	4.027
H(27A1)	-0.1439	0.3592	0.0535	4.737
H(27B1)	-0.0388	0.4494	0.0415	4.737
H(27C1)	-0.1771	0.4440	-0.0051	4.737

$$B_{eq} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

Table S3. Anisotropic Displacement Parameters for **4b**.

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
I(1)	0.02632(13)	0.02900(13)	0.03156(13)	-0.00887(7)	-0.00101(9)	0.00082(7)
Ni(1)	0.0190(2)	0.0247(2)	0.0195(2)	-0.00478(13)	0.0021(1)	-0.00073(12)
N(1)	0.0206(11)	0.0243(12)	0.0213(12)	-0.0025(9)	0.0001(9)	-0.0002(8)
N(2)	0.0206(11)	0.0221(12)	0.0181(11)	-0.0014(9)	0.0008(9)	0.0011(8)
N(3)	0.0297(13)	0.0314(13)	0.0171(11)	-0.0088(10)	0.0058(9)	-0.0028(9)
C(1)	0.034(2)	0.043(2)	0.025(2)	-0.016(1)	0.0098(13)	-0.0027(12)
C(2)	0.039(2)	0.035(2)	0.020(1)	-0.012(1)	0.0103(12)	0.0021(11)
C(3)	0.030(2)	0.023(1)	0.0208(13)	0.0000(11)	0.0074(11)	0.0003(10)
C(4)	0.026(1)	0.0228(13)	0.0188(13)	-0.0030(11)	0.0030(10)	0.0000(9)
C(5)	0.026(1)	0.0207(13)	0.0175(12)	-0.0047(11)	0.0047(10)	-0.0020(9)
C(6)	0.0204(13)	0.0228(13)	0.0169(12)	-0.0024(10)	0.0016(10)	-0.0013(9)
C(7)	0.0212(13)	0.026(1)	0.0160(13)	-0.0037(10)	-0.0007(10)	0.0015(9)
C(8)	0.0169(12)	0.0228(13)	0.0198(13)	-0.0038(10)	-0.0002(10)	0.0008(9)
C(9)	0.0197(13)	0.0253(13)	0.0167(12)	-0.0017(10)	0.0010(10)	0.0017(9)
C(10)	0.0205(13)	0.0202(12)	0.0163(12)	-0.0012(10)	0.0005(9)	-0.0001(9)
C(11)	0.0182(12)	0.0182(12)	0.0190(12)	-0.0001(10)	-0.0001(10)	-0.0007(9)
C(12)	0.0213(13)	0.0199(13)	0.0206(13)	0.0000(10)	0.0001(10)	0.0011(9)
C(13)	0.022(1)	0.0207(13)	0.0195(13)	0.0013(10)	-0.0017(10)	-0.0001(9)
C(14)	0.0197(13)	0.033(2)	0.025(1)	-0.0034(12)	-0.0051(11)	0.0016(11)
C(15)	0.0201(13)	0.033(2)	0.027(2)	-0.0050(12)	-0.0006(11)	0.0020(11)
C(16)	0.027(1)	0.027(1)	0.0182(13)	0.0022(12)	-0.0043(11)	0.0034(10)
C(17)	0.032(2)	0.042(2)	0.024(2)	-0.003(1)	-0.0063(13)	0.0002(12)
C(18)	0.052(2)	0.033(2)	0.034(2)	0.014(2)	0.002(2)	0.0078(13)
C(19)	0.033(2)	0.042(2)	0.025(2)	-0.007(1)	0.0007(12)	0.0082(12)
C(20)	0.0165(12)	0.029(2)	0.0215(13)	-0.0053(11)	0.0004(10)	0.0020(10)
C(21)	0.021(2)	0.046(2)	0.039(2)	-0.0015(13)	0.0000(13)	0.008(1)
C(22)	0.025(2)	0.059(2)	0.026(2)	-0.012(2)	0.0040(12)	0.005(1)
C(23)	0.033(2)	0.036(2)	0.040(2)	-0.014(1)	0.011(2)	-0.0078(13)
C(24)	0.040(2)	0.032(2)	0.0186(13)	0.0013(13)	0.0016(12)	0.0049(11)
C(25)	0.085(4)	0.041(2)	0.048(2)	-0.011(2)	-0.012(2)	0.021(2)
C(26)	0.032(2)	0.044(2)	0.025(2)	0.008(1)	0.0030(13)	0.0036(13)
C(27)	0.035(2)	0.065(2)	0.021(2)	-0.004(2)	0.0065(13)	-0.007(1)

The general temperature factor expression: $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$

Table S4. Bond lengths (Å) for **4b**.

atom	atom	distance	atom	atom	distance
I(1)	Ni(1)	2.5765(4)	Ni(1)	N(1)	2.027(2)
Ni(1)	N(2)	1.915(2)	Ni(1)	N(3)	2.038(2)
N(1)	C(11)	1.359(4)	N(1)	C(15)	1.343(3)
N(2)	C(6)	1.345(3)	N(2)	C(10)	1.349(4)
N(3)	C(1)	1.343(4)	N(3)	C(5)	1.346(4)
C(1)	C(2)	1.373(4)	C(2)	C(3)	1.393(4)
C(3)	C(4)	1.391(4)	C(3)	C(24)	1.535(4)
C(4)	C(5)	1.390(4)	C(5)	C(6)	1.483(4)
C(6)	C(7)	1.383(4)	C(7)	C(8)	1.401(4)
C(8)	C(9)	1.405(4)	C(8)	C(20)	1.530(4)
C(9)	C(10)	1.392(4)	C(10)	C(11)	1.487(4)
C(11)	C(12)	1.393(4)	C(12)	C(13)	1.399(4)
C(13)	C(14)	1.395(5)	C(13)	C(16)	1.538(4)
C(14)	C(15)	1.382(4)	C(16)	C(17)	1.542(4)
C(16)	C(18)	1.531(5)	C(16)	C(19)	1.528(5)
C(20)	C(21)	1.541(4)	C(20)	C(22)	1.524(5)
C(20)	C(23)	1.537(4)	C(24)	C(25)	1.527(6)
C(24)	C(26)	1.525(5)	C(24)	C(27)	1.542(5)

Table S5. Bond angles (°) for **4b**.

