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**A New Synthetic Route to Enantiomerically Pure Axially Chiral 2,2'-Bipyridine
N,N'-Dioxides. Highly Efficient Catalysts for Asymmetric Allylation of
Aldehydes with Allyl(trichloro)silanes**

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Supporting Information

X-ray crystallographic data for (*R*_{nap}*S*_{pyr})-6a

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Figure 1. ORTEP drawing of (*R*_{nap},*S*_{pyr})-**6a** with atom-numbering scheme

Table 1. Experimental Details

A. Crystal Data

Empirical Formula	$\text{N}_2\text{O}_4\text{C}_{53}\text{H}_{38}$
Formula Weight	766.89
Crystal Color, Habit	colorless, platelet
Crystal Dimensions	0.40 x 0.30 x 0.10 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 150.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	$a = 34.2(1) \text{ \AA}$ $b = 11.82(3) \text{ \AA}$ $c = 10.60(2) \text{ \AA}$ $V = 4280.2(2) \text{ \AA}^3$
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.190 g/cm ³
F_{000}	1608.00
$\mu(\text{MoK}\alpha)$	0.75 cm ⁻¹

B. Intensity Measurements

Diffractionmeter	Rigaku RAXIS-RAPID
Radiation	MoK α ($\lambda = 0.71075 \text{ \AA}$)
	graphite monochromated
Detector Aperture	270 mm x 256 mm
Data Images	74 exposures
ω oscillation Range ($\chi = 45.0, \phi = 0.0$)	130.0 - 190.0°
Exposure Rate	300.0 sec./°
ω oscillation Range ($\chi = 45.0, \phi = 180.0$)	0.0 - 162.0°
Exposure Rate	300.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm

$2\theta_{\max}$	50.4°
No. of Reflections Measured	Total: 22455
	Unique: 4320 ($R_{\text{int}} = 0.107$)
Corrections	Lorentz-polarization
	Secondary Extinction
	(coefficient: 5.69080e+002)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
Least Squares Weights	1
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 0.01\sigma(I)$)	3709
No. Variables	528
Reflection/Parameter Ratio	7.02
Residuals: R_1 ($I > 2.00\sigma(I)$)	0.089
Residuals: wR_2 ($I > 0.01\sigma(I)$)	0.220
Goodness of Fit Indicator	1.27
Max Shift/Error in Final Cycle	0.01
Maximum peak in Final Diff. Map	0.39 e/Å ³
Minimum peak in Final Diff. Map	-1.64 e/Å ³

Table 2. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$

atom	x	y	z	B_{eq}
O(1)	-1.0369(2)	-0.0299(7)	-0.6525(7)	6.5(2)
O(2)	-1.0062(2)	0.2134(7)	-0.5156(6)	5.6(2)
O(3)	-1.0016(2)	-0.0604(6)	-0.4774(6)	5.0(2)
O(5)	-1.0412(2)	0.1851(7)	-0.3409(7)	6.2(2)
N(1)	-0.8751(3)	0.0392(8)	-0.3663(8)	5.3(2)
N(2)	-0.8749(3)	0.1345(7)	-0.6194(9)	5.6(2)
C(1)	-0.9268(3)	-0.142(1)	-0.378(1)	5.6(3)
C(2)	-0.4226(7)	-0.081(2)	-0.491(3)	16.5(8)
C(3)	-0.4653(5)	-0.079(2)	-0.485(2)	9.5(4)
C(4)	-0.4975(5)	-0.116(1)	-0.389(2)	9.7(4)
C(5)	-0.5384(5)	-0.103(2)	-0.416(2)	10.4(5)
C(6)	-0.5506(6)	-0.055(2)	-0.541(2)	12.9(6)
C(7)	-1.0392(3)	0.2001(9)	-0.452(1)	4.8(3)
C(8)	-0.9318(3)	-0.0523(8)	-0.457(1)	4.9(2)
C(9)	-0.9068(3)	0.134(1)	-0.539(1)	5.1(3)
C(10)	-0.9653(3)	-0.0560(9)	-0.553(1)	4.7(2)
C(11)	-1.0709(3)	-0.0572(9)	-0.454(1)	4.5(2)
C(12)	-0.9356(3)	0.217(1)	-0.540(1)	5.1(3)
C(13)	-1.0366(3)	-0.0464(8)	-0.541(1)	4.4(2)
C(14)	-1.1010(3)	0.019(1)	-0.451(1)	5.2(3)
C(15)	-1.0692(4)	-0.155(1)	-0.374(1)	5.6(3)
C(16)	-0.9325(4)	0.303(1)	-0.629(1)	5.8(3)
C(17)	-1.1018(3)	0.1184(9)	-0.542(1)	4.7(2)
C(18)	-0.8363(4)	0.220(1)	-0.781(1)	5.9(3)
C(19)	-0.9706(3)	0.2160(9)	-0.443(1)	5.0(2)
C(20)	-0.9054(3)	0.0346(9)	-0.449(1)	4.9(2)
C(21)	-0.8729(3)	0.219(1)	-0.701(1)	5.7(3)
C(22)	-0.9011(3)	0.305(1)	-0.708(1)	5.7(3)
C(23)	-0.8692(3)	-0.047(1)	-0.285(1)	5.2(3)
C(24)	-1.1320(4)	0.005(1)	-0.359(1)	6.5(3)
C(25)	-0.8964(4)	-0.140(1)	-0.288(1)	6.3(3)
C(26)	-0.5195(5)	-0.030(2)	-0.608(2)	9.5(4)
C(27)	-0.8362(4)	-0.038(1)	-0.198(1)	5.8(3)
C(28)	-1.0755(3)	0.291(1)	-0.624(1)	6.0(3)
C(29)	-0.8000(4)	0.202(1)	-0.731(1)	6.6(3)
C(30)	-1.0742(3)	0.198(1)	-0.535(1)	5.2(3)
C(31)	-1.1629(4)	0.082(1)	-0.336(2)	8.6(4)

Table 2. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(32)	-1.0999(4)	-0.169(1)	-0.290(1)	6.8(4)
C(33)	-0.8039(4)	0.029(1)	-0.230(1)	7.1(4)
C(34)	-0.8353(4)	-0.095(1)	-0.087(1)	7.6(4)
C(35)	-1.1341(4)	0.121(1)	-0.628(1)	6.2(3)
C(36)	-0.8390(5)	0.254(1)	-0.910(1)	7.4(4)
C(37)	-0.7657(4)	0.207(1)	-0.800(2)	7.7(4)
C(38)	-0.8028(5)	0.262(1)	-0.978(1)	8.8(5)
C(39)	-0.7691(5)	-0.027(1)	-0.047(2)	9.9(6)
C(40)	-1.1945(5)	0.040(2)	-0.729(2)	10.4(5)
C(41)	-1.1631(5)	-0.107(2)	-0.188(1)	8.7(5)
C(42)	-0.8024(5)	-0.086(1)	-0.011(1)	9.5(5)
C(43)	-0.4822(5)	-0.040(2)	-0.591(2)	10.1(5)
C(44)	-1.1632(4)	0.035(1)	-0.642(1)	7.1(3)
C(45)	-1.1368(4)	0.214(1)	-0.715(1)	7.3(4)
C(46)	-1.1305(4)	-0.097(1)	-0.281(1)	7.4(4)
C(47)	-0.7684(5)	0.242(1)	-0.924(2)	9.6(5)
C(48)	-1.1081(4)	0.297(1)	-0.708(1)	8.0(4)
C(50)	-1.1680(6)	0.215(2)	-0.809(2)	10.9(6)
C(51)	-1.1961(6)	0.130(2)	-0.815(2)	12.2(7)
C(52)	-0.7696(4)	0.036(1)	-0.157(2)	9.1(5)
C(56)	-1.1910(6)	0.061(2)	-0.250(2)	11.6(7)
C(57)	-1.1911(6)	-0.036(2)	-0.177(2)	12.1(7)
H(1)	-0.7451(4)	0.049(1)	-0.169(2)	10.9(5)
H(2)	-0.8617(4)	-0.131(1)	-0.071(1)	9.2(4)
H(4)	-0.8989(3)	0.384(1)	-0.769(1)	6.9(3)
H(6)	-1.1621(4)	-0.029(1)	-0.589(1)	8.5(4)
H(8)	-0.9654(3)	-0.1366(9)	-0.607(1)	5.7(3)
H(9)	-0.9631(3)	0.0185(9)	-0.600(1)	5.7(3)
H(10)	-1.0524(4)	-0.208(1)	-0.390(1)	6.7(3)
H(11)	-0.9504(4)	0.351(1)	-0.628(1)	6.9(3)
H(13)	-0.9700(3)	0.2779(9)	-0.386(1)	6.1(3)
H(16)	-0.8631(5)	0.264(1)	-0.954(1)	8.9(4)
H(17)	-0.8023(5)	0.291(1)	-1.061(1)	10.5(5)
H(18)	-0.7453(5)	0.242(1)	-0.974(2)	11.6(6)
H(19)	-0.7410(4)	0.191(1)	-0.762(2)	9.3(4)
H(20)	-0.7980(4)	0.182(1)	-0.644(1)	7.9(4)
H(21)	-0.8942(4)	-0.198(1)	-0.227(1)	7.6(3)

