Supporting Information

Late Transition Metal Complexes of BINOL-Derived Salens: Synthesis, Structure, and Reactivity

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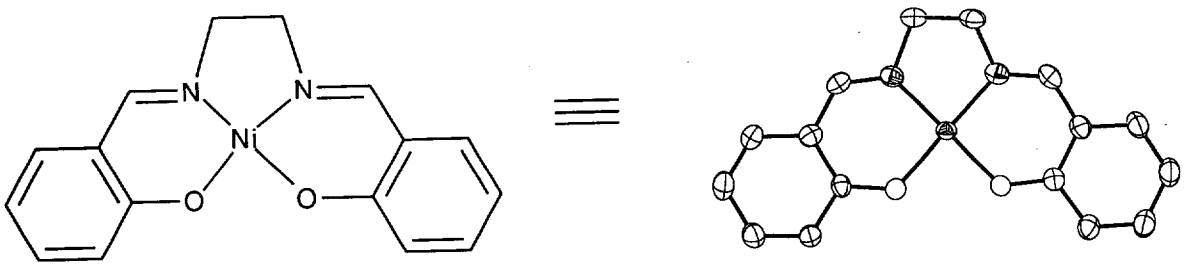
X-ray Structure Determination of Compound 801



Compound 801, $NiC_{16}H_{14}N_2O_2$, crystallizes in the orthorhombic space group Pbca (systematic absences hk0: h=odd, 0kl: k=odd, and h0l: l=odd) with a=7.42900(10)Å, b=13.7402(2)Å, c=26.0687(4)Å, V=2660.99(7)Å^3, Z=8 and d_{calc}=1.622 g/cm^3. X-ray intensity data were collected on an Rigaku R-AXIS IIc area detector employing graphite-monochromated Mo-K_α radiation (λ=0.71069 Å) at a temperature of 200°K. Indexing was performed from a series of 1° oscillation images with exposures of 4 minutes per frame. A hemispere of data was collected using 5° oscillation angles with exposures of 250 seconds per frame and a crystal-to-detector distance of 82 mm. Oscillation images were processed using bioteX[1], producing a listing of unaveraged F^2 and $\sigma(F^2)$ values which were then passed to the teXsan[2] program package for further processing and structure solution on a Silicon Graphics Indigo R4000 computer. A

total of 17857 reflections were measured over the ranges $5.92 \leq 2\theta \leq 54.96$ °, $-9 \leq h \leq 9$, $-15 \leq k \leq 17$, $-30 \leq l \leq 33$ yielding 3032 unique reflections ($R_{int} = 0.0524$). The intensity data were corrected for Lorentz and polarization effects but not for absorption.

The structure was solved by direct methods (SIR92[3]). Refinement was by full-matrix least squares based on F^2 using SHELXL-93[4]. All reflections were used during refinement (F^2's that were experimentally negative were replaced by $F^2 = 0$). The weighting scheme used was $w=1/[\sigma^2(F_o^2)+ 0.0307P^2 + 6.0940P]$ where $P = (F_o^2 + 2F_c^2)/3$. Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined isotropically. Refinement converged to $R_1=0.0629$ and $wR_2=0.1198$ for 2785 reflections for which $F > 4\sigma(F)$ and $R_1=0.0720$, $wR_2=0.1253$ and GOF = 1.304 for all 3032 unique, non-zero reflections and 246 variables[5]. The maximum Δ/σ in the final cycle of least squares was -0.001 and the two most prominent peaks in the final difference Fourier were +0.298 and -0.610 e/Å^3.

Table 1. lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in Table 2. Anisotropic thermal parameters are in Table 3. Tables 4. and 5. list bond distances and bond angles. Figure 1. is an ORTEP[6] representation of the molecule with 50% probability thermal ellipsoids displayed.

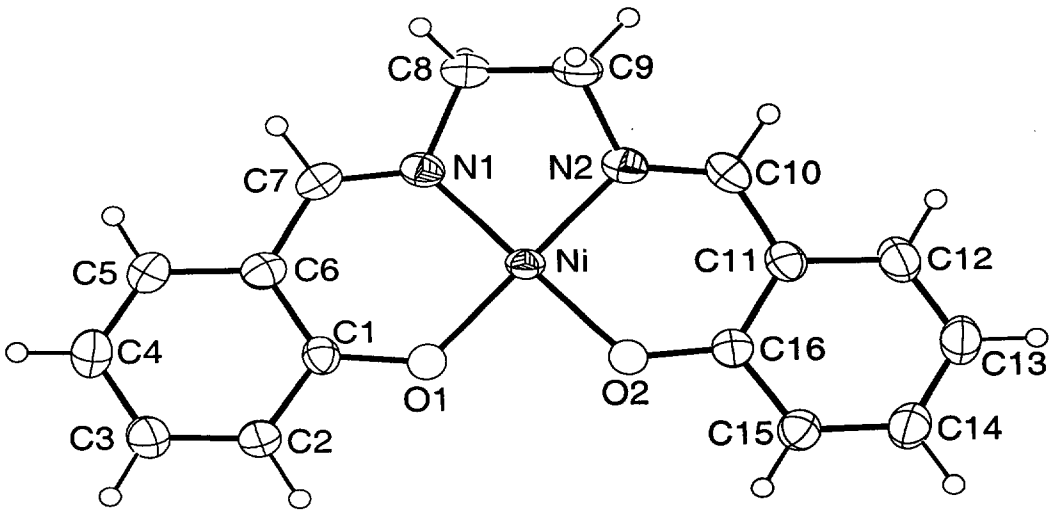


Figure 1. ORTEP drawing of the title compound with 50% probability thermal ellipsoids.

References

1. bioteX: A suite of Programs for the Collection, Reduction and Interpretation of Imaging Plate Data, Molecular Structure Corporation (1995).

2. teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

3. SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidoro, G. (1994). *J. Appl. Cryst.*, **27**, 435.

4. SHELXL-93: Program for the Refinement of Crystal Structures, Sheldrick, G.M. (1993), University of Göttingen, Germany.

5. $R_1 = \hat{A} \, ||F_o| - |F_c|| \, / \, \hat{A} \, |F_o|$

   $wR_2 = \{ \hat{A} \, w \, (F_o^2 - F_c^2)^2 \, / \, \hat{A} \, w(F_o^2)^2 \}^{1/2}$

   $GOF = \{ \hat{A} \, w \, (F_o^2 - F_c^2)^2 \, / \, (n - p) \}^{1/2}$
   where n = the number of reflections and p = the number of parameters refined.

6. "ORTEP-II: A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations". C.K. Johnson (1976) ORNL-5138.

Table 1. Summary of Structure Determination of Compound 801

Formula:	$NiC_{16}H_{14}N_2O_2$
Formula weight:	325.00
Crystal class:	orthorhombic
Space group:	Pbca (#61)
Z	8
Cell constants:	
a	7.42900(10)Å
b	13.7402(2)Å
c	26.0687(4)Å
V	2660.99(7)Å^3
μ	14.63 cm^{-1}
crystal size, mm	0.48 x 0.45 x 0.01
D_{calc}	1.622 g/cm^3
F(000)	1344
Radiation:	Mo-K_α (λ=0.71069Å)
2θ range	5.92 – 54.96 °
hkl collected:	-9≤ h ≤9; -15≤ k ≤17; -30≤ l ≤33
No. reflections measured:	17857
No. unique reflections:	3032 (R_{int}=0.0524)
No. observed reflections	2785 (F>4σ)
No. reflections used in refinement	3032
No. parameters	246
R indices (F>4σ)	R_1=0.0629
	wR_2=0.1198
R indices (all data)	R_1=0.0720
	wR_2=0.1253
GOF:	1.304
Final Difference Peaks, e/Å^3	+0.298, -0.610

Table 2. Refined Positional Parameters for Compound 801

Atom	x	y	z	U_{eq}, Å^2
Ni	0.69005(6)	0.54811(3)	0.51201(2)	0.0236(2)
C1	0.6231(5)	0.6290(3)	0.61074(14)	0.0258(7)
C2	0.5303(5)	0.6979(3)	0.6414(2)	0.0297(8)
C3	0.5406(6)	0.6951(3)	0.6940(2)	0.0365(9)
C4	0.6431(7)	0.6240(4)	0.7192(2)	0.0434(11)
C5	0.7290(6)	0.5550(3)	0.6903(2)	0.0383(10)
C6	0.7194(5)	0.5543(3)	0.6363(2)	0.0295(8)
C7	0.7976(5)	0.4748(3)	0.6085(2)	0.0286(8)
C8	0.8781(5)	0.3765(3)	0.5371(2)	0.0303(8)
C9	0.7973(6)	0.3610(3)	0.4846(2)	0.0330(8)
C10	0.7644(5)	0.4706(3)	0.4136(2)	0.0301(8)
C11	0.7025(5)	0.5556(3)	0.3877(2)	0.0300(8)
C12	0.7186(6)	0.5606(3)	0.3338(2)	0.0392(10)
C13	0.6409(7)	0.6345(4)	0.3060(2)	0.0445(11)
C14	0.5386(6)	0.7046(3)	0.3320(2)	0.0384(10)
C15	0.5229(6)	0.7025(3)	0.3844(2)	0.0317(8)
C16	0.6086(5)	0.6297(3)	0.41458(14)	0.0267(8)
N1	0.7918(4)	0.4643(2)	0.55938(12)	0.0265(6)
N2	0.7585(4)	0.4583(2)	0.46287(13)	0.0287(6)
O1	0.6153(4)	0.6376(2)	0.56055(10)	0.0286(6)
O2	0.5936(4)	0.6335(2)	0.46446(10)	0.0276(5)
H2	0.459(6)	0.748(3)	0.624(2)	0.035(11)
H3	0.483(7)	0.745(4)	0.713(2)	0.050(14)
H4	0.649(7)	0.622(4)	0.755(2)	0.06(2)
H5	0.798(7)	0.507(4)	0.706(2)	0.046(14)
H7	0.854(6)	0.426(3)	0.628(2)	0.031(11)
H8a	0.860(6)	0.323(3)	0.559(2)	0.027(10)
H8b	1.004(6)	0.390(3)	0.536(2)	0.035(11)
H9b	0.685(6)	0.323(3)	0.487(2)	0.033(11)
H9a	0.879(7)	0.323(4)	0.459(2)	0.046(13)
H10	0.820(6)	0.420(3)	0.394(2)	0.034(11)
H12	0.780(8)	0.509(4)	0.315(2)	0.06(2)
H13	0.658(8)	0.638(4)	0.269(2)	0.08(2)
H14	0.470(6)	0.754(3)	0.312(2)	0.043(13)
H15	0.454(6)	0.748(3)	0.403(2)	0.042(13)

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table 3. Refined Thermal Parameters (U's) for Compound 801