atom	atom	atom	angle	atom	atom	atom	angle
I(1)	Ni(1)	N(3)	99.96(8)	I(1)	Ni(1)	N(1)	103.35(6)
I(1)	Ni(1)	N(2)	160.15(7)	N(3)	Ni(1)	N(1)	156.5(1)
N(2)	Ni(1)	N(1)	79.12(9)	Ni(1)	N(1)	C(11)	115.0(2)
Ni(1)	N(1)	C(15)	127.7(2)	N(3)	Ni(1)	N(2)	79.8(1)
Ni(1)	N(2)	C(6)	119.6(2)	Ni(1)	N(2)	C(10)	120.3(2)
Ni(1)	N(3)	C(1)	128.6(2)	Ni(1)	N(3)	C(5)	114.2(2)
N(1)	C(11)	C(10)	113.2(2)	C(15)	N(1)	C(11)	117.3(2)
N(1)	C(11)	C(12)	122.2(3)	N(1)	C(15)	C(14)	123.3(3)
N(2)	C(6)	C(5)	112.2(3)	C(10)	N(2)	C(6)	120.0(2)
N(2)	C(6)	C(7)	121.4(3)	N(2)	C(10)	C(11)	111.2(3)
N(2)	C(10)	C(9)	121.3(2)	C(5)	N(3)	C(1)	116.6(2)
N(3)	C(1)	C(2)	123.4(3)	N(3)	C(5)	C(6)	113.9(2)
N(3)	C(5)	C(4)	123.2(3)	C(1)	C(2)	C(3)	120.6(3)
C(2)	C(3)	C(4)	116.3(3)	C(2)	C(3)	C(24)	121.4(3)
C(3)	C(4)	C(5)	120.0(3)	C(24)	C(3)	C(4)	122.3(3)
C(3)	C(24)	C(25)	109.8(3)	C(3)	C(24)	C(27)	107.0(3)
C(3)	C(24)	C(26)	112.4(3)	C(4)	C(5)	C(6)	122.8(3)
C(5)	C(6)	C(7)	126.3(2)	C(6)	C(7)	C(8)	119.9(2)
C(7)	C(8)	C(9)	117.7(3)	C(7)	C(8)	C(20)	118.5(2)
C(8)	C(9)	C(10)	119.4(3)	C(20)	C(8)	C(9)	123.7(3)
C(8)	C(20)	C(21)	109.4(2)	C(8)	C(20)	C(23)	108.1(3)
C(8)	C(20)	C(22)	112.2(2)	C(9)	C(10)	C(11)	127.4(2)
C(10)	C(11)	C(12)	124.3(3)	C(11)	C(12)	C(13)	120.1(3)
C(12)	C(13)	C(14)	116.7(3)	C(12)	C(13)	C(16)	122.7(3)
C(13)	C(14)	C(15)	120.1(3)	C(16)	C(13)	C(14)	120.4(3)
C(13)	C(16)	C(18)	107.6(3)	C(13)	C(16)	C(19)	112.0(2)
C(13)	C(16)	C(17)	110.1(2)	C(18)	C(16)	C(17)	108.6(3)
C(19)	C(16)	C(17)	108.4(3)	C(19)	C(16)	C(18)	110.0(3)
C(23)	C(20)	C(21)	109.3(3)	C(22)	C(20)	C(21)	107.9(3)
C(23)	C(20)	C(22)	109.9(3)	C(27)	C(24)	C(25)	110.0(3)
C(26)	C(24)	C(25)	109.2(3)	C(27)	C(24)	C(26)	108.4(3)

Table S6. Torsion Angles (°) for **4b**.

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
I(1)	Ni(1)	N(1)	C(11)	151.4(2)	I(1)	Ni(1)	N(1)	C(15)	-30.6(3)
N(2)	Ni(1)	N(1)	C(11)	-8.4(2)	N(2)	Ni(1)	N(1)	C(15)	169.5(3)
N(3)	Ni(1)	N(1)	C(11)	-35.0(3)	N(3)	Ni(1)	N(1)	C(15)	143.0(2)
I(1)	Ni(1)	N(2)	C(6)	88.4(3)	I(1)	Ni(1)	N(2)	C(10)	-88.8(3)
N(1)	Ni(1)	N(2)	C(6)	-172.4(2)	N(1)	Ni(1)	N(2)	C(10)	10.4(2)
N(3)	Ni(1)	N(2)	C(6)	-2.8(2)	N(3)	Ni(1)	N(2)	C(10)	180.0(2)
I(1)	Ni(1)	N(3)	C(1)	15.0(3)	I(1)	Ni(1)	N(3)	C(5)	-155.4(2)
N(1)	Ni(1)	N(3)	C(1)	-158.6(2)	N(1)	Ni(1)	N(3)	C(5)	30.9(4)
N(2)	Ni(1)	N(3)	C(1)	174.9(3)	N(2)	Ni(1)	N(3)	C(5)	4.4(2)
Ni(1)	N(1)	C(11)	C(10)	5.6(3)	Ni(1)	N(1)	C(11)	C(12)	179.7(2)
C(15)	N(1)	C(11)	C(10)	-172.6(2)	C(15)	N(1)	C(11)	C(12)	1.6(4)
Ni(1)	N(1)	C(15)	C(14)	-175.8(3)	C(11)	N(1)	C(15)	C(14)	2.1(5)
Ni(1)	N(2)	C(6)	C(5)	0.7(3)	Ni(1)	N(2)	C(6)	C(7)	-176.5(2)
C(10)	N(2)	C(6)	C(5)	178.0(2)	C(10)	N(2)	C(6)	C(7)	0.8(4)
Ni(1)	N(2)	C(10)	C(9)	172.5(2)	Ni(1)	N(2)	C(10)	C(11)	-10.0(3)
C(6)	N(2)	C(10)	C(9)	-4.7(4)	C(6)	N(2)	C(10)	C(11)	172.7(2)
Ni(1)	N(3)	C(1)	C(2)	-169.8(3)	C(5)	N(3)	C(1)	C(2)	0.4(5)
Ni(1)	N(3)	C(5)	C(4)	171.9(2)	Ni(1)	N(3)	C(5)	C(6)	-5.3(3)
C(1)	N(3)	C(5)	C(4)	0.3(4)	C(1)	N(3)	C(5)	C(6)	-176.9(2)
N(3)	C(1)	C(2)	C(3)	-0.3(5)	C(1)	C(2)	C(3)	C(4)	-0.6(5)
C(1)	C(2)	C(3)	C(24)	-179.3(3)	C(2)	C(3)	C(4)	C(5)	1.2(4)
C(24)	C(3)	C(4)	C(5)	179.9(2)	C(2)	C(3)	C(24)	C(25)	-45.8(4)
C(2)	C(3)	C(24)	C(26)	-167.6(3)	C(2)	C(3)	C(24)	C(27)	73.5(4)
C(4)	C(3)	C(24)	C(25)	135.6(3)	C(4)	C(3)	C(24)	C(26)	13.8(4)
C(4)	C(3)	C(24)	C(27)	-105.1(3)	C(3)	C(4)	C(5)	N(3)	-1.2(4)
C(3)	C(4)	C(5)	C(6)	175.8(2)	N(3)	C(5)	C(6)	N(2)	3.1(3)
N(3)	C(5)	C(6)	C(7)	-179.8(3)	C(4)	C(5)	C(6)	N(2)	-174.1(2)
C(4)	C(5)	C(6)	C(7)	3.0(4)	N(2)	C(6)	C(7)	C(8)	3.6(4)
C(5)	C(6)	C(7)	C(8)	-173.1(3)	C(6)	C(7)	C(8)	C(9)	-4.0(4)
C(6)	C(7)	C(8)	C(20)	176.5(2)	C(7)	C(8)	C(9)	C(10)	0.3(4)
C(20)	C(8)	C(9)	C(10)	179.7(2)	C(7)	C(8)	C(20)	C(21)	-53.2(3)
C(7)	C(8)	C(20)	C(22)	-172.8(2)	C(7)	C(8)	C(20)	C(23)	65.8(3)
C(9)	C(8)	C(20)	C(21)	127.4(3)	C(9)	C(8)	C(20)	C(22)	7.7(4)
C(9)	C(8)	C(20)	C(23)	-113.7(3)	C(8)	C(9)	C(10)	N(2)	4.1(4)
C(8)	C(9)	C(10)	C(11)	-172.8(2)	N(2)	C(10)	C(11)	N(1)	2.3(3)
N(2)	C(10)	C(11)	C(12)	-171.7(3)	C(9)	C(10)	C(11)	N(1)	179.5(3)
C(9)	C(10)	C(11)	C(12)	5.5(4)	N(1)	C(11)	C(12)	C(13)	-3.9(4)