Table 2. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

atom	x	y	z	B_{eq}
H(22)	-0.9449(3)	-0.203(1)	-0.381(1)	6.7(3)
H(23)	-0.8040(5)	-0.116(1)	0.072(1)	11.3(5)
H(24)	-0.7461(5)	-0.030(1)	0.003(2)	11.9(6)
H(25)	-0.8043(4)	0.070(1)	-0.307(1)	8.5(4)
H(26)	-1.1006(4)	-0.239(1)	-0.247(1)	8.2(4)
H(27)	-1.1640(5)	-0.175(2)	-0.140(1)	10.4(5)
H(28)	-1.2119(6)	-0.051(2)	-0.119(2)	14.6(8)
H(29)	-1.2098(6)	0.118(2)	-0.233(2)	13.9(7)
H(30)	-1.2127(5)	-0.020(2)	-0.741(2)	12.5(6)
H(31)	-1.2202(6)	0.144(2)	-0.856(2)	14.6(8)
H(32)	-1.1677(6)	0.265(2)	-0.879(2)	13.1(6)
H(33)	-1.1088(4)	0.355(1)	-0.771(1)	9.6(4)
H(34)	-1.0560(3)	0.349(1)	-0.619(1)	7.3(3)
H(35)	-0.9690(3)	0.1470(9)	-0.398(1)	6.1(3)
H(39)	-1.1643(4)	0.149(1)	-0.386(2)	10.3(5)

$$B_{\text{eq}} = 8/3 p^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$$

Table 3. Anisotropic Displacement Parameters

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	0.091(5)	0.098(6)	0.057(5)	0.003(5)	0.001(4)	-0.004(5)
O(2)	0.069(4)	0.091(5)	0.053(4)	-0.007(4)	0.005(4)	0.002(4)
O(3)	0.064(4)	0.070(4)	0.056(4)	-0.001(4)	-0.007(4)	-0.011(4)
O(5)	0.091(5)	0.091(6)	0.053(4)	0.011(5)	0.008(4)	0.002(4)
N(1)	0.075(5)	0.067(6)	0.061(5)	0.000(5)	-0.009(5)	0.002(5)
N(2)	0.079(6)	0.061(5)	0.074(6)	-0.001(5)	-0.007(5)	0.038(5)
C(1)	0.081(7)	0.056(6)	0.074(8)	-0.002(6)	-0.011(7)	-0.003(6)
C(7)	0.076(7)	0.055(6)	0.052(6)	0.012(6)	-0.001(6)	-0.002(6)
C(8)	0.088(7)	0.040(5)	0.059(6)	0.002(5)	-0.009(6)	-0.003(5)
C(9)	0.060(6)	0.073(7)	0.061(7)	-0.006(6)	0.004(6)	0.009(6)
C(10)	0.059(5)	0.053(6)	0.067(6)	-0.007(5)	0.005(5)	-0.006(6)
C(11)	0.067(6)	0.058(6)	0.045(5)	0.004(5)	-0.012(5)	0.003(5)
C(12)	0.058(6)	0.082(8)	0.053(6)	0.003(6)	-0.003(5)	-0.011(6)
C(13)	0.082(7)	0.037(5)	0.049(6)	0.007(5)	-0.009(6)	-0.006(5)
C(14)	0.066(6)	0.070(7)	0.061(6)	-0.006(6)	-0.009(6)	0.002(6)
C(15)	0.098(9)	0.060(7)	0.055(7)	-0.001(6)	0.003(7)	-0.007(6)
C(16)	0.094(8)	0.062(7)	0.064(7)	-0.002(6)	-0.006(7)	0.012(6)
C(17)	0.071(6)	0.059(6)	0.048(6)	0.004(6)	-0.002(5)	-0.001(5)
C(18)	0.095(9)	0.070(7)	0.058(7)	-0.024(7)	0.014(7)	-0.003(6)
C(19)	0.076(7)	0.048(6)	0.068(7)	-0.004(5)	-0.013(6)	-0.001(6)
C(20)	0.075(7)	0.061(6)	0.049(6)	0.003(6)	-0.003(6)	0.005(6)
C(21)	0.072(7)	0.076(8)	0.066(7)	-0.006(6)	0.004(6)	0.007(7)
C(22)	0.076(7)	0.066(7)	0.076(8)	-0.014(6)	0.000(7)	0.006(7)
C(23)	0.079(7)	0.066(7)	0.052(6)	0.009(6)	-0.004(6)	0.000(6)
C(24)	0.088(8)	0.083(8)	0.076(8)	-0.017(7)	0.005(7)	0.011(7)
C(25)	0.105(9)	0.079(8)	0.057(7)	0.010(8)	0.006(7)	0.021(7)
C(27)	0.083(8)	0.070(7)	0.067(7)	0.020(7)	-0.001(6)	0.022(6)
C(28)	0.086(8)	0.084(8)	0.059(7)	-0.003(7)	-0.009(6)	-0.002(7)
C(29)	0.074(8)	0.10(1)	0.073(8)	-0.011(7)	-0.005(7)	0.021(8)
C(30)	0.067(6)	0.067(7)	0.064(7)	0.014(6)	0.006(6)	-0.001(6)
C(31)	0.090(9)	0.10(1)	0.13(1)	0.031(9)	0.03(1)	-0.00(1)
C(32)	0.094(9)	0.084(9)	0.081(9)	0.011(8)	-0.022(8)	0.016(8)
C(33)	0.091(9)	0.10(1)	0.079(9)	-0.003(8)	0.002(8)	-0.005(9)
C(34)	0.077(8)	0.14(1)	0.073(8)	-0.001(8)	-0.025(7)	0.025(9)
C(35)	0.086(8)	0.087(9)	0.062(7)	0.014(7)	-0.007(7)	-0.012(7)
C(36)	0.13(1)	0.070(8)	0.081(9)	0.008(8)	-0.003(9)	0.013(7)
C(37)	0.070(8)	0.10(1)	0.12(1)	0.007(7)	-0.001(8)	0.03(1)

Table 3. Anisotropic Displacement Parameters (continued)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(38)	0.12(1)	0.12(1)	0.08(1)	0.03(1)	0.04(1)	0.03(1)
C(39)	0.14(1)	0.11(1)	0.13(1)	0.01(1)	-0.07(1)	-0.03(1)
C(40)	0.11(1)	0.12(1)	0.17(2)	0.00(1)	-0.08(1)	-0.01(1)
C(41)	0.11(1)	0.14(1)	0.08(1)	-0.01(1)	0.018(9)	0.02(1)
C(42)	0.17(1)	0.12(1)	0.07(1)	0.01(1)	-0.03(1)	0.01(1)
C(44)	0.097(9)	0.080(9)	0.091(9)	-0.011(8)	-0.018(8)	0.002(8)
C(45)	0.10(1)	0.09(1)	0.080(9)	-0.007(9)	-0.011(8)	0.010(9)
C(46)	0.079(8)	0.11(1)	0.09(1)	-0.008(8)	-0.001(8)	0.005(9)
C(47)	0.13(1)	0.10(1)	0.14(2)	0.03(1)	0.05(1)	0.03(1)
C(48)	0.11(1)	0.10(1)	0.09(1)	0.010(9)	-0.008(9)	0.045(9)
C(50)	0.17(2)	0.14(2)	0.10(1)	0.05(1)	-0.05(1)	0.03(1)
C(51)	0.17(2)	0.11(1)	0.19(2)	-0.00(1)	-0.08(2)	0.04(2)
C(52)	0.09(1)	0.13(1)	0.13(1)	0.01(1)	-0.03(1)	-0.02(1)
C(56)	0.13(1)	0.12(1)	0.19(2)	0.03(1)	0.07(1)	-0.02(2)
C(57)	0.14(2)	0.16(2)	0.17(2)	0.02(2)	0.08(1)	0.00(2)

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

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O(1)	C(13)	1.20(1)	O(2)	C(7)	1.32(1)
O(2)	C(19)	1.44(1)	O(3)	C(10)	1.48(1)
O(3)	C(13)	1.38(1)	O(5)	C(7)	1.20(1)
N(1)	C(20)	1.36(1)	N(1)	C(23)	1.35(1)
N(2)	C(9)	1.38(1)	N(2)	C(21)	1.33(1)
C(1)	C(8)	1.36(1)	C(1)	C(25)	1.41(2)
C(2)	C(3)	1.46(3)	C(3)	C(4)	1.56(2)
C(3)	C(43)	1.35(2)	C(4)	C(5)	1.44(2)
C(5)	C(6)	1.50(3)	C(6)	C(26)	1.31(2)
C(7)	C(30)	1.48(2)	C(8)	C(10)	1.53(1)
C(8)	C(20)	1.37(1)	C(9)	C(12)	1.39(1)
C(9)	C(20)	1.51(1)	C(11)	C(13)	1.50(2)
C(11)	C(14)	1.37(1)	C(11)	C(15)	1.43(1)
C(12)	C(16)	1.40(2)	C(12)	C(19)	1.57(1)
C(14)	C(17)	1.52(1)	C(14)	C(24)	1.45(2)
C(15)	C(32)	1.39(2)	C(16)	C(22)	1.36(2)
C(17)	C(30)	1.34(1)	C(17)	C(35)	1.43(2)
C(18)	C(21)	1.51(2)	C(18)	C(29)	1.37(2)
C(18)	C(36)	1.43(2)	C(21)	C(22)	1.40(2)
C(23)	C(25)	1.44(2)	C(23)	C(27)	1.46(2)
C(24)	C(31)	1.42(2)	C(24)	C(46)	1.45(2)
C(26)	C(43)	1.29(2)	C(27)	C(33)	1.40(2)
C(27)	C(34)	1.35(2)	C(28)	C(30)	1.46(2)
C(28)	C(48)	1.43(2)	C(29)	C(37)	1.38(2)
C(31)	C(56)	1.35(2)	C(32)	C(46)	1.35(2)
C(33)	C(52)	1.41(2)	C(34)	C(42)	1.39(2)
C(35)	C(44)	1.43(2)	C(35)	C(45)	1.44(2)
C(36)	C(38)	1.43(2)	C(37)	C(47)	1.38(2)
C(38)	C(47)	1.33(2)	C(39)	C(42)	1.39(2)
C(39)	C(52)	1.38(2)	C(40)	C(44)	1.41(2)
C(40)	C(51)	1.40(2)	C(41)	C(46)	1.49(2)
C(41)	C(57)	1.28(2)	C(45)	C(48)	1.39(2)
C(45)	C(50)	1.46(2)	C(50)	C(51)	1.39(2)
C(56)	C(57)	1.39(3)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(1)	H(22)	0.95(2)	C(10)	H(8)	1.11(2)
C(10)	H(9)	1.02(2)	C(15)	H(10)	0.87(1)
C(16)	H(11)	0.83(1)	C(19)	H(13)	0.95(1)
C(19)	H(35)	0.95(1)	C(22)	H(4)	1.13(2)
C(25)	H(21)	0.95(2)	C(28)	H(34)	0.95(2)
C(29)	H(20)	0.95(2)	C(31)	H(39)	0.95(2)
C(32)	H(26)	0.95(2)	C(33)	H(25)	0.95(2)
C(34)	H(2)	1.01(2)	C(36)	H(16)	0.95(2)
C(37)	H(19)	0.95(2)	C(38)	H(17)	0.95(2)
C(39)	H(24)	0.95(2)	C(40)	H(30)	0.95(2)
C(41)	H(27)	0.95(2)	C(42)	H(23)	0.95(2)
C(44)	H(6)	0.95(2)	C(47)	H(18)	0.95(2)
C(48)	H(33)	0.95(2)	C(50)	H(32)	0.95(3)
C(51)	H(31)	0.95(3)	C(52)	H(1)	0.86(2)
C(56)	H(29)	0.95(3)	C(57)	H(28)	0.95(3)