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni	0.0267(2)	0.0188(2)	0.0253(2)	0.0000(2)	0.0022(2)	0.0003(2)
C1	0.029(2)	0.026(2)	0.022(2)	-0.0016(14)	-0.0001(14)	-0.005(2)
C2	0.034(2)	0.026(2)	0.029(2)	0.001(2)	0.000(2)	0.000(2)
C3	0.045(2)	0.035(2)	0.030(2)	-0.001(2)	0.005(2)	0.001(2)
C4	0.054(3)	0.049(3)	0.027(2)	0.003(2)	-0.001(2)	0.000(2)
C5	0.047(3)	0.038(2)	0.030(2)	0.003(2)	-0.007(2)	0.006(2)
C6	0.028(2)	0.027(2)	0.033(2)	0.001(2)	-0.003(2)	-0.002(2)
C7	0.026(2)	0.026(2)	0.034(2)	0.007(2)	-0.002(2)	0.000(2)
C8	0.026(2)	0.024(2)	0.041(2)	-0.001(2)	0.001(2)	0.003(2)
C9	0.038(2)	0.021(2)	0.041(2)	0.000(2)	0.008(2)	0.002(2)
C10	0.029(2)	0.029(2)	0.032(2)	-0.008(2)	0.004(2)	-0.004(2)
C11	0.031(2)	0.031(2)	0.028(2)	-0.003(2)	0.001(2)	-0.004(2)
C12	0.047(3)	0.042(2)	0.029(2)	-0.005(2)	0.005(2)	-0.001(2)
C13	0.061(3)	0.046(3)	0.026(2)	0.001(2)	0.000(2)	-0.003(2)
C14	0.046(3)	0.039(2)	0.030(2)	0.003(2)	-0.006(2)	-0.004(2)
C15	0.035(2)	0.030(2)	0.030(2)	0.000(2)	-0.004(2)	-0.004(2)
C16	0.028(2)	0.025(2)	0.027(2)	0.0001(14)	0.0008(14)	-0.008(2)
N1	0.026(2)	0.021(2)	0.032(2)	-0.0014(13)	0.0033(12)	-0.0017(12)
N2	0.028(2)	0.023(2)	0.034(2)	-0.0021(14)	0.0034(14)	-0.0004(13)
O1	0.0355(14)	0.0257(13)	0.0245(12)	0.0008(11)	-0.0012(11)	0.0017(11)
O2	0.0334(14)	0.0253(12)	0.0241(12)	-0.0005(11)	0.0014(11)	0.0029(11)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

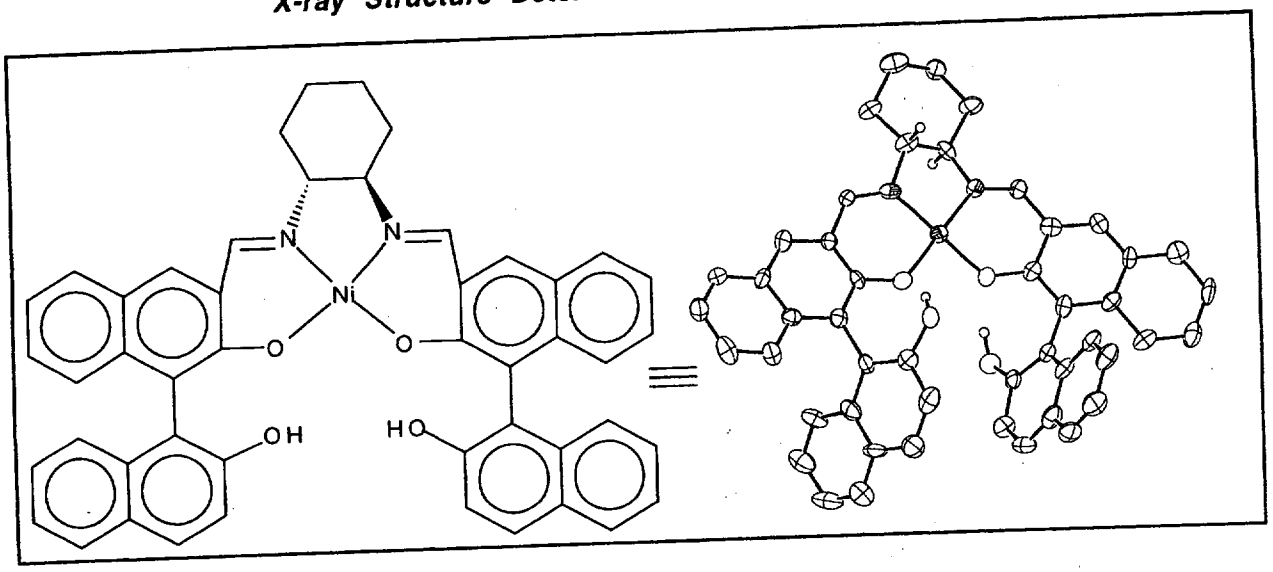
Table 4. Bond Distances in Compound 801, Å

Ni-O1	1.850(3)	Ni-N2	1.850(3)	Ni-N1	1.850(3)
Ni-O2	1.851(3)	C1-O1	1.315(4)	C1-C2	1.418(5)
C1-C6	1.418(5)	C2-C3	1.374(5)	C2-H2	0.99(4)
C3-C4	1.401(6)	C3-H3	0.95(5)	C4-C5	1.369(6)
C4-H4	0.93(5)	C5-C6	1.410(5)	C5-H5	0.93(5)
C6-C7	1.434(5)	C7-N1	1.290(5)	C7-H7	0.94(4)
C8-N1	1.484(5)	C8-C9	1.510(6)	C8-H8a	0.94(4)
C8-H8b	0.95(5)	C9-N2	1.481(5)	C9-H9b	0.98(4)
C9-H9a	1.05(5)	C10-N2	1.296(5)	C10-C11	1.426(6)
C10-H10	0.96(4)	C11-C12	1.411(5)	C11-C16	1.419(5)
C12-C13	1.375(6)	C12-H12	0.97(6)	C13-C14	1.400(7)
C13-H13	0.96(6)	C14-C15	1.373(5)	C14-H14	0.99(5)
C15-C16	1.423(5)	C15-H15	0.95(5)	C16-O2	1.306(4)