Table S6. Torsion angles ($^{\circ}$) -- continued for **4b**.

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(10)	C(11)	C(12)	C(13)	169.6(2)	C(11)	C(12)	C(13)	C(14)	2.5(4)
C(11)	C(12)	C(13)	C(16)	-172.7(2)	C(12)	C(13)	C(14)	C(15)	1.0(5)
C(16)	C(13)	C(14)	C(15)	176.3(3)	C(12)	C(13)	C(16)	C(17)	-140.6(3)
C(12)	C(13)	C(16)	C(18)	101.2(3)	C(12)	C(13)	C(16)	C(19)	-19.9(4)
C(14)	C(13)	C(16)	C(17)	44.4(4)	C(14)	C(13)	C(16)	C(18)	-73.8(3)
C(14)	C(13)	C(16)	C(19)	165.1(3)	C(13)	C(14)	C(15)	N(1)	-3.4(5)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

X-ray data analysis for **3**: Because of the weak data obtained for **3** (as explicitly noted in the Communication text), all atoms except for the Ni atoms were refined isotropically. The refinement was also performed in the lowest space group symmetry possible, hence multiple molecules were found in the asymmetric unit.

Table S7. Crystal data and structure refinement for **3**.

Empirical formula	C ₉₆ H ₈₄ N ₁₈ Ni ₆
Formula weight	1842.07
Temperature	173(2) K
Wavelength	0.71070 Å
Crystal system, space group	Primitive, P-1
Unit cell dimensions	a = 13.80(5) Å alpha = 73.6(3) deg. b = 18.43(6) Å beta = 68.1(3) deg. c = 18.41(7) Å gamma = 68.0(2) deg.
Volume	3974(24) Å ³
Z, Calculated density	3, 2.309 Mg/m ³
Absorption coefficient	2.184 mm ⁻¹
F(000)	2862
Crystal size	0.05 x 0.10 x 0.20 mm
Theta range for data collection	2.34 to 26.00 deg.
Limiting indices	-13 ≤ h ≤ 17, -22 ≤ k ≤ 21, -22 ≤ l ≤ 22
Reflections collected / unique	22117 / 14277 [R(int) = 0.1536]
Completeness to theta = 26.00	91.5 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	14277 / 0 / 1088
Goodness-of-fit on F ²	1.173
Final R indices [I > 2sigma(I)]	R1 = 0.1867, wR2 = 0.2776
R indices (all data)	R1 = 0.3490, wR2 = 0.3508
Largest diff. peak and hole	0.562 and -0.660 e.Å ⁻³

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.

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

	x	y	z	U(eq)
Ni(1)	2440(2)	2650(2)	1566(2)	29(1)
Ni(2)	1652(2)	2352(2)	3431(2)	30(1)
Ni(3)	9873(2)	1399(2)	7825(2)	31(1)
Ni(4)	12204(2)	68(2)	7702(2)	28(1)
Ni(5)	4094(3)	3602(2)	7178(2)	32(1)
Ni(6)	4974(2)	4933(2)	7298(2)	27(1)
N(1)	1976(16)	3702(12)	1759(9)	41(6)
N(2)	2975(15)	2344(13)	3447(9)	40(6)
N(3)	2481(14)	1301(9)	3232(10)	32(5)
N(4)	1175(17)	3379(10)	3689(9)	41(5)
N(5)	3279(15)	1590(10)	1319(9)	36(5)
N(6)	3799(12)	2651(8)	1540(9)	16(4)
N(7)	4768(17)	2912(11)	7891(10)	35(5)
N(8)	3010(14)	3911(11)	8095(11)	36(5)
N(9)	10576(15)	2127(11)	7093(10)	39(5)
N(10)	12470(15)	-288(10)	6741(11)	35(5)
N(11)	12337(15)	542(10)	8422(10)	34(5)
N(12)	10040(13)	1074(11)	6885(9)	30(5)
N(13)	9840(13)	1951(10)	8592(10)	32(5)
N(14)	5668(17)	4253(10)	8035(12)	43(6)
N(15)	3884(16)	5318(9)	8229(10)	30(5)
N(16)	12937(13)	786(8)	6936(9)	23(4)
N(17)	5353(16)	3087(9)	6440(10)	33(5)
C(1)	4340(20)	1361(13)	1296(11)	25(6)
C(2)	5000(30)	624(17)	1151(13)	79(11)
C(3)	4720(20)	106(12)	1010(15)	62(9)
C(4)	3610(30)	342(14)	1069(13)	53(8)
C(5)	2900(30)	1066(12)	1217(12)	53(9)
C(6)	994(18)	4276(14)	1849(12)	36(6)
C(7)	739(19)	5023(14)	1987(13)	45(7)
C(8)	1550(20)	5272(14)	1964(13)	48(7)
C(9)	2610(20)	4728(13)	1850(13)	53(9)
C(10)	2805(19)	3973(11)	1721(13)	33(6)
C(11)	4650(20)	1986(14)	1419(11)	41(7)
C(12)	5700(20)	1981(17)	1382(15)	62(8)
C(13)	5770(30)	2722(18)	1482(16)	65(9)
C(14)	4900(30)	3357(18)	1581(14)	65(9)
C(15)	3790(20)	3388(11)	1641(11)	29(6)
C(16)	2170(20)	718(12)	3123(11)	32(6)
C(17)	2770(20)	-27(12)	2997(16)	53(8)