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(7)	O(2)	C(19)	117.0(8)	C(10)	O(3)	C(13)	117.1(7)
C(20)	N(1)	C(23)	119.8(1)	C(9)	N(2)	C(21)	116.6(1)
C(8)	C(1)	C(25)	120.1(1)	C(2)	C(3)	C(4)	136.6(2)
C(2)	C(3)	C(43)	113.4(2)	C(4)	C(3)	C(43)	109.9(2)
C(3)	C(4)	C(5)	121.4(2)	C(4)	C(5)	C(6)	119.5(2)
C(5)	C(6)	C(26)	109.6(2)	O(2)	C(7)	O(5)	124.5(1)
O(2)	C(7)	C(30)	113.1(9)	O(5)	C(7)	C(30)	122.3(1)
C(1)	C(8)	C(10)	118.9(1)	C(1)	C(8)	C(20)	117.4(1)
C(10)	C(8)	C(20)	123.6(1)	N(2)	C(9)	C(12)	123.3(1)
N(2)	C(9)	C(20)	111.7(9)	C(12)	C(9)	C(20)	125.1(1)
O(3)	C(10)	C(8)	105.5(8)	C(13)	C(11)	C(14)	123.2(1)
C(13)	C(11)	C(15)	113.6(1)	C(14)	C(11)	C(15)	123.2(1)
C(9)	C(12)	C(16)	117.8(1)	C(9)	C(12)	C(19)	122.0(1)
C(16)	C(12)	C(19)	120.2(1)	O(1)	C(13)	O(3)	120.6(1)
O(1)	C(13)	C(11)	128.1(1)	O(3)	C(13)	C(11)	111.3(8)
C(11)	C(14)	C(17)	120.4(1)	C(11)	C(14)	C(24)	119.3(1)
C(17)	C(14)	C(24)	120.2(1)	C(11)	C(15)	C(32)	116.5(1)
C(12)	C(16)	C(22)	119.4(1)	C(14)	C(17)	C(30)	119.8(1)
C(14)	C(17)	C(35)	116.0(1)	C(30)	C(17)	C(35)	124.1(1)
C(21)	C(18)	C(29)	122.0(1)	C(21)	C(18)	C(36)	119.3(1)
C(29)	C(18)	C(36)	118.3(1)	O(2)	C(19)	C(12)	107.2(8)
N(1)	C(20)	C(8)	124.8(1)	N(1)	C(20)	C(9)	113.6(9)
C(8)	C(20)	C(9)	121.5(1)	N(2)	C(21)	C(18)	114.5(1)
N(2)	C(21)	C(22)	123.4(1)	C(18)	C(21)	C(22)	122.0(1)
C(16)	C(22)	C(21)	119.5(1)	N(1)	C(23)	C(25)	117.8(1)
N(1)	C(23)	C(27)	117.6(1)	C(25)	C(23)	C(27)	124.7(1)
C(14)	C(24)	C(31)	125.7(1)	C(14)	C(24)	C(46)	116.8(1)
C(31)	C(24)	C(46)	117.5(1)	C(1)	C(25)	C(23)	120.0(1)
C(6)	C(26)	C(43)	134.9(2)	C(23)	C(27)	C(33)	119.8(1)
C(23)	C(27)	C(34)	121.8(1)	C(33)	C(27)	C(34)	118.3(1)
C(30)	C(28)	C(48)	117.7(1)	C(18)	C(29)	C(37)	123.8(1)
C(7)	C(30)	C(17)	127.9(1)	C(7)	C(30)	C(28)	113.3(1)
C(17)	C(30)	C(28)	118.6(1)	C(24)	C(31)	C(56)	121.8(2)
C(15)	C(32)	C(46)	123.7(1)	C(27)	C(33)	C(52)	124.0(1)
C(27)	C(34)	C(42)	119.0(1)	C(17)	C(35)	C(44)	125.9(1)
C(17)	C(35)	C(45)	118.6(1)	C(44)	C(35)	C(45)	115.3(1)
C(18)	C(36)	C(38)	116.4(1)	C(29)	C(37)	C(47)	117.2(1)
C(36)	C(38)	C(47)	122.1(1)	C(42)	C(39)	C(52)	119.5(2)
C(44)	C(40)	C(51)	118.8(2)	C(46)	C(41)	C(57)	124.6(2)
C(34)	C(42)	C(39)	122.8(2)	C(3)	C(43)	C(26)	124.6(2)
C(35)	C(44)	C(40)	124.7(1)	C(35)	C(45)	C(48)	117.5(1)
C(35)	C(45)	C(50)	119.5(1)	C(48)	C(45)	C(50)	122.9(2)
C(24)	C(46)	C(32)	120.4(1)	C(24)	C(46)	C(41)	114.7(1)
C(32)	C(46)	C(41)	124.8(2)	C(37)	C(47)	C(38)	121.8(2)
C(28)	C(48)	C(45)	123.3(1)	C(45)	C(50)	C(51)	121.8(2)
C(40)	C(51)	C(50)	119.6(2)	C(33)	C(52)	C(39)	116.1(2)
C(31)	C(56)	C(57)	122.3(2)	C(41)	C(57)	C(56)	119.1(2)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(8)	C(1)	H(22)	118.9(1)	C(25)	C(1)	H(22)	120.9(1)
O(3)	C(10)	H(8)	104.3(1)	C(8)	C(10)	H(8)	111.5(1)
O(3)	C(10)	H(9)	111.1(1)	C(8)	C(10)	H(9)	104.3(1)
H(8)	C(10)	H(9)	119.5(1)	C(11)	C(15)	H(10)	119.9(1)
C(32)	C(15)	H(10)	122.4(2)	C(12)	C(16)	H(11)	115.5(1)
C(22)	C(16)	H(11)	125.1(2)	O(2)	C(19)	H(13)	112.0(1)
C(12)	C(19)	H(13)	113.1(1)	O(2)	C(19)	H(35)	107.6(1)
C(12)	C(19)	H(35)	107.1(1)	H(13)	C(19)	H(35)	109.5(1)
C(16)	C(22)	H(4)	114.7(1)	C(21)	C(22)	H(4)	125.6(1)
C(1)	C(25)	H(21)	120.7(2)	C(23)	C(25)	H(21)	119.2(2)
C(30)	C(28)	H(34)	118.8(1)	C(48)	C(28)	H(34)	123.3(2)
C(18)	C(29)	H(20)	118.7(2)	C(37)	C(29)	H(20)	117.5(2)
C(24)	C(31)	H(39)	118.8(2)	C(56)	C(31)	H(39)	119.4(2)
C(15)	C(32)	H(26)	116.0(2)	C(46)	C(32)	H(26)	119.7(2)
C(27)	C(33)	H(25)	119.0(2)	C(52)	C(33)	H(25)	117.0(2)
C(27)	C(34)	H(2)	110.0(2)	C(42)	C(34)	H(2)	130.5(2)
C(18)	C(36)	H(16)	123.6(2)	C(38)	C(36)	H(16)	119.8(2)
C(29)	C(37)	H(19)	121.7(2)	C(47)	C(37)	H(19)	121.0(2)
C(36)	C(38)	H(17)	120.5(2)	C(47)	C(38)	H(17)	117.0(2)
C(42)	C(39)	H(24)	120.5(2)	C(52)	C(39)	H(24)	120.0(2)
C(44)	C(40)	H(30)	123.7(2)	C(51)	C(40)	H(30)	116.8(2)
C(46)	C(41)	H(27)	117.1(2)	C(57)	C(41)	H(27)	118.1(2)
C(34)	C(42)	H(23)	117.7(2)	C(39)	C(42)	H(23)	119.3(2)
C(35)	C(44)	H(6)	118.5(2)	C(40)	C(44)	H(6)	116.8(2)
C(37)	C(47)	H(18)	118.4(2)	C(38)	C(47)	H(18)	119.3(2)
C(28)	C(48)	H(33)	119.1(2)	C(45)	C(48)	H(33)	117.1(2)
C(45)	C(50)	H(32)	122.3(2)	C(51)	C(50)	H(32)	114.8(2)
C(40)	C(51)	H(31)	118.0(2)	C(50)	C(51)	H(31)	119.5(3)
C(33)	C(52)	H(1)	137.7(2)	C(39)	C(52)	H(1)	102.1(2)
C(31)	C(56)	H(29)	118.7(2)	C(57)	C(56)	H(29)	118.7(3)
C(41)	C(57)	H(28)	120.3(3)	C(56)	C(57)	H(28)	120.7(3)