Table 5. Bond Angles in Compound 801, °

O1-Ni-N2	178.47(13)	O1-Ni-N1	94.58(13)	N2-Ni-N1	86.26(14)
O1-Ni-O2	85.45(11)	N2-Ni-O2	93.75(13)	N1-Ni-O2	178.59(13)
O1-C1-C2	118.7(3)	O1-C1-C6	123.7(3)	C2-C1-C6	117.6(3)
C3-C2-C1	121.2(4)	C3-C2-H2	121(3)	C1-C2-H2	118(3)
C2-C3-C4	121.1(4)	C2-C3-H3	118(3)	C4-C3-H3	120(3)
C5-C4-C3	118.6(4)	C5-C4-H4	121(3)	C3-C4-H4	121(3)
C4-C5-C6	122.0(4)	C4-C5-H5	120(3)	C6-C5-H5	118(3)
C5-C6-C1	119.4(4)	C5-C6-C7	119.3(4)	C1-C6-C7	121.2(3)
N1-C7-C6	125.0(3)	N1-C7-H7	118(3)	C6-C7-H7	118(3)
N1-C8-C9	107.3(3)	N1-C8-H8a	110(3)	C9-C8-H8a	112(3)
N1-C8-H8b	106(3)	C9-C8-H8b	112(3)	H8a-C8-H8b	108(4)
N2-C9-C8	107.2(3)	N2-C9-H9b	110(3)	C8-C9-H9b	111(3)
N2-C9-H9a	109(3)	C8-C9-H9a	115(3)	H9b-C9-H9a	106(4)
N2-C10-C11	124.4(4)	N2-C10-H10	117(3)	C11-C10-H10	118(3)
C12-C11-C16	119.9(4)	C12-C11-C10	118.9(4)	C16-C11-C10	120.8(3)
C13-C12-C11	121.6(4)	C13-C12-H12	118(3)	C11-C12-H12	120(3)
C12-C13-C14	118.8(4)	C12-C13-H13	120(4)	C14-C13-H13	121(4)
C15-C14-C13	120.9(4)	C15-C14-H14	119(3)	C13-C14-H14	120(3)
C14-C15-C16	121.8(4)	C14-C15-H15	123(3)	C16-C15-H15	115(3)
O2-C16-C11	124.2(3)	O2-C16-C15	118.9(3)	C11-C16-C15	116.8(3)
C7-N1-C8	117.7(3)	C7-N1-Ni	127.4(3)	C8-N1-Ni	114.9(2)
C10-N2-C9	119.4(3)	C10-N2-Ni	127.5(3)	C9-N2-Ni	113.0(3)
C1-O1-Ni	127.5(2)	C16-O2-Ni	127.5(2)		

X-ray Structure Determination of Compound 836



Compound 836, $NiC_{49}H_{38}N_2O_4Cl_6$, crystallizes in the monoclinic space group $P2_1$ (systematic absences 0k0: k=odd) with a=14.9158(5)Å, b=17.2044(8)Å, c=18.3523(6)Å, β=97.040(3)°, V=4674.0(3)Å^3, Z=4 and d_{calc}=1.407 g/cm^3. X-ray intensity data were collected on an Rigaku R-AXIS IIc area detector employing graphite-monochromated Mo-K_α radiation (λ=0.71069 Å) at a temperature of 200°K. Indexing was performed from a series of 1° oscillation images with exposures of 200 seconds per frame. A hemisphere of data was collected using 5° oscillation angles with exposures of 1500 seconds per frame and a crystal-to-detector distance of 82 mm. Oscillation images were processed using bioteX[1], producing a listing of unaveraged F^2 and $\sigma(F^2)$ values which were then passed to the teXsan[2] program package for further processing and structure solution on a Silicon Graphics Indigo R4000 computer. A total of 19661 reflections were measured over the ranges $5.06 \le 2\theta \le 50.7$ °, $-17 \le h \le 17$, $-19 \le k \le 20$, $-21 \le l \le 22$ yielding 13389 unique reflections (R_{int} = 0.0650). The intensity data were corrected for Lorentz and polarization effects but not for absorption.

The structure was solved by direct methods (SIR92[3]). The asymmetric unit includes six molecules of disordered methylene chloride solvent. The data were corrected for the presence of disordered solvent using SQUEEZE[4]. Refinement was by full-matrix least squares based on F^2 using SHELXL-93[5]. All reflections were used during refinement (F^2's that were experimentally negative were replaced by F^2 = 0). The weighting scheme used was $w=1/[\sigma^2(F_o^2)+ 0.1035P^2 + 14.8947P]$ where $P = (F_o^2$

+ $2F_c^2$)/3 . Non-hydrogen atoms were refined anisotropically and hydrogen atoms were refined using a "riding" model. Refinement converged to R_1=0.0948 and wR_2=0.2276 for 10993 reflections for which F > 4σ(F) and R_1=0.1100, wR_2=0.2414 and GOF = 1.075 for all 13389 unique, non-zero reflections and 992 variables[6]. The maximum Δ/σ in the final cycle of least squares was 0.005 and the two most prominent peaks in the final difference Fourier were +0.422 and -0.386 e/Å^3.

Table 1. lists cell information, data collection parameters, and refinement data. Final positional and equivalent isotropic thermal parameters are given in Table 2. Anisotropic thermal parameters are in Table 3. Tables 4. and 5. list bond distances and bond angles. Figures 1. and 2 are ORTEP[7] representations of the molecule with 30% probability thermal ellipsoids displayed.