C(18)	3770(20)	-213(16)	3031(14)	66(9)
C(19)	4202(19)	260(17)	3163(13)	59(9)
C(20)	3553(18)	1054(16)	3243(14)	69(11)
C(21)	3860(20)	1704(15)	3352(14)	40(7)
C(22)	4850(20)	1679(19)	3362(18)	74(10)
C(23)	4980(30)	2310(30)	3501(13)	100(15)
C(24)	4050(20)	3003(19)	3629(17)	66(9)
C(25)	3120(20)	2977(13)	3586(11)	32(7)
C(26)	2030(19)	3632(16)	3744(13)	43(7)
C(27)	720(30)	4923(16)	4021(12)	55(9)
C(28)	-30(20)	4668(14)	3954(15)	52(7)
C(29)	240(20)	3959(12)	3788(14)	51(8)
C(30)	1750(30)	4406(15)	3865(15)	76(11)
C(31)	170(20)	2378(15)	3544(15)	64(8)
C(32)	1064(19)	2653(11)	1455(15)	53(8)
C(33)	5647(19)	3186(14)	5651(12)	37(6)
C(34)	6590(20)	2772(13)	5214(13)	53(8)
C(35)	7400(30)	2208(14)	5489(15)	58(9)
C(36)	3250(20)	3472(12)	8803(11)	30(6)
C(37)	9427(17)	1835(11)	9396(11)	27(5)
C(38)	12930(20)	106(15)	6047(12)	44(7)
C(39)	4276(19)	5745(11)	6553(12)	39(6)
N(18)	6326(13)	4384(8)	6589(9)	23(4)
C(41)	5120(20)	4309(13)	8800(14)	45(8)
C(42)	4020(20)	4935(12)	8966(17)	47(8)
C(43)	4297(18)	2880(10)	8686(12)	26(6)
C(44)	6196(19)	2496(11)	6768(14)	29(6)
C(45)	4790(20)	2345(12)	9244(15)	46(7)
C(46)	5780(20)	1835(13)	8985(12)	34(6)
C(47)	2450(20)	3684(17)	9545(14)	53(8)
C(48)	12813(19)	1150(10)	8070(12)	27(6)
C(49)	13218(16)	1262(12)	7204(12)	23(5)
C(50)	12961(17)	1591(12)	8515(13)	41(7)
C(51)	11522(18)	-740(12)	8475(10)	31(6)
C(52)	5840(20)	2369(13)	7626(13)	32(6)
C(53)	6290(20)	1859(11)	8170(13)	36(6)
C(54)	7170(20)	2057(12)	6297(18)	52(8)
C(55)	3390(20)	5119(17)	9678(15)	51(8)
C(56)	5622(19)	3815(12)	9362(12)	36(6)
C(57)	6670(17)	3723(11)	7761(13)	21(5)
C(58)	7065(15)	3833(10)	6907(11)	18(5)
C(59)	8061(18)	3434(12)	6497(11)	28(5)
C(60)	6646(16)	4522(11)	5767(11)	20(5)
C(61)	10850(17)	2614(11)	7344(13)	27(5)
C(62)	11300(17)	3174(11)	6830(13)	30(6)
C(63)	10816(16)	2081(12)	6325(12)	30(6)
C(64)	11333(18)	2644(13)	5778(11)	39(7)
C(65)	12600(20)	1414(14)	9325(14)	49(8)
C(66)	11992(17)	852(15)	9737(12)	40(7)
C(67)	13760(18)	1764(11)	6690(12)	27(6)
C(68)	14038(17)	1752(12)	5870(13)	39(7)

C(69)	13790(20)	1208(12)	5629(13)	45(7)
C(70)	13234(18)	721(14)	6174(13)	33(6)
C(71)	13205(19)	-101(15)	5345(13)	46(7)
C(72)	12150(20)	-882(11)	6687(13)	44(7)
C(73)	12280(20)	-1098(16)	6007(15)	58(8)
C(74)	10424(16)	2518(12)	8218(11)	23(5)
C(75)	10498(16)	1494(12)	6174(11)	22(5)
C(76)	9004(17)	760(13)	8603(11)	42(7)
C(77)	9780(16)	471(13)	6766(13)	34(6)
C(78)	9880(20)	310(16)	6097(14)	61(9)
C(79)	2080(20)	4488(16)	8199(13)	39(7)
C(80)	2930(20)	5919(17)	8297(17)	65(8)
C(81)	2211(18)	6118(16)	8986(16)	63(9)
C(82)	2410(20)	5748(18)	9698(18)	79(10)
C(83)	8341(17)	3576(13)	5668(11)	29(6)
C(84)	11951(16)	450(14)	9255(14)	41(6)
C(85)	12850(20)	-744(19)	5355(16)	66(9)
C(86)	10350(20)	760(17)	5415(16)	59(8)
C(87)	10655(19)	1376(13)	5431(12)	35(6)
C(88)	9590(30)	2208(15)	9835(13)	66(10)
C(89)	10108(19)	2785(12)	9497(12)	34(6)
C(90)	10590(20)	2896(12)	8691(13)	41(7)
C(91)	6590(20)	3267(11)	9126(14)	39(7)
C(92)	7210(20)	3223(14)	8298(14)	42(6)
C(93)	7550(20)	4170(15)	5307(12)	48(7)
C(94)	11578(19)	3187(12)	6030(13)	37(6)
C(95)	1540(20)	4260(20)	9598(18)	80(11)
C(96)	1340(20)	4706(19)	8870(20)	84(11)
C(40)	3362(18)	4236(12)	6410(12)	35(6)

Table S9. Bond lengths [Å] and angles [deg] for **3**.

Ni(1)-N(6)	1.861(16)
Ni(1)-N(1)	1.89(2)
Ni(1)-N(5)	1.943(19)
Ni(1)-C(32)	1.98(2)
Ni(2)-N(2)	1.831(18)
Ni(2)-N(4)	1.893(19)
Ni(2)-N(3)	1.904(16)
Ni(2)-C(31)	1.96(3)
Ni(3)-N(9)	1.88(2)
Ni(3)-N(12)	1.894(16)
Ni(3)-C(76)	1.92(2)
Ni(3)-N(13)	1.940(18)
Ni(4)-N(11)	1.873(15)
Ni(4)-N(16)	1.910(18)
Ni(4)-N(10)	1.919(17)
Ni(4)-C(51)	2.00(2)
Ni(5)-N(7)	1.815(18)
Ni(5)-N(8)	1.85(2)
Ni(5)-N(17)	1.87(2)
Ni(5)-C(40)	1.907(19)
Ni(6)-N(14)	1.856(18)
Ni(6)-N(15)	1.92(2)
Ni(6)-N(18)	1.929(18)
Ni(6)-C(39)	1.949(19)
N(1)-C(6)	1.36(3)
N(1)-C(10)	1.38(2)
N(2)-C(21)	1.34(3)
N(2)-C(25)	1.36(2)
N(3)-C(16)	1.38(2)
N(3)-C(20)	1.38(3)
N(4)-C(29)	1.32(3)
N(4)-C(26)	1.47(3)
N(5)-C(5)	1.34(2)
N(5)-C(1)	1.35(3)
N(6)-C(11)	1.35(2)
N(6)-C(15)	1.41(2)
N(7)-C(43)	1.36(2)
N(7)-C(52)	1.43(3)
N(8)-C(79)	1.31(3)
N(8)-C(36)	1.41(2)
N(9)-C(61)	1.33(2)
N(9)-C(63)	1.35(2)
N(10)-C(38)	1.34(2)
N(10)-C(72)	1.37(2)
N(11)-C(48)	1.39(2)
N(11)-C(84)	1.41(3)
N(12)-C(75)	1.37(2)