Table 8. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(19)	O(2)	C(7)	O(5)	-3.5(2)	C(19)	O(2)	C(7)	C(30)	-179.8(1)
C(7)	O(2)	C(19)	C(12)	173.0(1)	C(13)	O(3)	C(10)	C(8)	170.2(1)
C(10)	O(3)	C(13)	O(1)	-1.1(2)	C(10)	O(3)	C(13)	C(11)	177.8(1)
C(23)	N(1)	C(20)	C(8)	0.9(2)	C(23)	N(1)	C(20)	C(9)	-176.6(1)
C(20)	N(1)	C(23)	C(25)	-1.6(2)	C(20)	N(1)	C(23)	C(27)	-180.0(1)
C(21)	N(2)	C(9)	C(12)	-0.7(2)	C(21)	N(2)	C(9)	C(20)	-178.8(1)
C(9)	N(2)	C(21)	C(18)	176.5(1)	C(9)	N(2)	C(21)	C(22)	-0.3(2)
C(25)	C(1)	C(8)	C(10)	-179.6(1)	C(25)	C(1)	C(8)	C(20)	2.6(2)
C(8)	C(1)	C(25)	C(23)	-3.4(2)	C(2)	C(3)	C(4)	C(5)	-178.8(4)
C(43)	C(3)	C(4)	C(5)	-1.7(4)	C(2)	C(3)	C(43)	C(26)	-179.5(3)
C(4)	C(3)	C(43)	C(26)	2.7(3)	C(3)	C(4)	C(5)	C(6)	0.8(4)
C(4)	C(5)	C(6)	C(26)	-0.6(4)	C(5)	C(6)	C(26)	C(43)	1.9(4)
O(2)	C(7)	C(30)	C(17)	125.1(2)	O(2)	C(7)	C(30)	C(28)	-49.2(2)
O(5)	C(7)	C(30)	C(17)	-51.2(2)	O(5)	C(7)	C(30)	C(28)	134.4(1)
C(1)	C(8)	C(10)	O(3)	62.6(2)	C(20)	C(8)	C(10)	O(3)	-119.7(2)
C(1)	C(8)	C(20)	N(1)	-1.4(2)	C(1)	C(8)	C(20)	C(9)	175.9(1)
C(10)	C(8)	C(20)	N(1)	-179.1(1)	C(10)	C(8)	C(20)	C(9)	-1.8(2)
N(2)	C(9)	C(12)	C(16)	1.8(2)	N(2)	C(9)	C(12)	C(19)	-177.4(1)
C(20)	C(9)	C(12)	C(16)	179.7(1)	C(20)	C(9)	C(12)	C(19)	0.4(2)
N(2)	C(9)	C(20)	N(1)	65.8(2)	N(2)	C(9)	C(20)	C(8)	-111.7(2)
C(12)	C(9)	C(20)	N(1)	-112.2(2)	C(12)	C(9)	C(20)	C(8)	70.2(2)
C(14)	C(11)	C(13)	O(1)	-49.7(2)	C(14)	C(11)	C(13)	O(3)	131.4(2)
C(15)	C(11)	C(13)	O(1)	130.4(2)	C(15)	C(11)	C(13)	O(3)	-48.5(2)
C(13)	C(11)	C(14)	C(17)	2.6(2)	C(13)	C(11)	C(14)	C(24)	-176.9(1)
C(15)	C(11)	C(14)	C(17)	-177.5(1)	C(15)	C(11)	C(14)	C(24)	3.0(2)
C(13)	C(11)	C(15)	C(32)	179.3(1)	C(14)	C(11)	C(15)	C(32)	-0.6(2)
C(9)	C(12)	C(16)	C(22)	-2.0(2)	C(19)	C(12)	C(16)	C(22)	177.3(1)
C(9)	C(12)	C(19)	O(2)	-122.0(2)	C(16)	C(12)	C(19)	O(2)	58.7(2)
C(11)	C(14)	C(17)	C(30)	-65.1(2)	C(11)	C(14)	C(17)	C(35)	117.3(2)
C(24)	C(14)	C(17)	C(30)	114.4(2)	C(24)	C(14)	C(17)	C(35)	-63.2(2)
C(11)	C(14)	C(24)	C(31)	174.1(2)	C(11)	C(14)	C(24)	C(46)	-4.9(2)
C(17)	C(14)	C(24)	C(31)	-5.5(3)	C(17)	C(14)	C(24)	C(46)	175.6(2)
C(11)	C(15)	C(32)	C(46)	0.3(3)	C(12)	C(16)	C(22)	C(21)	1.1(2)
C(14)	C(17)	C(30)	C(7)	5.0(2)	C(14)	C(17)	C(30)	C(28)	179.2(1)
C(35)	C(17)	C(30)	C(7)	-177.5(1)	C(35)	C(17)	C(30)	C(28)	-3.4(2)
C(14)	C(17)	C(35)	C(44)	-5.6(2)	C(14)	C(17)	C(35)	C(45)	179.1(2)
C(30)	C(17)	C(35)	C(44)	176.9(2)	C(30)	C(17)	C(35)	C(45)	1.6(3)

Table 8. Torsion angles (°) -- continued

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(29)	C(18)	C(21)	N(2)	-45.0(2)	C(29)	C(18)	C(21)	C(22)	131.9(2)
C(36)	C(18)	C(21)	N(2)	142.1(2)	C(36)	C(18)	C(21)	C(22)	-41.1(3)
C(21)	C(18)	C(29)	C(37)	-177.2(2)	C(36)	C(18)	C(29)	C(37)	-4.2(3)
C(21)	C(18)	C(36)	C(38)	174.8(2)	C(29)	C(18)	C(36)	C(38)	1.6(3)
N(2)	C(21)	C(22)	C(16)	0.0(2)	C(18)	C(21)	C(22)	C(16)	-176.5(2)
N(1)	C(23)	C(25)	C(1)	2.9(2)	C(27)	C(23)	C(25)	C(1)	-178.9(2)
N(1)	C(23)	C(27)	C(33)	-25.8(2)	N(1)	C(23)	C(27)	C(34)	156.4(2)
C(25)	C(23)	C(27)	C(33)	155.9(2)	C(25)	C(23)	C(27)	C(34)	-21.9(3)
C(14)	C(24)	C(31)	C(56)	178.8(2)	C(46)	C(24)	C(31)	C(56)	-2.2(3)
C(14)	C(24)	C(46)	C(32)	4.6(3)	C(14)	C(24)	C(46)	C(41)	-179.8(2)
C(31)	C(24)	C(46)	C(32)	-174.4(2)	C(31)	C(24)	C(46)	C(41)	1.2(3)
C(6)	C(26)	C(43)	C(3)	-3.4(5)	C(23)	C(27)	C(33)	C(52)	-174.9(2)
C(34)	C(27)	C(33)	C(52)	3.0(3)	C(23)	C(27)	C(34)	C(42)	177.6(2)
C(33)	C(27)	C(34)	C(42)	-0.3(3)	C(48)	C(28)	C(30)	C(7)	179.9(2)
C(48)	C(28)	C(30)	C(17)	5.0(3)	C(30)	C(28)	C(48)	C(45)	-5.1(3)
C(18)	C(29)	C(37)	C(47)	5.8(3)	C(24)	C(31)	C(56)	C(57)	0.7(4)
C(15)	C(32)	C(46)	C(24)	-2.4(3)	C(15)	C(32)	C(46)	C(41)	-177.5(2)
C(27)	C(33)	C(52)	C(39)	-0.5(3)	C(27)	C(34)	C(42)	C(39)	-5.0(3)
C(17)	C(35)	C(44)	C(40)	-179.4(2)	C(45)	C(35)	C(44)	C(40)	-3.9(3)
C(17)	C(35)	C(45)	C(48)	-1.3(3)	C(17)	C(35)	C(45)	C(50)	176.1(2)
C(44)	C(35)	C(45)	C(48)	-177.1(2)	C(44)	C(35)	C(45)	C(50)	0.3(3)
C(18)	C(36)	C(38)	C(47)	-1.0(3)	C(29)	C(37)	C(47)	C(38)	-5.0(3)
C(36)	C(38)	C(47)	C(37)	2.8(3)	C(52)	C(39)	C(42)	C(34)	7.5(3)
C(42)	C(39)	C(52)	C(33)	-4.6(3)	C(51)	C(40)	C(44)	C(35)	5.3(4)
C(44)	C(40)	C(51)	C(50)	-2.8(4)	C(57)	C(41)	C(46)	C(24)	1.6(4)
C(57)	C(41)	C(46)	C(32)	177.0(3)	C(46)	C(41)	C(57)	C(56)	-3.3(4)
C(35)	C(45)	C(48)	C(28)	3.3(3)	C(50)	C(45)	C(48)	C(28)	-174.1(2)
C(35)	C(45)	C(50)	C(51)	1.8(3)	C(48)	C(45)	C(50)	C(51)	179.1(2)
C(45)	C(50)	C(51)	C(40)	-0.6(4)	C(31)	C(56)	C(57)	C(41)	2.2(4)

Figure 2. ORTEP drawing of (*R**nap*,*S**pyr*)-**7a** with atom-numbering scheme

Table 9. Experimental Details

A. Crystal Data

Empirical Formula	N ₂ O ₄ C ₅₈ H ₄₂
Formula Weight	830.98
Crystal Color, Habit	colorless, block
Crystal Dimensions	0.40 X 0.20 X 0.10 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	3 stills @ 2.0 seconds
Detector Position	127.40 mm
Pixel Size	0.200 mm
Lattice Parameters	a = 8.9674(1) Å b = 20.8342(2) Å c = 23.2481(3) Å V = 4343.41(7) Å ³
Space Group	P2 ₁ 2 ₁ 2 ₁ (#19)
Z value	4
D _{calc}	1.271 g/cm ³
F ₀₀₀	1744.00
μ(MoKα)	0.79 cm ⁻¹

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71069 Å)
	graphite monochromated
Detector Aperture	270 mm x 256 mm
Data Images	74 exposures
ω oscillation Range (χ=45.0, φ=0.0)	130.0 - 190.0°
Exposure Rate	4.2 sec./°
Detector Swing Angle	0.00°
ω oscillation Range (χ=45.0, φ=180.0)	0.0 - 162.0°
Exposure Rate	4.2 sec./°
Detector Swing Angle	0.00°
Detector Position	127.40 mm
Pixel Size	0.200 mm
2θ _{max}	55.0°

No. of Reflections Measured

Total: 5495

Unique: 5463 ($R_{\text{int}} = 0.097$)

Corrections

Lorentz-polarization

Secondary Extinction

(coefficient: 6.22390×10^2)

C. Structure Solution and Refinement

Structure Solution

Direct Methods (SIR97)

Refinement

Full-matrix least-squares on F

Function Minimized

$\sum w (|F_o| - |F_c|)^2$

Least Squares Weights

$1/\sigma^2(F_o)$

Anomalous Dispersion

All non-hydrogen atoms

No. Observations ($I > 0.20\sigma(I)$)