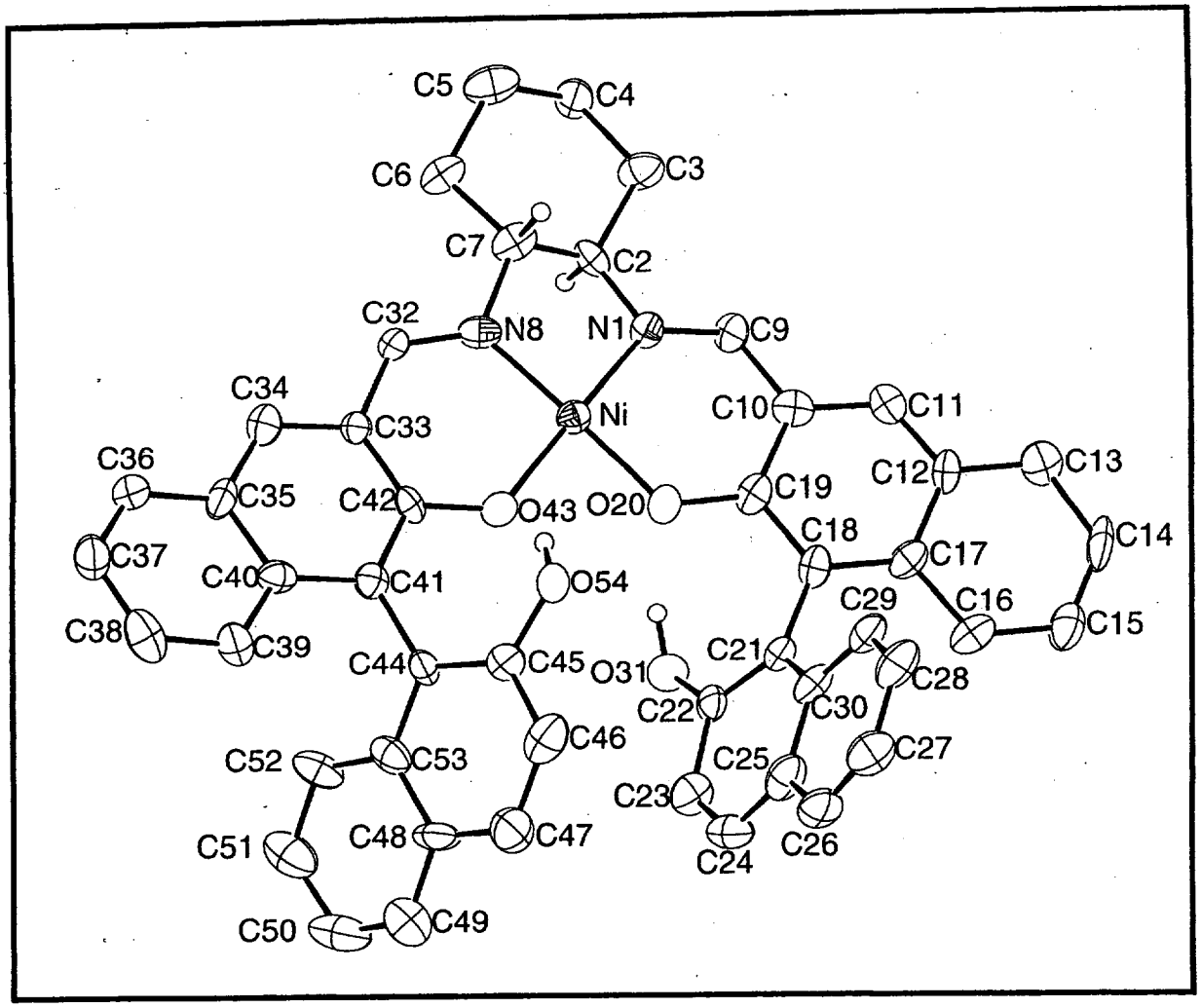


Figure 1. ORTEP drawing of molecule no. 1 of the asymmetric unit with 30% probability thermal ellipsoids.