N(12)-C(77)	1.38(2)
N(13)-C(37)	1.36(2)
N(13)-C(74)	1.42(3)
N(14)-C(41)	1.34(3)
N(14)-C(57)	1.37(3)
N(15)-C(80)	1.36(3)
N(15)-C(42)	1.39(3)
N(16)-C(70)	1.33(2)
N(16)-C(49)	1.34(2)
N(17)-C(33)	1.33(2)
N(17)-C(44)	1.45(2)
C(1)-C(2)	1.36(3)
C(1)-C(11)	1.47(3)
C(2)-C(3)	1.27(3)
C(3)-C(4)	1.40(3)
C(4)-C(5)	1.36(3)
C(6)-C(7)	1.36(3)
C(7)-C(8)	1.35(3)
C(8)-C(9)	1.41(3)
C(9)-C(10)	1.39(3)
C(10)-C(15)	1.37(3)
C(11)-C(12)	1.42(3)
C(12)-C(13)	1.47(3)
C(13)-C(14)	1.32(3)
C(14)-C(15)	1.48(3)
C(16)-C(17)	1.34(3)
C(17)-C(18)	1.32(3)
C(18)-C(19)	1.33(3)
C(19)-C(20)	1.42(3)
C(20)-C(21)	1.49(4)
C(21)-C(22)	1.35(3)
C(22)-C(23)	1.34(4)
C(23)-C(24)	1.44(4)
C(24)-C(25)	1.33(3)
C(25)-C(26)	1.52(3)
C(26)-C(30)	1.39(3)
C(27)-C(28)	1.34(3)
C(27)-C(30)	1.36(4)
C(28)-C(29)	1.31(3)
C(33)-C(34)	1.32(3)
C(34)-C(35)	1.36(3)
C(35)-C(54)	1.37(3)
C(36)-C(43)	1.43(3)
C(36)-C(47)	1.45(3)
C(37)-C(88)	1.32(3)
C(38)-C(71)	1.33(3)
C(38)-C(70)	1.44(3)
N(18)-C(58)	1.32(2)
N(18)-C(60)	1.39(2)
C(41)-C(56)	1.38(3)
C(41)-C(42)	1.51(3)

C(42)-C(55)	1.33(3)
C(43)-C(45)	1.39(3)
C(44)-C(54)	1.39(3)
C(44)-C(52)	1.45(3)
C(45)-C(46)	1.34(3)
C(46)-C(53)	1.40(3)
C(47)-C(95)	1.30(3)
C(48)-C(50)	1.41(3)
C(48)-C(49)	1.46(3)
C(49)-C(67)	1.34(3)
C(50)-C(65)	1.37(3)
C(52)-C(53)	1.33(3)
C(55)-C(82)	1.41(3)
C(56)-C(91)	1.34(3)
C(57)-C(92)	1.38(3)
C(57)-C(58)	1.44(3)
C(58)-C(59)	1.34(3)
C(59)-C(83)	1.40(2)
C(60)-C(93)	1.27(3)
C(61)-C(62)	1.36(3)
C(61)-C(74)	1.47(3)
C(62)-C(94)	1.37(3)
C(63)-C(64)	1.42(3)
C(63)-C(75)	1.44(3)
C(64)-C(94)	1.40(3)
C(65)-C(66)	1.44(3)
C(66)-C(84)	1.33(3)
C(67)-C(68)	1.42(3)
C(68)-C(69)	1.40(3)
C(69)-C(70)	1.35(3)
C(71)-C(85)	1.44(3)
C(72)-C(73)	1.35(3)
C(73)-C(85)	1.31(3)
C(74)-C(90)	1.38(3)
C(75)-C(87)	1.37(2)
C(77)-C(78)	1.29(3)
C(78)-C(86)	1.38(3)
C(79)-C(96)	1.33(3)
C(80)-C(81)	1.33(3)
C(81)-C(82)	1.37(3)
C(83)-C(93)	1.44(3)
C(86)-C(87)	1.36(3)
C(88)-C(89)	1.38(3)
C(89)-C(90)	1.37(3)
C(91)-C(92)	1.45(3)
C(95)-C(96)	1.43(4)
N(6)-Ni(1)-N(1)	83.7(7)
N(6)-Ni(1)-N(5)	82.0(8)
N(1)-Ni(1)-N(5)	165.5(9)
N(6)-Ni(1)-C(32)	173.2(9)

N(1)-Ni(1)-C(32)	98.3(8)
N(5)-Ni(1)-C(32)	95.7(9)
N(2)-Ni(2)-N(4)	83.2(10)
N(2)-Ni(2)-N(3)	81.3(10)
N(4)-Ni(2)-N(3)	164.3(9)
N(2)-Ni(2)-C(31)	173.3(9)
N(4)-Ni(2)-C(31)	93.5(10)
N(3)-Ni(2)-C(31)	101.6(10)
N(9)-Ni(3)-N(12)	82.2(9)
N(9)-Ni(3)-C(76)	173.2(9)
N(12)-Ni(3)-C(76)	100.3(9)
N(9)-Ni(3)-N(13)	83.0(9)
N(12)-Ni(3)-N(13)	165.1(8)
C(76)-Ni(3)-N(13)	94.2(9)
N(11)-Ni(4)-N(16)	82.8(8)
N(11)-Ni(4)-N(10)	160.9(9)
N(16)-Ni(4)-N(10)	79.5(8)
N(11)-Ni(4)-C(51)	98.8(8)
N(16)-Ni(4)-C(51)	176.3(8)
N(10)-Ni(4)-C(51)	98.5(8)
N(7)-Ni(5)-N(8)	81.9(9)
N(7)-Ni(5)-N(17)	83.3(9)
N(8)-Ni(5)-N(17)	165.1(7)
N(7)-Ni(5)-C(40)	174.0(8)
N(8)-Ni(5)-C(40)	99.8(9)
N(17)-Ni(5)-C(40)	94.8(9)
N(14)-Ni(6)-N(15)	82.3(9)
N(14)-Ni(6)-N(18)	80.4(9)
N(15)-Ni(6)-N(18)	162.3(7)
N(14)-Ni(6)-C(39)	173.4(8)
N(15)-Ni(6)-C(39)	95.2(9)
N(18)-Ni(6)-C(39)	101.6(9)
C(6)-N(1)-C(10)	113(2)
C(6)-N(1)-Ni(1)	132.0(15)
C(10)-N(1)-Ni(1)	114.9(16)
C(21)-N(2)-C(25)	115(2)
C(21)-N(2)-Ni(2)	122.5(17)
C(25)-N(2)-Ni(2)	122.5(18)
C(16)-N(3)-C(20)	113(2)
C(16)-N(3)-Ni(2)	130.7(16)
C(20)-N(3)-Ni(2)	115.7(18)
C(29)-N(4)-C(26)	110(2)
C(29)-N(4)-Ni(2)	134.5(19)
C(26)-N(4)-Ni(2)	115.1(16)
C(5)-N(5)-C(1)	118(2)
C(5)-N(5)-Ni(1)	127.0(18)
C(1)-N(5)-Ni(1)	114.7(16)
C(11)-N(6)-C(15)	128.6(19)
C(11)-N(6)-Ni(1)	118.3(15)
C(15)-N(6)-Ni(1)	113.1(13)
C(43)-N(7)-C(52)	117.1(18)