5116

No. Variables

620

Reflection/Parameter Ratio

8.25

Residuals: R; R_w

0.072 ; 0.044

Goodness of Fit Indicator

1.13

Max Shift/Error in Final Cycle

0.00

Maximum peak in Final Diff. Map

$0.68 \text{ e}^-/\text{\AA}^3$

Minimum peak in Final Diff. Map

$-2.30 \text{ e}^-/\text{\AA}^3$

Table 10. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$

atom	x	y	z	B_{eq}
O(1)	0.8514(5)	0.4020(3)	0.1673(2)	5.9(1)
O(2)	1.0441(5)	0.4086(3)	0.2272(2)	7.1(1)
O(3)	0.6964(4)	0.3989(2)	0.3022(2)	3.23(9)
O(4)	0.6835(5)	0.3781(2)	0.3952(2)	6.0(1)
N(1)	0.6985(6)	0.2413(3)	0.2623(2)	4.2(1)
N(2)	0.5700(5)	0.3145(2)	0.1431(2)	3.2(1)
C(1)	0.7298(6)	0.2819(3)	0.2207(3)	3.8(2)
C(2)	0.8702(7)	0.2905(4)	0.1946(3)	5.7(2)
C(3)	0.9802(9)	0.2504(6)	0.2144(3)	10.0(3)
C(4)	0.950(1)	0.2072(5)	0.2564(4)	9.9(3)
C(5)	0.8085(9)	0.2019(4)	0.2824(3)	6.6(2)
C(6)	0.6008(6)	0.3210(2)	0.1996(3)	3.0(1)
C(7)	0.5141(7)	0.3617(3)	0.2333(2)	3.5(1)
C(8)	0.3928(6)	0.3919(3)	0.2100(3)	4.4(2)
C(9)	0.3592(7)	0.3828(3)	0.1536(3)	4.5(2)
C(10)	0.4485(6)	0.3444(3)	0.1196(3)	3.3(1)
C(11)	0.769(1)	0.1584(4)	0.3295(3)	6.5(2)
C(12)	0.845(1)	0.1014(5)	0.3377(3)	13.9(4)
C(13)	0.809(2)	0.0640(5)	0.3831(3)	15.2(4)
C(14)	0.698(1)	0.0780(4)	0.4186(3)	8.7(3)
C(15)	0.6223(9)	0.1340(3)	0.4092(4)	6.8(2)
C(16)	0.6576(8)	0.1745(3)	0.3648(4)	5.8(2)
C(17)	0.4191(6)	0.3318(3)	0.0589(3)	3.3(1)
C(18)	0.3238(7)	0.3703(3)	0.0278(3)	4.5(2)
C(19)	0.3009(8)	0.3606(3)	-0.0304(3)	5.0(2)
C(20)	0.3736(8)	0.3117(3)	-0.0581(3)	4.8(2)
C(21)	0.4729(8)	0.2719(3)	-0.0281(3)	4.6(2)
C(22)	0.4919(7)	0.2832(3)	0.0297(3)	3.7(1)
C(23)	0.9014(7)	0.3405(4)	0.1485(3)	8.3(3)
C(24)	0.5513(6)	0.3686(2)	0.2971(2)	3.6(1)
C(25)	0.9306(7)	0.4303(4)	0.2096(3)	4.8(2)
C(26)	0.7509(8)	0.4004(3)	0.3562(3)	4.0(2)
C(27)	0.8715(5)	0.5108(2)	0.2835(2)	2.2(1)
C(28)	0.8551(6)	0.4907(3)	0.2272(2)	3.6(1)
C(29)	0.7672(7)	0.5260(5)	0.1888(3)	7.2(2)
C(30)	0.6971(8)	0.5802(5)	0.2051(4)	9.1(3)
C(31)	0.7140(7)	0.6034(3)	0.2624(4)	6.0(2)

Table 10. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

atom	x	y	z	B_{eq}
C(32)	0.640(1)	0.6606(4)	0.2799(5)	9.8(3)
C(33)	0.655(1)	0.6814(5)	0.3332(6)	12.7(4)
C(34)	0.7401(7)	0.6486(3)	0.3733(5)	9.0(3)
C(35)	0.8112(6)	0.5942(3)	0.3565(3)	5.2(2)
C(36)	0.7992(6)	0.5689(3)	0.3008(3)	3.9(1)
C(37)	0.9607(6)	0.4755(2)	0.3272(2)	2.3(1)
C(38)	0.9032(7)	0.4268(3)	0.3594(2)	3.1(1)
C(39)	0.9875(8)	0.3972(4)	0.4030(3)	6.0(2)
C(40)	1.1294(9)	0.4141(4)	0.4121(3)	6.6(2)
C(41)	1.1971(6)	0.4635(3)	0.3805(2)	3.4(1)
C(42)	1.3473(7)	0.4839(4)	0.3874(3)	5.4(2)
C(43)	1.4071(7)	0.5320(4)	0.3568(3)	5.7(2)
C(44)	1.3201(7)	0.5645(3)	0.3161(3)	5.6(2)
C(45)	1.1769(6)	0.5457(3)	0.3079(3)	4.4(2)
C(46)	1.1121(6)	0.4952(2)	0.3375(2)	2.3(1)
C(47)	0.677(2)	0.7453(8)	0.0210(6)	13.9(6)
C(48)	0.631(1)	0.7779(5)	0.0701(6)	10.6(4)
C(49)	0.714(2)	0.7705(6)	0.1178(6)	12.3(5)
C(50)	0.833(2)	0.7317(6)	0.1152(4)	15.0(5)
C(51)	0.872(2)	0.7019(7)	0.0651(7)	17.3(7)
C(52)	0.791(2)	0.7039(9)	0.0153(8)	16.1(7)
C(53)	0.731(1)	0.5259(5)	0.0187(4)	9.4(3)
C(54)	0.6669(9)	0.4691(5)	0.0215(4)	7.5(3)
C(55)	0.748(1)	0.4168(4)	0.0167(6)	12.4(4)
C(56)	0.8991(9)	0.4210(4)	0.0135(4)	9.0(3)
C(57)	0.9691(8)	0.4763(4)	0.0139(3)	5.5(2)
C(58)	0.8859(9)	0.5297(4)	0.0164(5)	11.5(4)
H(1)	1.0781(9)	0.2544(6)	0.1992(3)	12.0(5)
H(2)	1.025(1)	0.1778(5)	0.2680(4)	11.8(5)
H(3)	0.3316(6)	0.4178(3)	0.2340(3)	5.3(2)
H(4)	0.2793(7)	0.4054(3)	0.1360(3)	5.4(2)
H(5)	0.916(1)	0.0871(5)	0.3102(3)	16.7(6)
H(6)	0.864(2)	0.0254(5)	0.3888(3)	18.2(7)
H(7)	0.681(1)	0.0513(4)	0.4511(3)	10.4(4)
H(8)	0.5402(9)	0.1439(3)	0.4335(4)	8.2(3)
H(9)	0.6015(8)	0.2125(3)	0.3583(4)	6.9(2)
H(10)	0.2733(7)	0.4051(3)	0.0457(3)	5.4(2)

Table 10. Atomic coordinates and $B_{\text{iso}}/B_{\text{eq}}$ (continued)

atom	x	y	z	B_{eq}
H(11)	0.2348(8)	0.3876(3)	-0.0513(3)	6.0(2)
H(12)	0.3574(8)	0.3048(3)	-0.0980(3)	5.7(2)
H(13)	0.5252(8)	0.2381(3)	-0.0467(3)	5.5(2)
H(14)	0.5552(7)	0.2554(3)	0.0510(3)	4.4(2)
H(15)	0.8494(7)	0.3285(4)	0.1146(3)	10.0(4)
H(16)	1.0054(7)	0.3417(4)	0.1409(3)	10.0(4)
H(17)	0.5530(6)	0.3280(2)	0.3157(2)	4.3(2)
H(18)	0.4778(6)	0.3950(2)	0.3146(2)	4.3(2)
H(19)	0.7542(7)	0.5102(5)	0.1509(3)	8.7(3)
H(20)	0.6378(8)	0.6028(5)	0.1779(4)	11.0(4)
H(21)	0.577(1)	0.6844(4)	0.2550(5)	11.8(5)
H(22)	0.608(1)	0.7205(5)	0.3443(6)	15.2(7)
H(23)	0.7450(7)	0.6654(3)	0.4113(5)	10.8(4)
H(24)	0.8709(6)	0.5721(3)	0.3838(3)	6.3(2)
H(25)	0.9461(8)	0.3643(4)	0.4264(3)	7.2(2)
H(26)	1.1883(9)	0.3928(4)	0.4402(3)	7.9(3)
H(27)	1.4074(7)	0.4622(4)	0.4149(3)	6.5(2)
H(28)	1.5076(7)	0.5444(4)	0.3634(3)	6.8(2)
H(29)	1.3631(7)	0.5985(3)	0.2945(3)	6.7(2)
H(30)	1.1183(6)	0.5684(3)	0.2806(3)	5.3(2)
H(31)	0.618(2)	0.7485(8)	-0.0127(6)	16.7(7)
H(32)	0.549(1)	0.8072(5)	0.0686(6)	12.7(4)
H(33)	0.678(2)	0.7871(6)	0.1534(6)	14.7(5)
H(34)	0.902(2)	0.7340(6)	0.1460(4)	18.0(6)
H(35)	0.949(2)	0.6704(7)	0.0657(7)	20.7(9)
H(36)	0.819(2)	0.6839(9)	-0.0198(8)	19.4(9)
H(37)	0.673(1)	0.5640(5)	0.0207(4)	11.2(4)
H(38)	0.5614(9)	0.4667(5)	0.0248(4)	9.0(3)
H(39)	0.697(1)	0.3769(4)	0.0148(6)	14.9(5)
H(40)	0.9557(9)	0.3824(4)	0.0139(4)	10.8(4)
H(41)	1.0739(8)	0.4788(4)	0.0084(3)	6.6(2)
H(42)	0.9347(9)	0.5702(4)	0.0178(5)	13.8(5)