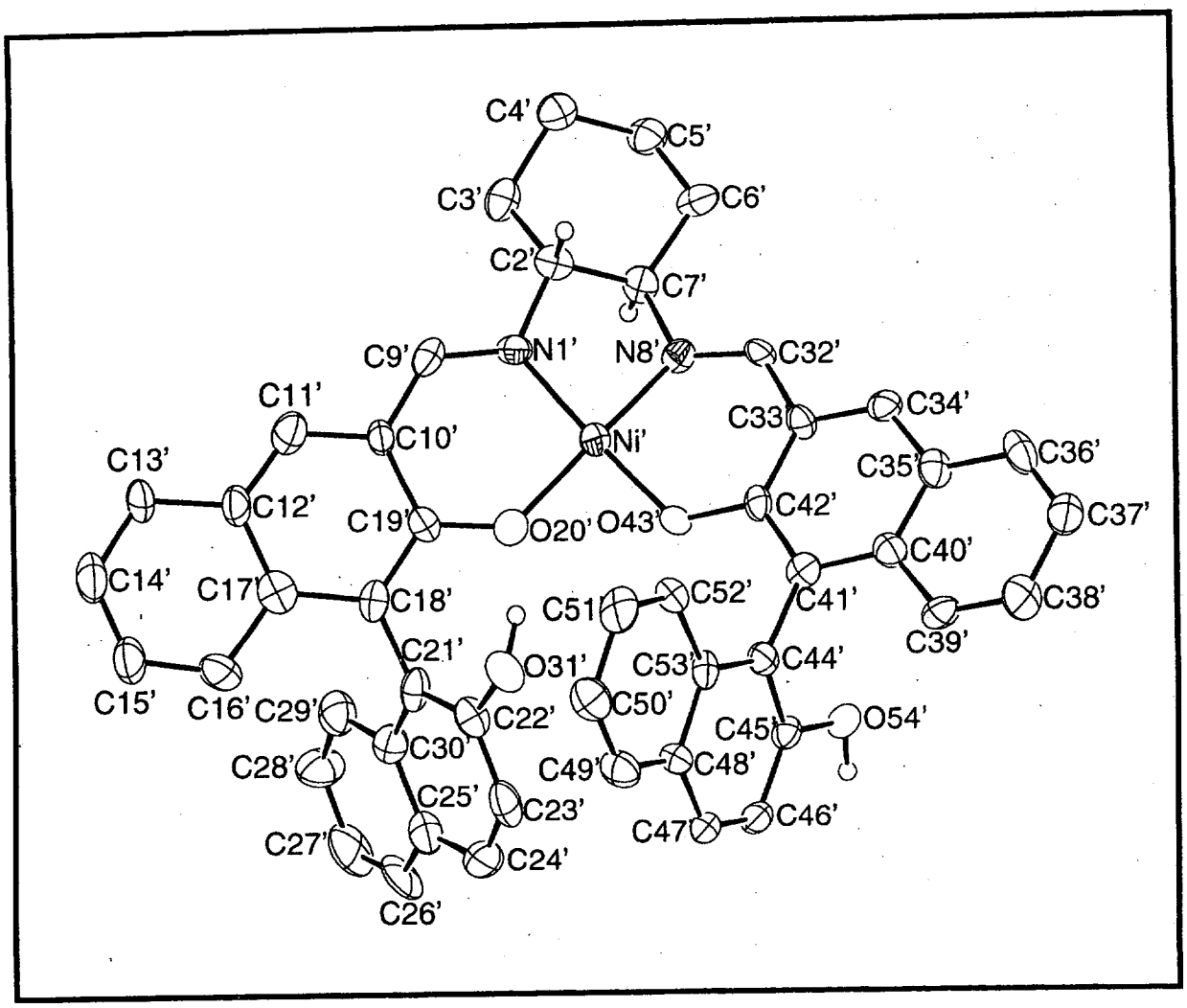


Figure 2. ORTEP drawing of molecule no. 2 of the asymmetric unit with 30% probability thermal ellipsoids.

Three of the hydroxyl's in the asymmetric unit participate in intramolecular hydrogen bonding (O31 to O20, O54 to O43 and O31' to O20'); O54' forms an intermolecular hydrogen bond to O54. The hydroxyl hydrogen atoms could not be located from difference Fourier maps, but their positions were inferred from the O(donor)···O(acceptor) distances and C—O(donor)···O(acceptor) angles which are listed below:

O31···O20	2.652(10) Å	C22—O31···O20	89.6(5)°
O54···O43	2.603(9) Å	C45—O54···O43	92.1(5)°
O31'···O20'	2.695(10) Å	C22'—O31'···O20'	87.9(6)°
O54'···O54	2.660(9) Å	C45'—O54'···O54	116.3(6)°

Hydrogen positions were calculated by assuming approximately linear hydrogen bonds while maintaining the tetrahedral angle for C—O—H. The hydrogen parameters are as follows:

H31···O20	1.833 Å	O31—H31···O20	150.3°
H54···O43	1.739 Å	O54—H54···O43	155.1°
H31'···O20'	1.876 Å	O31'—H31'···O20'	149.5°
H54'···O54	1.772 Å	O54'—H54'···O54	169.8°

References

1. bioteX: A suite of Programs for the Collection, Reduction and Interpretation of Imaging Plate Data, Molecular Structure Corporation (1995).

2. teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

3. SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidoro, G. (1994). *J. Appl. Cryst.*, **27**, 435.

4. SQUEEZE: P. v.d. Sluis & A.L. Spek (1990). *Acta. Cryst.*, **A46**, 194.

5. SHELXL-93: Program for the Refinement of Crystal Structures, Sheldrick, G.M. (1993), University of Göttingen, Germany.

6. $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$

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

   $GOF = \{ \sum w (F_o^2 - F_c^2)^2 / (n - p) \}^{1/2}$

   where n = the number of reflections and p = the number of parameters refined.

7. "ORTEP-II: A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations". C.K. Johnson (1976) ORNL-5138.

Table 1. Summary of Structure Determination of Compound 836

Formula:	$NiC_{49}H_{38}N_2O_4Cl_6$
Formula weight:	990.22
Crystal class:	monoclinic
Space group:	$P2_1$ (#4)
Z	4
Cell constants:	
a	14.9158(5)Å
b	17.2044(8)Å
c	18.3523(6)Å
β	97.040(3)°
V	4674.0(3)Å^3
μ	8.04 cm^{-1}
crystal size, mm	0.42 x 0.10 x 0.03
D_{calc}	1.407 g/cm^3
F(000)	2032
Radiation:	Mo-K_α (λ=0.71069Å)
2θ range	5.06 – 50.7 °
hkl collected:	-17≤ h ≤17; -19≤ k ≤20; -21≤ l ≤22
No. reflections measured:	19661
No. unique reflections:	13389 (R_{int}=0.0650)
No. observed reflections	10993 (F>4σ)
No. reflections used in refinement	13389
No. parameters	992
R indices (F>4σ)	R_1=0.0948
	wR_2=0.2276
R indices (all data)	R_1=0.1100
	wR_2=0.2414
GOF:	1.075
Final Difference Peaks, e/Å^3	+0.422, -0.386