C(43)-N(7)-Ni(5)	122.6(17)
C(52)-N(7)-Ni(5)	120.3(14)
C(79)-N(8)-C(36)	115(2)
C(79)-N(8)-Ni(5)	131.2(16)
C(36)-N(8)-Ni(5)	114.1(15)
C(61)-N(9)-C(63)	124(2)
C(61)-N(9)-Ni(3)	120.5(15)
C(63)-N(9)-Ni(3)	115.0(16)
C(38)-N(10)-C(72)	115.1(19)
C(38)-N(10)-Ni(4)	118.8(15)
C(72)-N(10)-Ni(4)	125.8(16)
C(48)-N(11)-C(84)	113.4(16)
C(48)-N(11)-Ni(4)	114.3(13)
C(84)-N(11)-Ni(4)	131.9(16)
C(75)-N(12)-C(77)	111.0(17)
C(75)-N(12)-Ni(3)	117.3(14)
C(77)-N(12)-Ni(3)	131.6(15)
C(37)-N(13)-C(74)	118.5(18)
C(37)-N(13)-Ni(3)	130.1(16)
C(74)-N(13)-Ni(3)	111.1(13)
C(41)-N(14)-C(57)	125(2)
C(41)-N(14)-Ni(6)	116.7(18)
C(57)-N(14)-Ni(6)	118.1(16)
C(80)-N(15)-C(42)	112(2)
C(80)-N(15)-Ni(6)	129.5(16)
C(42)-N(15)-Ni(6)	118.7(17)
C(70)-N(16)-C(49)	124(2)
C(70)-N(16)-Ni(4)	117.3(15)
C(49)-N(16)-Ni(4)	117.9(14)
C(33)-N(17)-C(44)	113(2)
C(33)-N(17)-Ni(5)	131.5(17)
C(44)-N(17)-Ni(5)	115.6(14)
N(5)-C(1)-C(2)	120(2)
N(5)-C(1)-C(11)	113(2)
C(2)-C(1)-C(11)	127(2)
C(3)-C(2)-C(1)	126(3)
C(2)-C(3)-C(4)	113(2)
C(5)-C(4)-C(3)	124(2)
N(5)-C(5)-C(4)	119(3)
N(1)-C(6)-C(7)	128(2)
C(8)-C(7)-C(6)	118(2)
C(7)-C(8)-C(9)	118(2)
C(10)-C(9)-C(8)	120(2)
C(15)-C(10)-N(1)	112.2(19)
C(15)-C(10)-C(9)	125(2)
N(1)-C(10)-C(9)	123(2)
N(6)-C(11)-C(12)	119(2)
N(6)-C(11)-C(1)	112(2)
C(12)-C(11)-C(1)	129(2)
C(11)-C(12)-C(13)	117(2)
C(14)-C(13)-C(12)	121(3)

C(13)-C(14)-C(15)	125(3)
C(10)-C(15)-N(6)	115.6(19)
C(10)-C(15)-C(14)	134(2)
N(6)-C(15)-C(14)	110(2)
C(17)-C(16)-N(3)	130(2)
C(18)-C(17)-C(16)	113(2)
C(17)-C(18)-C(19)	126(3)
C(18)-C(19)-C(20)	119(2)
N(3)-C(20)-C(19)	119(3)
N(3)-C(20)-C(21)	112(2)
C(19)-C(20)-C(21)	129(2)
N(2)-C(21)-C(22)	124(2)
N(2)-C(21)-C(20)	108(2)
C(22)-C(21)-C(20)	128(3)
C(23)-C(22)-C(21)	121(3)
C(22)-C(23)-C(24)	118(3)
C(25)-C(24)-C(23)	117(3)
C(24)-C(25)-N(2)	126(3)
C(24)-C(25)-C(26)	125(2)
N(2)-C(25)-C(26)	109.1(19)
C(30)-C(26)-N(4)	118(2)
C(30)-C(26)-C(25)	132(2)
N(4)-C(26)-C(25)	110(2)
C(28)-C(27)-C(30)	115(3)
C(29)-C(28)-C(27)	120(3)
C(28)-C(29)-N(4)	132(3)
C(27)-C(30)-C(26)	125(3)
C(34)-C(33)-N(17)	124(2)
C(33)-C(34)-C(35)	126(2)
C(34)-C(35)-C(54)	115(2)
N(8)-C(36)-C(43)	114.5(19)
N(8)-C(36)-C(47)	117(2)
C(43)-C(36)-C(47)	128.2(18)
C(88)-C(37)-N(13)	122(2)
C(71)-C(38)-N(10)	125(2)
C(71)-C(38)-C(70)	125(2)
N(10)-C(38)-C(70)	110.4(19)
C(58)-N(18)-C(60)	114.9(17)
C(58)-N(18)-Ni(6)	117.7(13)
C(60)-N(18)-Ni(6)	127.4(13)
N(14)-C(41)-C(56)	118(2)
N(14)-C(41)-C(42)	116(2)
C(56)-C(41)-C(42)	126(2)
C(55)-C(42)-N(15)	128(2)
C(55)-C(42)-C(41)	126(2)
N(15)-C(42)-C(41)	106(2)
N(7)-C(43)-C(45)	124(2)
N(7)-C(43)-C(36)	106.8(17)
C(45)-C(43)-C(36)	130(2)
C(54)-C(44)-C(52)	125(2)
C(54)-C(44)-N(17)	122(2)