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

Table 11. Anisotropic Displacement Parameters

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	0.042(3)	0.159(5)	0.023(2)	-0.047(3)	0.009(2)	-0.023(3)
O(2)	0.030(2)	0.165(5)	0.077(4)	0.007(3)	-0.011(3)	-0.071(4)
O(3)	0.042(2)	0.039(2)	0.041(2)	-0.018(2)	0.010(2)	-0.005(2)
O(4)	0.084(4)	0.095(4)	0.051(3)	-0.036(3)	0.006(3)	0.032(3)
N(1)	0.051(4)	0.058(3)	0.052(4)	0.012(3)	-0.010(3)	-0.031(3)
N(2)	0.025(2)	0.051(3)	0.045(3)	-0.011(2)	0.008(3)	-0.017(3)
C(1)	0.022(3)	0.078(5)	0.046(4)	0.006(3)	-0.008(3)	-0.048(4)
C(2)	0.029(4)	0.141(7)	0.045(4)	0.013(4)	-0.000(4)	-0.061(5)
C(3)	0.048(5)	0.28(1)	0.047(5)	0.055(8)	-0.009(5)	-0.088(8)
C(4)	0.101(8)	0.21(1)	0.062(6)	0.101(8)	-0.037(6)	-0.092(8)
C(5)	0.071(5)	0.123(7)	0.056(5)	0.069(5)	-0.025(5)	-0.068(5)
C(6)	0.040(3)	0.029(3)	0.044(4)	-0.018(3)	0.010(3)	-0.014(3)
C(7)	0.041(3)	0.054(4)	0.039(4)	-0.025(3)	0.019(3)	-0.023(3)
C(8)	0.026(3)	0.078(5)	0.064(5)	-0.001(3)	0.018(4)	-0.010(4)
C(9)	0.030(3)	0.092(5)	0.051(4)	0.000(4)	0.013(4)	-0.005(4)
C(10)	0.026(3)	0.047(3)	0.052(4)	-0.016(3)	0.009(3)	-0.013(3)
C(11)	0.107(7)	0.107(6)	0.031(4)	0.059(6)	-0.023(5)	-0.040(5)
C(12)	0.28(1)	0.21(1)	0.044(5)	0.20(1)	-0.021(8)	-0.033(7)
C(13)	0.39(2)	0.156(9)	0.036(5)	0.20(1)	-0.025(9)	-0.006(6)
C(14)	0.18(1)	0.089(6)	0.057(5)	0.065(7)	-0.039(7)	-0.038(5)
C(15)	0.074(5)	0.055(4)	0.129(8)	0.016(5)	-0.021(6)	-0.017(5)
C(16)	0.065(5)	0.048(4)	0.106(7)	0.012(4)	-0.014(5)	-0.020(5)
C(17)	0.029(3)	0.052(4)	0.045(4)	-0.018(3)	0.003(3)	-0.003(3)
C(18)	0.044(4)	0.054(4)	0.074(5)	0.004(4)	-0.010(4)	-0.003(4)
C(19)	0.058(5)	0.058(4)	0.072(5)	0.006(4)	-0.002(5)	0.026(4)
C(20)	0.082(5)	0.059(4)	0.040(4)	-0.016(4)	0.004(4)	0.006(4)
C(21)	0.069(5)	0.050(4)	0.054(4)	-0.010(4)	0.003(4)	0.016(4)
C(22)	0.046(4)	0.055(4)	0.039(4)	-0.007(3)	0.005(4)	0.000(3)
C(23)	0.034(4)	0.24(1)	0.042(5)	-0.051(6)	0.022(4)	-0.074(7)
C(24)	0.036(3)	0.044(3)	0.057(4)	-0.019(3)	0.021(3)	-0.021(3)
C(25)	0.031(3)	0.126(6)	0.024(4)	-0.032(4)	0.003(3)	-0.017(4)
C(26)	0.065(5)	0.039(3)	0.046(4)	-0.002(3)	-0.005(4)	0.008(4)
C(27)	0.020(2)	0.025(3)	0.038(3)	-0.009(2)	-0.006(3)	0.021(3)
C(28)	0.029(3)	0.080(5)	0.028(3)	-0.017(3)	0.003(3)	0.011(4)
C(29)	0.028(4)	0.20(1)	0.047(5)	-0.023(5)	-0.017(4)	0.070(6)
C(30)	0.029(4)	0.19(1)	0.131(9)	-0.002(6)	-0.012(6)	0.132(9)
C(31)	0.021(3)	0.064(4)	0.145(8)	-0.006(3)	-0.007(5)	0.068(6)

Table 11. Anisotropic Displacement Parameters (continued)

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(32)	0.024(4)	0.082(7)	0.27(2)	-0.009(5)	-0.026(8)	0.092(9)
C(33)	0.029(4)	0.055(5)	0.40(2)	0.021(4)	-0.04(1)	-0.04(1)
C(34)	0.028(4)	0.060(5)	0.25(1)	0.005(4)	-0.022(6)	-0.082(6)
C(35)	0.026(3)	0.037(3)	0.137(7)	0.008(3)	-0.022(4)	-0.024(4)
C(36)	0.020(3)	0.029(3)	0.098(5)	-0.004(3)	-0.021(4)	0.019(4)
C(37)	0.039(3)	0.018(2)	0.030(3)	0.006(2)	-0.008(3)	-0.008(2)
C(38)	0.046(3)	0.049(3)	0.023(3)	0.007(3)	-0.005(3)	0.009(3)
C(39)	0.074(5)	0.094(6)	0.061(5)	0.012(5)	-0.012(5)	0.040(5)
C(40)	0.081(6)	0.108(6)	0.063(5)	0.035(5)	-0.014(5)	0.052(5)
C(41)	0.035(3)	0.067(4)	0.027(3)	0.032(3)	-0.018(3)	-0.018(3)
C(42)	0.032(4)	0.117(7)	0.056(5)	0.030(4)	-0.024(4)	-0.031(5)
C(43)	0.026(3)	0.099(6)	0.091(6)	0.013(4)	-0.008(4)	-0.056(5)
C(44)	0.030(4)	0.072(5)	0.112(7)	-0.008(4)	-0.006(4)	-0.001(5)
C(45)	0.027(3)	0.047(4)	0.092(6)	-0.007(3)	-0.012(4)	-0.002(4)
C(46)	0.036(3)	0.029(3)	0.022(3)	0.004(3)	-0.006(3)	-0.015(2)
C(47)	0.24(2)	0.18(1)	0.11(1)	-0.11(1)	0.05(1)	-0.06(1)
C(48)	0.16(1)	0.087(7)	0.16(1)	-0.023(8)	0.01(1)	-0.011(9)
C(49)	0.20(1)	0.16(1)	0.11(1)	0.09(1)	0.07(1)	0.030(9)
C(50)	0.32(2)	0.19(1)	0.053(6)	0.16(1)	0.02(1)	0.045(7)
C(51)	0.34(3)	0.13(1)	0.19(2)	0.12(1)	0.06(2)	-0.03(1)
C(52)	0.23(2)	0.19(2)	0.20(2)	-0.05(1)	0.10(2)	-0.13(1)
C(53)	0.071(6)	0.109(7)	0.18(1)	0.001(6)	0.059(7)	0.017(8)
C(54)	0.054(5)	0.131(8)	0.101(7)	-0.030(6)	0.000(5)	0.019(7)
C(55)	0.081(7)	0.068(6)	0.32(2)	-0.030(6)	0.05(1)	0.031(9)
C(56)	0.061(5)	0.102(7)	0.18(1)	-0.019(6)	0.004(7)	0.067(7)
C(57)	0.038(4)	0.106(6)	0.064(5)	-0.015(5)	0.004(4)	0.015(5)
C(58)	0.069(6)	0.085(6)	0.28(1)	-0.009(6)	0.087(8)	-0.012(9)

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 12. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
O(1)	C(23)	1.427(8)	O(1)	C(25)	1.348(7)
O(2)	C(25)	1.187(7)	O(3)	C(24)	1.451(6)
O(3)	C(26)	1.348(7)	O(4)	C(26)	1.185(7)
N(1)	C(1)	1.316(8)	N(1)	C(5)	1.365(8)
N(2)	C(6)	1.347(6)	N(2)	C(10)	1.370(7)
C(1)	C(2)	1.409(8)	C(1)	C(6)	1.498(8)
C(2)	C(3)	1.37(1)	C(2)	C(23)	1.52(1)
C(3)	C(4)	1.36(1)	C(4)	C(5)	1.41(1)
C(5)	C(11)	1.46(1)	C(6)	C(7)	1.393(7)
C(7)	C(8)	1.370(8)	C(7)	C(24)	1.526(7)
C(8)	C(9)	1.357(8)	C(9)	C(10)	1.382(7)
C(10)	C(17)	1.458(7)	C(11)	C(12)	1.38(1)
C(11)	C(16)	1.340(9)	C(12)	C(13)	1.35(1)
C(13)	C(14)	1.33(1)	C(14)	C(15)	1.367(9)
C(15)	C(16)	1.369(9)	C(17)	C(18)	1.376(7)
C(17)	C(22)	1.384(7)	C(18)	C(19)	1.385(8)
C(19)	C(20)	1.370(8)	C(20)	C(21)	1.403(8)
C(21)	C(22)	1.375(7)	C(25)	C(28)	1.486(9)
C(26)	C(38)	1.475(8)	C(27)	C(28)	1.383(7)
C(27)	C(36)	1.430(7)	C(27)	C(37)	1.487(6)
C(28)	C(29)	1.399(8)	C(29)	C(30)	1.35(1)
C(30)	C(31)	1.43(1)	C(31)	C(32)	1.43(1)
C(31)	C(36)	1.376(8)	C(32)	C(33)	1.32(1)
C(33)	C(34)	1.39(1)	C(34)	C(35)	1.358(8)
C(35)	C(36)	1.403(8)	C(37)	C(38)	1.362(7)
C(37)	C(46)	1.438(7)	C(38)	C(39)	1.407(8)
C(39)	C(40)	1.34(1)	C(40)	C(41)	1.403(9)
C(41)	C(42)	1.421(8)	C(41)	C(46)	1.421(7)
C(42)	C(43)	1.341(9)	C(43)	C(44)	1.402(9)
C(44)	C(45)	1.356(7)	C(45)	C(46)	1.386(7)
C(47)	C(48)	1.39(1)	C(47)	C(52)	1.35(2)
C(48)	C(49)	1.35(1)	C(49)	C(50)	1.34(1)
C(50)	C(51)	1.37(1)	C(51)	C(52)	1.37(2)
C(53)	C(54)	1.32(1)	C(53)	C(58)	1.39(1)
C(54)	C(55)	1.31(1)	C(55)	C(56)	1.36(1)
C(56)	C(57)	1.312(9)	C(57)	C(58)	1.342(9)