Table 2. Refined Positional Parameters for Compound 836

Atom	x	y	z	U_{eq}, Å^2
Ni	0.37295(7)	0.41431(7)	0.98828(6)	0.0411(3)
O20	0.3783(5)	0.3753(4)	1.0815(3)	0.050(2)
O31	0.2605(4)	0.3928(4)	1.1774(4)	0.055(2)
O43	0.3682(4)	0.5109(4)	1.0352(3)	0.047(2)
O54	0.4942(4)	0.5461(4)	1.1410(4)	0.047(2)
N1	0.3731(5)	0.3178(5)	0.9428(4)	0.042(2)
N8	0.3713(5)	0.4573(5)	0.8961(4)	0.046(2)
C2	0.3461(6)	0.3227(6)	0.8631(5)	0.047(2)
H2	0.2803(6)	0.3289(6)	0.8552(5)	0.063
C3	0.3695(8)	0.2552(7)	0.8176(5)	0.061(3)
H3a	0.3403(8)	0.2087(7)	0.8330(5)	0.082
H3b	0.4343(8)	0.2467(7)	0.8252(5)	0.082
C4	0.3392(10)	0.2698(6)	0.7350(5)	0.067(3)
H4a	0.2738(10)	0.2712(6)	0.7259(5)	0.089
H4b	0.3604(10)	0.2279(6)	0.7061(5)	0.089
C5	0.3787(8)	0.3484(8)	0.7120(6)	0.072(4)
H5a	0.4441(8)	0.3446(8)	0.7164(6)	0.095
H5b	0.3570(8)	0.3588(8)	0.6609(6)	0.095
C6	0.3527(7)	0.4150(8)	0.7587(5)	0.059(3)
H6a	0.2875(7)	0.4211(8)	0.7528(5)	0.079
H6b	0.3792(7)	0.4630(8)	0.7437(5)	0.079
C7	0.3874(6)	0.3972(6)	0.8399(5)	0.054(3)
H7	0.4528(6)	0.3891(6)	0.8431(5)	0.071
C9	0.3882(7)	0.2543(6)	0.9738(6)	0.049(2)
H9	0.3902(7)	0.2113(6)	0.9433(6)	0.065
C10	0.4035(6)	0.2390(6)	1.0534(5)	0.049(2)
C11	0.4189(7)	0.1643(6)	1.0814(6)	0.053(3)
H11	0.4211(7)	0.1237(6)	1.0482(6)	0.070
C12	0.4306(7)	0.1476(6)	1.1522(5)	0.047(2)
C13	0.4406(7)	0.0693(7)	1.1758(6)	0.061(3)
H13	0.4435(7)	0.0290(7)	1.1423(6)	0.080
C14	0.4461(8)	0.0543(7)	1.2536(8)	0.070(4)
H14	0.4571(8)	0.0037(7)	1.2703(8)	0.093
C15	0.4358(8)	0.1112(7)	1.3038(7)	0.069(3)
H15	0.4366(8)	0.0989(7)	1.3533(7)	0.091
C16	0.4242(7)	0.1880(7)	1.2802(5)	0.058(3)
H16	0.4184(7)	0.2265(7)	1.3148(5)	0.078
C17	0.4208(6)	0.2098(6)	1.2039(5)	0.048(2)
C18	0.4119(6)	0.2872(6)	1.1809(5)	0.049(2)

C19	0.3969(6)	0.3035(6)	1.1052(5)	0.045(2)
C21	0.4067(7)	0.3495(6)	1.2361(5)	0.053(3)
C22	0.3312(7)	0.3966(5)	1.2335(5)	0.046(2)
C23	0.3204(7)	0.4452(7)	1.2929(6)	0.062(3)
H23	0.2664(7)	0.4721(7)	1.2932(6)	0.082
C24	0.3877(8)	0.4544(7)	1.3512(6)	0.063(3)
H24	0.3779(8)	0.4846(7)	1.3915(6)	0.084
C25	0.4682(8)	0.4185(7)	1.3485(5)	0.063(3)
C26	0.5446(10)	0.4324(7)	1.4031(6)	0.071(4)
H26	0.5374(10)	0.4647(7)	1.4426(6)	0.095
C27	0.6248(8)	0.4007(8)	1.3988(6)	0.073(3)
H27	0.6729(8)	0.4134(8)	1.4339(6)	0.097
C28	0.6386(8)	0.3488(7)	1.3428(6)	0.071(4)
H28	0.6950(8)	0.3265(7)	1.3405(6)	0.094
C29	0.5648(7)	0.3311(7)	1.2898(5)	0.056(2)
H29	0.5733(7)	0.2955(7)	1.2531(5)	0.074
C30	0.4810(7)	0.3639(7)	1.2900(5)	0.056(3)
C32	0.3610(7)	0.5297(6)	0.8779(5)	0.046(2)
H32	0.3554(7)	0.5419(6)	0.8282(5)	0.061
C33	0.3578(6)	0.5930(5)	0.9296(5)	0.042(2)
C34	0.3538(8)	0.6660(7)	0.9003(6)	0.061(3)
H34	0.3475(8)	0.6719(7)	0.8495(6)	0.081
C35	0.3593(7)	0.7333(6)	0.9458(5)	0.050(2)
C36	0.3669(7)	0.8084(6)	0.9171(6)	0.058(3)
H36	0.3623(7)	0.8143(6)	0.8664(6)	0.077
C37	0.3804(8)	0.8716(7)	0.9590(7)	0.067(3)
H37	0.3839(8)	0.9204(7)	0.9378(7)	0.089
C38	0.3895(7)	0.8630(7)	1.0377(8)	0.071(4)
H38	0.3995(7)	0.9063(7)	1.0680(8)	0.094
C39	0.3832(7)	0.7895(6)	1.0677(6)	0.058(3)
H39	0.3883(7)	0.7841(6)	1.1185(6)	0.077
C40	0.3693(6)	0.7223(6)	1.0228(5)	0.047(2)
C41	0.3651(6)	0.6442(6)	1.0515(5)	0.043(2)
C42	0.3627(5)	0.5812(5)	1.0049(5)	0.035(2)
C44	0.3681(6)	0.6375(5)	1.1346(5)	0.044(2)
C45	0.4374(7)	0.5948(6)	1.1732(6)	0.049(2)
C46	0.4565(10)	0.5999(8)	1.2487(7)	0.077(4)
H46	0.5079(10)	0.5758(8)	1.2721(7)	0.103
C47	0.3989(9)	0.6415(8)	1.2912(7)	0.077(4)
H47	0.4123(9)	0.6466(8)	1.3419(7)	0.103
C48	0.3198(9)	0.6749(7)	1.2526(6)	0.069(3)
C49	0.2612(12)	0.7095(9)	1.2922(9)	0.094(4)
H49	0.2749(12)	0.7132(9)	1.3429(9)	0.124