C(52)-C(44)-N(17)	112(2)
C(46)-C(45)-C(43)	119(2)
C(45)-C(46)-C(53)	119(2)
C(95)-C(47)-C(36)	124(2)
N(11)-C(48)-C(50)	122.7(19)
N(11)-C(48)-C(49)	114.7(15)
C(50)-C(48)-C(49)	122(2)
N(16)-C(49)-C(67)	120.3(19)
N(16)-C(49)-C(48)	109.9(18)
C(67)-C(49)-C(48)	129.8(18)
C(65)-C(50)-C(48)	118(2)
C(53)-C(52)-N(7)	118(2)
C(53)-C(52)-C(44)	133(2)
N(7)-C(52)-C(44)	108.8(18)
C(52)-C(53)-C(46)	123(2)
C(35)-C(54)-C(44)	120(2)
C(42)-C(55)-C(82)	116(2)
C(91)-C(56)-C(41)	119(2)
N(14)-C(57)-C(92)	119(2)
N(14)-C(57)-C(58)	112.2(18)
C(92)-C(57)-C(58)	128(2)
N(18)-C(58)-C(59)	124.9(19)
N(18)-C(58)-C(57)	111.5(18)
C(59)-C(58)-C(57)	123.6(18)
C(58)-C(59)-C(83)	118(2)
C(93)-C(60)-N(18)	126.8(19)
N(9)-C(61)-C(62)	122(2)
N(9)-C(61)-C(74)	109(2)
C(62)-C(61)-C(74)	128(2)
C(61)-C(62)-C(94)	119(2)
N(9)-C(63)-C(64)	114(2)
N(9)-C(63)-C(75)	116.2(19)
C(64)-C(63)-C(75)	129(2)
C(94)-C(64)-C(63)	122(2)
C(50)-C(65)-C(66)	123(2)
C(84)-C(66)-C(65)	113(2)
C(49)-C(67)-C(68)	117.4(19)
C(69)-C(68)-C(67)	120(2)
C(70)-C(69)-C(68)	120(2)
N(16)-C(70)-C(69)	118(2)
N(16)-C(70)-C(38)	114(2)
C(69)-C(70)-C(38)	128(2)
C(38)-C(71)-C(85)	115(2)
C(73)-C(72)-N(10)	125(2)
C(85)-C(73)-C(72)	116(2)
C(90)-C(74)-N(13)	118.3(18)
C(90)-C(74)-C(61)	126(2)
N(13)-C(74)-C(61)	115.7(19)
C(87)-C(75)-N(12)	127(2)
C(87)-C(75)-C(63)	124(2)
N(12)-C(75)-C(63)	109.1(17)

C(78)-C(77)-N(12)	127(2)
C(77)-C(78)-C(86)	117(3)
N(8)-C(79)-C(96)	129(3)
C(81)-C(80)-N(15)	124(3)
C(80)-C(81)-C(82)	122(2)
C(81)-C(82)-C(55)	117(3)
C(59)-C(83)-C(93)	117.7(19)
C(66)-C(84)-N(11)	129(2)
C(73)-C(85)-C(71)	123(2)
C(87)-C(86)-C(78)	122(2)
C(86)-C(87)-C(75)	115(2)
C(37)-C(88)-C(89)	121(2)
C(90)-C(89)-C(88)	119(2)
C(89)-C(90)-C(74)	121(2)
C(56)-C(91)-C(92)	123(2)
C(57)-C(92)-C(91)	115(2)
C(60)-C(93)-C(83)	117.3(19)
C(62)-C(94)-C(64)	118(2)
C(47)-C(95)-C(96)	117(3)
C(79)-C(96)-C(95)	117(3)

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.
The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni(1)	43(2)	14(2)	30(2)	-3(1)	-17(2)	-2(1)
Ni(2)	31(2)	34(2)	24(2)	4(1)	-6(2)	-16(2)
Ni(3)	28(2)	36(2)	23(2)	0(1)	-4(2)	-8(2)
Ni(4)	32(2)	27(2)	26(2)	-8(1)	-8(2)	-9(1)
Ni(5)	42(2)	40(2)	23(2)	0(2)	-11(2)	-25(2)
Ni(6)	28(2)	25(2)	24(2)	-3(1)	-6(2)	-7(1)
N(1)	42(14)	85(16)	0(9)	19(9)	11(10)	-60(13)
N(2)	15(12)	95(17)	10(9)	11(10)	-5(10)	-30(12)
N(3)	21(11)	6(9)	30(11)	-21(8)	30(9)	14(8)
N(4)	56(16)	30(12)	9(10)	-6(8)	12(10)	-3(11)
N(5)	41(13)	32(11)	8(9)	23(8)	-18(10)	9(10)
N(6)	6(9)	0(8)	33(10)	-18(7)	-13(9)	27(7)
N(7)	63(16)	43(12)	25(11)	-8(10)	-22(12)	-35(12)
N(8)	7(11)	51(13)	65(14)	-9(11)	-23(11)	-14(10)
N(9)	33(13)	58(14)	24(11)	8(10)	-8(11)	-24(11)
N(10)	37(13)	20(10)	43(13)	-33(10)	1(11)	6(9)
N(11)	47(14)	45(12)	32(11)	-25(10)	-16(11)	-18(11)
N(12)	12(11)	56(12)	2(8)	-31(9)	27(8)	0(9)
N(13)	0(10)	27(10)	25(10)	-19(8)	18(9)	32(8)
N(14)	62(16)	36(12)	61(15)	-9(11)	-50(14)	-15(11)
N(15)	58(15)	14(10)	35(11)	7(9)	-24(12)	-27(10)
N(16)	16(10)	11(9)	20(10)	-14(8)	15(9)	9(8)
N(17)	60(15)	15(10)	29(11)	6(8)	-1(11)	-35(10)
C(1)	64(18)	35(14)	13(11)	21(10)	-23(13)	-60(14)
C(2)	150(30)	47(19)	18(14)	-16(14)	-16(18)	0(20)
C(3)	70(20)	4(11)	80(20)	-46(13)	-11(18)	40(13)
C(4)	100(30)	37(16)	31(15)	-23(13)	-13(18)	-21(17)
C(5)	140(30)	5(12)	34(14)	2(11)	-25(17)	-46(15)
C(6)	6(13)	62(17)	40(14)	-43(13)	4(12)	4(12)
C(7)	18(15)	55(17)	61(17)	-58(14)	-4(14)	17(12)
C(8)	60(20)	33(15)	42(16)	8(12)	-28(16)	-1(15)
C(9)	120(30)	24(14)	65(18)	43(13)	-68(19)	-67(16)
C(10)	40(16)	0(11)	60(17)	13(10)	-22(14)	-13(11)
C(11)	33(17)	56(17)	8(11)	12(11)	7(12)	-10(14)
C(12)	32(18)	80(20)	58(19)	-9(16)	-4(16)	-11(16)
C(13)	60(20)	70(20)	90(20)	-20(19)	-40(20)	-18(19)
C(14)	70(20)	80(20)	45(18)	17(16)	-39(19)	-20(20)
C(15)	70(20)	12(11)	13(11)	3(9)	-26(13)	-17(12)
C(16)	66(19)	15(12)	16(11)	28(10)	-14(13)	-34(12)
C(17)	45(18)	0(11)	110(20)	-12(13)	-35(18)	8(11)
C(18)	60(20)	60(20)	35(16)	13(14)	-24(18)	13(17)