Table 13. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.95(1)	C(4)	H(2)	0.95(1)
C(8)	H(3)	0.950(8)	C(9)	H(4)	0.950(7)
C(12)	H(5)	0.95(1)	C(13)	H(6)	0.95(1)
C(14)	H(7)	0.950(9)	C(15)	H(8)	0.950(9)
C(16)	H(9)	0.950(9)	C(18)	H(10)	0.950(8)
C(19)	H(11)	0.950(8)	C(20)	H(12)	0.950(8)
C(21)	H(13)	0.950(7)	C(22)	H(14)	0.950(7)
C(23)	H(15)	0.950(7)	C(23)	H(16)	0.950(7)
C(24)	H(17)	0.950(7)	C(24)	H(18)	0.950(7)
C(29)	H(19)	0.95(1)	C(30)	H(20)	0.95(1)
C(32)	H(21)	0.95(1)	C(33)	H(22)	0.95(1)
C(34)	H(23)	0.950(8)	C(35)	H(24)	0.950(8)
C(39)	H(25)	0.95(1)	C(40)	H(26)	0.950(9)
C(42)	H(27)	0.950(9)	C(43)	H(28)	0.950(9)
C(44)	H(29)	0.950(7)	C(45)	H(30)	0.950(7)
C(47)	H(31)	0.95(2)	C(48)	H(32)	0.95(1)
C(49)	H(33)	0.95(1)	C(50)	H(34)	0.95(1)
C(51)	H(35)	0.95(2)	C(52)	H(36)	0.95(2)
C(53)	H(37)	0.95(1)	C(54)	H(38)	0.95(1)
C(55)	H(39)	0.95(1)	C(56)	H(40)	0.950(9)
C(57)	H(41)	0.950(9)	C(58)	H(42)	0.950(9)

Table 14. Bond angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(23)	O(1)	C(25)	116.8(6)	C(24)	O(3)	C(26)	114.3(5)
C(1)	N(1)	C(5)	118.9(7)	C(6)	N(2)	C(10)	120.4(5)
N(1)	C(1)	C(2)	126.1(7)	N(1)	C(1)	C(6)	115.2(5)
C(2)	C(1)	C(6)	118.7(7)	C(1)	C(2)	C(3)	114.9(8)
C(1)	C(2)	C(23)	123.7(7)	C(3)	C(2)	C(23)	121.4(7)
C(2)	C(3)	C(4)	120.1(9)	C(3)	C(4)	C(5)	122.7(9)
N(1)	C(5)	C(4)	117.2(8)	N(1)	C(5)	C(11)	117.1(7)
C(4)	C(5)	C(11)	125.8(8)	N(2)	C(6)	C(1)	115.1(5)
N(2)	C(6)	C(7)	119.7(6)	C(1)	C(6)	C(7)	125.2(6)
C(6)	C(7)	C(8)	120.0(6)	C(6)	C(7)	C(24)	118.9(6)
C(8)	C(7)	C(24)	121.1(5)	C(7)	C(8)	C(9)	119.7(6)
C(8)	C(9)	C(10)	120.4(7)	N(2)	C(10)	C(9)	119.7(6)
N(2)	C(10)	C(17)	116.7(5)	C(9)	C(10)	C(17)	123.6(6)
C(5)	C(11)	C(12)	121.3(8)	C(5)	C(11)	C(16)	118.9(8)
C(12)	C(11)	C(16)	119.8(9)	C(11)	C(12)	C(13)	119.3(1)
C(12)	C(13)	C(14)	122.4(9)	C(13)	C(14)	C(15)	117.5(9)
C(14)	C(15)	C(16)	122.1(9)	C(11)	C(16)	C(15)	118.7(8)
C(10)	C(17)	C(18)	121.0(6)	C(10)	C(17)	C(22)	121.4(6)
C(18)	C(17)	C(22)	117.4(6)	C(17)	C(18)	C(19)	121.4(7)
C(18)	C(19)	C(20)	119.8(7)	C(19)	C(20)	C(21)	120.6(6)
C(20)	C(21)	C(22)	117.6(7)	C(17)	C(22)	C(21)	123.2(7)
O(1)	C(23)	C(2)	110.0(5)	O(3)	C(24)	C(7)	108.4(4)
O(1)	C(25)	O(2)	122.5(8)	O(1)	C(25)	C(28)	109.3(6)
O(2)	C(25)	C(28)	128.2(6)	O(3)	C(26)	O(4)	121.3(6)
O(3)	C(26)	C(38)	113.0(6)	O(4)	C(26)	C(38)	125.5(6)
C(28)	C(27)	C(36)	118.3(5)	C(28)	C(27)	C(37)	123.6(5)
C(36)	C(27)	C(37)	118.2(5)	C(25)	C(28)	C(27)	118.0(5)
C(25)	C(28)	C(29)	121.8(6)	C(27)	C(28)	C(29)	120.2(6)
C(28)	C(29)	C(30)	121.7(8)	C(29)	C(30)	C(31)	119.7(8)
C(30)	C(31)	C(32)	120.0(9)	C(30)	C(31)	C(36)	119.2(8)
C(32)	C(31)	C(36)	120.8(9)	C(31)	C(32)	C(33)	119.7(1)
C(32)	C(33)	C(34)	121.6(1)	C(33)	C(34)	C(35)	118.5(9)
C(34)	C(35)	C(36)	122.9(7)	C(27)	C(36)	C(31)	120.8(7)
C(27)	C(36)	C(35)	122.8(5)	C(31)	C(36)	C(35)	116.4(6)
C(27)	C(37)	C(38)	122.7(5)	C(27)	C(37)	C(46)	118.7(5)
C(38)	C(37)	C(46)	118.6(5)	C(26)	C(38)	C(37)	126.9(5)
C(26)	C(38)	C(39)	111.8(6)	C(37)	C(38)	C(39)	121.3(6)

Table 14. Bond angles(°) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(38)	C(39)	C(40)	120.7(7)	C(39)	C(40)	C(41)	121.5(7)
C(40)	C(41)	C(42)	124.8(6)	C(40)	C(41)	C(46)	118.5(6)
C(42)	C(41)	C(46)	116.7(6)	C(41)	C(42)	C(43)	122.9(7)
C(42)	C(43)	C(44)	119.8(6)	C(43)	C(44)	C(45)	118.8(7)
C(44)	C(45)	C(46)	123.2(7)	C(37)	C(46)	C(41)	119.4(5)
C(37)	C(46)	C(45)	122.0(5)	C(41)	C(46)	C(45)	118.5(5)
C(48)	C(47)	C(52)	128.4(2)	C(47)	C(48)	C(49)	117.0(1)
C(48)	C(49)	C(50)	118.2(1)	C(49)	C(50)	C(51)	121.5(1)
C(50)	C(51)	C(52)	124.6(2)	C(47)	C(52)	C(51)	110.0(1)
C(54)	C(53)	C(58)	119.3(9)	C(53)	C(54)	C(55)	119.7(8)
C(54)	C(55)	C(56)	120.4(9)	C(55)	C(56)	C(57)	122.1(9)
C(56)	C(57)	C(58)	117.6(7)	C(53)	C(58)	C(57)	120.6(9)

Table 15. Bond angles involving hydrogens(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	119.2(6)	C(4)	C(3)	H(1)	120.7(6)
C(3)	C(4)	H(2)	119.4(6)	C(5)	C(4)	H(2)	117.8(6)
C(7)	C(8)	H(3)	119.1(4)	C(9)	C(8)	H(3)	121.3(4)
C(8)	C(9)	H(4)	120.9(4)	C(10)	C(9)	H(4)	118.5(4)
C(11)	C(12)	H(5)	120.3(6)	C(13)	C(12)	H(5)	120.2(6)
C(12)	C(13)	H(6)	118.4(6)	C(14)	C(13)	H(6)	119.1(5)
C(13)	C(14)	H(7)	119.1(5)	C(15)	C(14)	H(7)	123.1(6)
C(14)	C(15)	H(8)	118.4(6)	C(16)	C(15)	H(8)	119.5(5)
C(11)	C(16)	H(9)	120.4(5)	C(15)	C(16)	H(9)	120.8(5)
C(17)	C(18)	H(10)	120.6(4)	C(19)	C(18)	H(10)	117.9(4)
C(18)	C(19)	H(11)	120.4(4)	C(20)	C(19)	H(11)	119.8(4)
C(19)	C(20)	H(12)	119.9(4)	C(21)	C(20)	H(12)	119.6(4)
C(20)	C(21)	H(13)	121.6(4)	C(22)	C(21)	H(13)	120.8(4)
C(17)	C(22)	H(14)	118.1(4)	C(21)	C(22)	H(14)	118.6(4)
O(1)	C(23)	H(15)	109.7(4)	C(2)	C(23)	H(15)	108.4(4)
O(1)	C(23)	H(16)	110.1(3)	C(2)	C(23)	H(16)	109.2(4)
H(15)	C(23)	H(16)	109.5(4)	O(3)	C(24)	H(17)	109.7(3)
C(7)	C(24)	H(17)	111.2(3)	O(3)	C(24)	H(18)	109.6(3)
C(7)	C(24)	H(18)	108.5(3)	H(17)	C(24)	H(18)	109.5(3)
C(28)	C(29)	H(19)	118.6(5)	C(30)	C(29)	H(19)	119.6(6)
C(29)	C(30)	H(20)	119.4(6)	C(31)	C(30)	H(20)	120.9(5)
C(31)	C(32)	H(21)	122.8(6)	C(33)	C(32)	H(21)	117.5(7)
C(32)	C(33)	H(22)	119.4(7)	C(34)	C(33)	H(22)	119.0(6)
C(33)	C(34)	H(23)	117.9(6)	C(35)	C(34)	H(23)	123.5(6)
C(34)	C(35)	H(24)	118.5(6)	C(36)	C(35)	H(24)	118.6(3)
C(38)	C(39)	H(25)	121.2(4)	C(40)	C(39)	H(25)	118.1(5)
C(39)	C(40)	H(26)	121.0(5)	C(41)	C(40)	H(26)	117.5(4)
C(41)	C(42)	H(27)	118.1(4)	C(43)	C(42)	H(27)	119.0(4)
C(42)	C(43)	H(28)	119.8(4)	C(44)	C(43)	H(28)	120.3(4)
C(43)	C(44)	H(29)	119.5(4)	C(45)	C(44)	H(29)	121.7(5)
C(44)	C(45)	H(30)	118.3(5)	C(46)	C(45)	H(30)	118.5(3)
C(48)	C(47)	H(31)	118.4(1)	C(52)	C(47)	H(31)	112.9(1)
C(47)	C(48)	H(32)	120.8(1)	C(49)	C(48)	H(32)	122.0(8)
C(48)	C(49)	H(33)	119.3(8)	C(50)	C(49)	H(33)	121.6(9)
C(49)	C(50)	H(34)	117.2(1)	C(51)	C(50)	H(34)	119.5(1)
C(50)	C(51)	H(35)	119.5(9)	C(52)	C(51)	H(35)	114.6(1)
C(47)	C(52)	H(36)	124.4(1)	C(51)	C(52)	H(36)	125.1(1)

Table 15. Bond angles involving hydrogens(°) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
C(54)	C(53)	H(37)	120.4(6)	C(58)	C(53)	H(37)	120.1(7)
C(53)	C(54)	H(38)	119.2(6)	C(55)	C(54)	H(38)	121.1(5)
C(54)	C(55)	H(39)	117.4(5)	C(56)	C(55)	H(39)	122.2(7)
C(55)	C(56)	H(40)	118.5(6)	C(57)	C(56)	H(40)	119.2(5)
C(56)	C(57)	H(41)	121.4(5)	C(58)	C(57)	H(41)	120.7(5)
C(53)	C(58)	H(42)	120.6(7)	C(57)	C(58)	H(42)	118.8(5)

Table 16. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(25)	O(1)	C(23)	C(2)	71.2(1)	C(23)	O(1)	C(25)	O(2)	6.5(1)
C(23)	O(1)	C(25)	C(28)	-174.9(8)	C(26)	O(3)	C(24)	C(7)	-172.0(7)
C(24)	O(3)	C(26)	O(4)	0.4(1)	C(24)	O(3)	C(26)	C(38)	175.4(6)
C(5)	N(1)	C(1)	C(2)	-1.6(2)	C(5)	N(1)	C(1)	C(6)	177.2(8)
C(1)	N(1)	C(5)	C(4)	-0.6(1)	C(1)	N(1)	C(5)	C(11)	178.8(9)
C(10)	N(2)	C(6)	C(1)	175.6(7)	C(10)	N(2)	C(6)	C(7)	-4.2(1)
C(6)	N(2)	C(10)	C(9)	1.7(1)	C(6)	N(2)	C(10)	C(17)	-176.7(7)
N(1)	C(1)	C(2)	C(3)	2.2(1)	N(1)	C(1)	C(2)	C(23)	-177.1(8)
C(6)	C(1)	C(2)	C(3)	-176.6(8)	C(6)	C(1)	C(2)	C(23)	4.2(1)
N(1)	C(1)	C(6)	N(2)	-121.4(8)	N(1)	C(1)	C(6)	C(7)	58.4(1)
C(2)	C(1)	C(6)	N(2)	57.5(1)	C(2)	C(1)	C(6)	C(7)	-122.7(1)
C(1)	C(2)	C(3)	C(4)	-0.6(2)	C(23)	C(2)	C(3)	C(4)	178.7(1)
C(1)	C(2)	C(23)	O(1)	51.3(1)	C(3)	C(2)	C(23)	O(1)	-127.8(1)
C(2)	C(3)	C(4)	C(5)	-1.4(2)	C(3)	C(4)	C(5)	N(1)	2.0(2)
C(3)	C(4)	C(5)	C(11)	-177.2(1)	N(1)	C(5)	C(11)	C(12)	153.7(1)
N(1)	C(5)	C(11)	C(16)	-25.9(1)	C(4)	C(5)	C(11)	C(12)	-27.1(2)
C(4)	C(5)	C(11)	C(16)	153.4(1)	N(2)	C(6)	C(7)	C(8)	4.0(1)
N(2)	C(6)	C(7)	C(24)	-179.7(6)	C(1)	C(6)	C(7)	C(8)	-175.8(8)
C(1)	C(6)	C(7)	C(24)	0.5(1)	C(6)	C(7)	C(8)	C(9)	-1.1(1)
C(24)	C(7)	C(8)	C(9)	-177.4(7)	C(6)	C(7)	C(24)	O(3)	65.8(9)
C(8)	C(7)	C(24)	O(3)	-118.0(9)	C(7)	C(8)	C(9)	C(10)	-1.4(1)
C(8)	C(9)	C(10)	N(2)	1.1(1)	C(8)	C(9)	C(10)	C(17)	179.4(7)
N(2)	C(10)	C(17)	C(18)	-164.4(7)	N(2)	C(10)	C(17)	C(22)	11.9(1)
C(9)	C(10)	C(17)	C(18)	17.3(1)	C(9)	C(10)	C(17)	C(22)	-166.3(8)
C(5)	C(11)	C(12)	C(13)	177.2(1)	C(16)	C(11)	C(12)	C(13)	-3.3(2)
C(5)	C(11)	C(16)	C(15)	-179.3(9)	C(12)	C(11)	C(16)	C(15)	1.2(2)
C(11)	C(12)	C(13)	C(14)	4.2(2)	C(12)	C(13)	C(14)	C(15)	-2.7(2)
C(13)	C(14)	C(15)	C(16)	0.4(2)	C(14)	C(15)	C(16)	C(11)	0.3(2)
C(10)	C(17)	C(18)	C(19)	176.8(8)	C(22)	C(17)	C(18)	C(19)	0.3(1)
C(10)	C(17)	C(22)	C(21)	-176.6(7)	C(18)	C(17)	C(22)	C(21)	-0.1(1)
C(17)	C(18)	C(19)	C(20)	0.2(1)	C(18)	C(19)	C(20)	C(21)	-0.9(1)
C(19)	C(20)	C(21)	C(22)	1.1(1)	C(20)	C(21)	C(22)	C(17)	-0.5(1)
O(1)	C(25)	C(28)	C(27)	150.2(7)	O(1)	C(25)	C(28)	C(29)	-28.5(1)
O(2)	C(25)	C(28)	C(27)	-31.3(1)	O(2)	C(25)	C(28)	C(29)	150.0(8)
O(3)	C(26)	C(38)	C(37)	36.3(1)	O(3)	C(26)	C(38)	C(39)	-146.3(7)
O(4)	C(26)	C(38)	C(37)	-148.9(8)	O(4)	C(26)	C(38)	C(39)	28.5(1)
C(36)	C(27)	C(28)	C(25)	179.9(7)	C(36)	C(27)	C(28)	C(29)	-1.3(1)

Table 16. Torsion angles (°) -- continued

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(37)	C(27)	C(28)	C(25)	0.2(1)	C(37)	C(27)	C(28)	C(29)	178.9(7)
C(28)	C(27)	C(36)	C(31)	0.8(1)	C(28)	C(27)	C(36)	C(35)	-178.7(8)
C(37)	C(27)	C(36)	C(31)	-179.4(7)	C(37)	C(27)	C(36)	C(35)	1.1(1)
C(28)	C(27)	C(37)	C(38)	-86.4(1)	C(28)	C(27)	C(37)	C(46)	96.2(9)
C(36)	C(27)	C(37)	C(38)	93.8(1)	C(36)	C(27)	C(37)	C(46)	-83.6(9)
C(25)	C(28)	C(29)	C(30)	179.1(1)	C(27)	C(28)	C(29)	C(30)	0.3(1)
C(28)	C(29)	C(30)	C(31)	1.1(2)	C(29)	C(30)	C(31)	C(32)	-179.8(1)
C(29)	C(30)	C(31)	C(36)	-1.6(2)	C(30)	C(31)	C(32)	C(33)	179.3(1)
C(36)	C(31)	C(32)	C(33)	1.0(2)	C(30)	C(31)	C(36)	C(27)	0.6(2)
C(30)	C(31)	C(36)	C(35)	-179.9(1)	C(32)	C(31)	C(36)	C(27)	178.8(1)
C(32)	C(31)	C(36)	C(35)	-1.6(2)	C(31)	C(32)	C(33)	C(34)	-0.5(2)
C(32)	C(33)	C(34)	C(35)	0.7(2)	C(33)	C(34)	C(35)	C(36)	-1.5(2)
C(34)	C(35)	C(36)	C(27)	-178.6(9)	C(34)	C(35)	C(36)	C(31)	1.9(2)
C(27)	C(37)	C(38)	C(26)	1.5(1)	C(27)	C(37)	C(38)	C(39)	-175.7(7)
C(46)	C(37)	C(38)	C(26)	178.9(7)	C(46)	C(37)	C(38)	C(39)	1.7(1)
C(27)	C(37)	C(46)	C(41)	177.7(6)	C(27)	C(37)	C(46)	C(45)	-0.2(1)
C(38)	C(37)	C(46)	C(41)	0.1(1)	C(38)	C(37)	C(46)	C(45)	-177.7(7)
C(26)	C(38)	C(39)	C(40)	179.1(9)	C(37)	C(38)	C(39)	C(40)	-3.3(1)
C(38)	C(39)	C(40)	C(41)	2.9(1)	C(39)	C(40)	C(41)	C(42)	-179.6(9)
C(39)	C(40)	C(41)	C(46)	-1.0(1)	C(40)	C(41)	C(42)	C(43)	-179.1(1)
C(46)	C(41)	C(42)	C(43)	2.4(1)	C(40)	C(41)	C(46)	C(37)	-0.5(1)
C(40)	C(41)	C(46)	C(45)	177.4(8)	C(42)	C(41)	C(46)	C(37)	178.2(7)
C(42)	C(41)	C(46)	C(45)	-3.9(1)	C(41)	C(42)	C(43)	C(44)	0.1(1)
C(42)	C(43)	C(44)	C(45)	-1.0(1)	C(43)	C(44)	C(45)	C(46)	-0.8(1)
C(44)	C(45)	C(46)	C(37)	-178.8(7)	C(44)	C(45)	C(46)	C(41)	3.3(1)
C(52)	C(47)	C(48)	C(49)	4.0(4)	C(48)	C(47)	C(52)	C(51)	-6.4(3)
C(47)	C(48)	C(49)	C(50)	-1.4(3)	C(48)	C(49)	C(50)	C(51)	2.3(3)
C(49)	C(50)	C(51)	C(52)	-5.7(3)	C(50)	C(51)	C(52)	C(47)	7.1(3)
C(58)	C(53)	C(54)	C(55)	-6.1(2)	C(54)	C(53)	C(58)	C(57)	3.5(2)
C(53)	C(54)	C(55)	C(56)	5.2(2)	C(54)	C(55)	C(56)	C(57)	-1.4(2)
C(55)	C(56)	C(57)	C(58)	-1.3(2)	C(56)	C(57)	C(58)	C(53)	0.3(2)