C(19)	36(17)	100(20)	49(17)	-15(15)	-58(16)	14(16)
C(20)	0(13)	63(19)	40(16)	32(14)	25(12)	42(13)
C(21)	44(18)	39(16)	52(17)	28(13)	-31(16)	-36(14)
C(22)	25(18)	100(30)	110(30)	-30(20)	-30(20)	-21(17)
C(23)	40(20)	260(50)	0(13)	20(20)	21(14)	-100(30)
C(24)	40(20)	100(20)	80(20)	-13(19)	-16(19)	-46(19)
C(25)	72(19)	43(15)	20(12)	36(11)	-34(14)	-69(15)
C(26)	18(15)	70(20)	33(15)	-3(14)	2(13)	-22(15)
C(27)	90(30)	39(17)	5(12)	-16(12)	18(15)	-8(18)
C(28)	40(19)	23(15)	70(20)	-28(13)	11(16)	9(13)
C(29)	60(20)	3(11)	53(17)	-4(11)	4(15)	13(12)
C(30)	180(40)	35(17)	52(18)	-18(15)	-10(20)	-90(20)
C(31)	90(20)	56(18)	55(18)	-3(15)	-13(18)	-45(18)
C(32)	70(20)	0(11)	90(20)	-3(12)	-30(18)	-4(12)
C(33)	34(16)	67(17)	12(12)	-34(12)	24(12)	-28(14)
C(34)	110(30)	20(13)	18(13)	-15(11)	-4(16)	-11(15)
C(35)	100(30)	29(15)	23(15)	-25(12)	32(16)	-33(16)
C(36)	70(19)	35(13)	10(12)	2(10)	-33(14)	-25(13)
C(37)	25(14)	28(12)	13(11)	8(10)	-4(11)	-4(10)
C(38)	52(19)	62(18)	0(11)	-7(12)	21(12)	-26(15)
C(39)	47(17)	28(13)	24(13)	7(10)	-12(13)	-1(12)
N(18)	23(11)	0(8)	32(11)	-9(7)	1(10)	8(7)
C(41)	100(20)	29(14)	34(15)	-3(12)	-43(17)	-34(15)
C(42)	80(20)	8(12)	70(20)	7(13)	-50(20)	-12(13)
C(43)	42(16)	2(10)	22(12)	23(9)	-17(12)	-5(10)
C(44)	42(16)	0(10)	57(16)	0(10)	-31(15)	-7(10)
C(45)	80(20)	15(13)	48(17)	11(12)	-16(17)	-29(14)
C(46)	59(19)	31(14)	3(11)	3(10)	2(13)	-19(13)
C(47)	60(20)	90(20)	27(15)	27(15)	-13(16)	-67(19)
C(48)	60(17)	0(10)	42(14)	-18(10)	-35(14)	-1(10)
C(49)	19(13)	30(13)	30(13)	-9(11)	-15(12)	-9(10)
C(50)	29(15)	39(15)	44(16)	23(12)	-22(14)	-11(12)
C(51)	41(16)	42(14)	6(11)	-12(10)	20(11)	-30(12)
C(52)	51(18)	26(13)	28(14)	12(11)	-15(14)	-30(13)
C(53)	58(18)	4(10)	60(17)	-2(11)	-34(16)	-12(11)
C(54)	25(16)	7(12)	110(30)	-27(14)	-9(18)	9(11)
C(55)	60(20)	80(20)	29(15)	-8(15)	-6(16)	-48(18)
C(56)	55(18)	27(13)	17(12)	-19(10)	2(13)	-4(12)
C(57)	7(12)	15(11)	39(14)	5(10)	-5(12)	-10(9)
C(58)	0(11)	7(10)	17(11)	11(8)	24(9)	-6(8)
C(59)	29(15)	41(14)	17(12)	-4(10)	9(11)	-29(12)
C(60)	4(12)	22(11)	4(10)	5(8)	24(9)	0(9)
C(61)	27(15)	7(11)	39(14)	6(10)	-13(13)	-1(10)
C(62)	38(16)	11(11)	34(14)	-15(10)	10(12)	-12(11)
C(63)	0(11)	17(12)	21(12)	20(10)	18(10)	14(9)
C(64)	37(16)	49(15)	7(11)	-19(11)	-7(12)	26(12)
C(65)	60(20)	55(17)	35(15)	7(13)	-43(16)	-5(15)
C(66)	14(14)	80(20)	0(11)	-23(12)	18(10)	2(13)
C(67)	44(16)	10(11)	24(12)	10(9)	-14(13)	-11(11)
C(68)	23(14)	28(13)	47(15)	39(11)	-23(13)	-6(11)
C(69)	100(20)	18(13)	23(13)	0(11)	-7(15)	-42(15)

C(70)	23(15)	52(16)	19(13)	-20(12)	4(12)	-6(12)
C(71)	34(17)	80(20)	28(14)	-21(14)	-5(13)	-18(15)
C(72)	90(20)	13(12)	39(15)	-31(11)	-19(15)	0(12)
C(73)	90(20)	90(20)	31(15)	-17(15)	-18(17)	-66(19)
C(74)	12(13)	21(12)	3(10)	9(9)	9(10)	12(10)
C(75)	11(12)	41(14)	12(11)	-13(10)	9(10)	-10(11)
C(76)	21(14)	69(17)	3(11)	13(11)	15(11)	-11(13)
C(77)	13(13)	57(16)	47(15)	-14(13)	-18(13)	-12(12)
C(78)	100(30)	90(20)	27(15)	-29(15)	-6(17)	-60(20)
C(79)	18(15)	90(20)	8(12)	-17(13)	37(11)	-46(15)
C(80)	50(20)	80(20)	56(19)	-23(17)	-10(18)	0(17)
C(81)	0(13)	90(20)	60(20)	-69(17)	21(14)	40(13)
C(82)	50(20)	100(20)	60(20)	-40(18)	-19(19)	27(19)
C(83)	14(12)	65(16)	10(11)	-49(11)	50(10)	-37(12)
C(84)	1(12)	64(17)	43(15)	-46(14)	16(12)	11(11)
C(85)	70(20)	110(30)	29(16)	-46(18)	5(16)	-30(20)
C(86)	42(19)	90(20)	39(17)	4(16)	-20(16)	-18(17)
C(87)	58(18)	48(15)	22(12)	-11(11)	-25(13)	-25(14)
C(88)	140(30)	54(18)	26(15)	18(13)	-66(19)	-34(19)
C(89)	59(18)	23(13)	10(12)	-17(10)	-6(13)	4(12)
C(90)	53(18)	20(13)	47(16)	-1(11)	-37(16)	11(12)
C(91)	70(20)	0(10)	37(15)	0(10)	-18(15)	-4(12)
C(92)	30(16)	51(16)	48(16)	-14(13)	0(14)	-22(13)
C(93)	43(18)	90(20)	0(11)	5(12)	4(12)	-32(16)
C(94)	51(18)	17(12)	34(14)	-15(11)	-6(14)	0(11)
C(95)	0(15)	170(30)	60(20)	-60(20)	13(15)	0(18)
C(96)	40(20)	130(30)	110(30)	-50(20)	-50(20)	-1(19)
C(40)	45(16)	35(13)	43(14)	-5(11)	-27(14)	-18(12)