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C50	0.1831(12)	0.7386(10)	1.2594(9)	0.104(5)
H50	0.1391(12)	0.7562(10)	1.2872(9)	0.138
C51	0.1685(9)	0.7423(8)	1.1823(9)	0.084(4)
H51	0.1178(9)	0.7676(8)	1.1589(9)	0.112
C52	0.2275(8)	0.7094(7)	1.1426(7)	0.067(3)
H52	0.2148(8)	0.7088(7)	1.0918(7)	0.089
C53	0.3077(7)	0.6760(6)	1.1752(6)	0.056(3)
Ni'	0.89557(7)	0.82702(7)	1.15444(6)	0.0426(3)
O20'	0.9068(5)	0.7920(4)	1.2507(4)	0.053(2)
O31'	0.9247(6)	0.6472(4)	1.3067(4)	0.063(2)
O43'	0.8479(4)	0.7305(4)	1.1279(3)	0.046(2)
O54'	0.6513(4)	0.5748(4)	1.0916(4)	0.050(2)
N1'	0.9563(5)	0.9211(5)	1.1771(4)	0.046(2)
N8'	0.8679(5)	0.8691(5)	1.0622(4)	0.044(2)
C2'	0.9614(7)	0.9712(5)	1.1140(5)	0.047(2)
H2'	1.0129(7)	0.9550(5)	1.0893(5)	0.062
C3'	0.9688(7)	1.0597(6)	1.1294(6)	0.058(3)
H3a'	1.0232(7)	1.0708(6)	1.1623(6)	0.078
H3b'	0.9172(7)	1.0773(6)	1.1524(6)	0.078
C4'	0.9717(7)	1.1028(7)	1.0544(6)	0.063(3)
H4a'	0.9772(7)	1.1584(7)	1.0626(6)	0.084
H4b'	1.0233(7)	1.0853(7)	1.0315(6)	0.084
C5'	0.8827(7)	1.0845(7)	1.0036(6)	0.059(3)
H5a'	0.8315(7)	1.1033(7)	1.0265(6)	0.078
H5b'	0.8831(7)	1.1115(7)	0.9573(6)	0.078
C6'	0.8721(7)	0.9980(6)	0.9894(7)	0.059(3)
H6a'	0.9201(7)	0.9795(6)	0.9627(7)	0.079
H6b'	0.8148(7)	0.9876(6)	0.9601(7)	0.079
C7'	0.8763(7)	0.9553(6)	1.0643(6)	0.047(2)
H7'	0.8262(7)	0.9751(6)	1.0888(6)	0.062
C9'	1.0049(6)	0.9366(6)	1.2406(5)	0.051(2)
H9'	1.0430(6)	0.9796(6)	1.2422(5)	0.068
C10'	1.0043(7)	0.8936(5)	1.3066(5)	0.046(2)
C11'	1.0557(7)	0.9211(8)	1.3688(6)	0.064(3)
H11'	1.0920(7)	0.9645(8)	1.3649(6)	0.086
C12'	1.0551(7)	0.8871(6)	1.4355(5)	0.056(3)
C13'	1.1115(7)	0.9149(9)	1.5007(5)	0.074(3)
H13'	1.1499(7)	0.9570(9)	1.4977(5)	0.098
C14'	1.1070(8)	0.8779(9)	1.5671(6)	0.077(4)
H14'	1.1425(8)	0.8965(9)	1.6086(6)	0.103
C15'	1.0528(9)	0.8153(9)	1.5740(6)	0.076(4)
H15'	1.0540(9)	0.7918(9)	1.6197(6)	0.101

C16'	0.9960(9)	0.7856(7)	1.5154(6)	0.070(3)
H16'	0.9590(9)	0.7431(7)	1.5215(6)	0.093
C17'	0.9955(7)	0.8227(7)	1.4431(6)	0.060(3)
C18'	0.9361(6)	0.7941(6)	1.3791(5)	0.048(2)
C19'	0.9475(6)	0.8236(6)	1.3118(4)	0.047(2)
C21'	0.8667(7)	0.7351(5)	1.3874(5)	0.049(2)
C22'	0.8702(7)	0.6676(7)	1.3539(6)	0.057(3)
C23'	0.8094(9)	0.6067(7)	1.3664(6)	0.070(3)
H23'	0.8147(9)	0.5588(7)	1.3438(6)	0.094
C24'	0.7433(10)	0.6170(7)	1.4112(7)	0.076(4)
H24'	0.7043(10)	0.5764(7)	1.4185(7)	0.101
C25'	0.7343(9)	0.6891(8)	1.4461(6)	0.071(3)
C26'	0.6638(10)	0.7145(12)	1.4879(6)	0.096(5)
H26'	0.6195(10)	0.6779(12)	1.4945(6)	0.128
C27'	0.6548(13)	0.7816(12)	1.5172(7)	0.112(6)
H27'	0.6098(13)	0.7903(12)	1.5472(7)	0.149
C28'	0.7125(8)	0.8398(9)	1.5032(7)	0.078(4)
H28'	0.7036(8)	0.8894(9)	1.5211(7)	0.104
C29'	0.7834(7)	0.8272(8)	1.4634(6)	0.068(3)
H29'	0.8226(7)	0.8676(8)	1.4561(6)	0.090
C30'	0.7972(7)	0.7520(6)	1.4331(6)	0.054(3)
C32'	0.8482(6)	0.8310(7)	1.0004(4)	0.046(2)
H32'	0.8431(6)	0.8591(7)	0.9569(4)	0.061
C33'	0.8341(6)	0.7487(6)	0.9959(5)	0.043(2)
C34'	0.8179(6)	0.7192(6)	0.9276(5)	0.046(2)
H34'	0.8161(6)	0.7526(6)	0.8876(5)	0.061
C35'	0.8031(6)	0.6373(6)	0.9147(5)	0.049(2)
C36'	0.7923(6)	0.6037(8)	0.8452(5)	0.060(3)
H36'	0.7937(6)	0.6352(8)	0.8042(5)	0.080
C37'	0.7795(7)	0.5236(7)	0.8355(6)	0.062(3)
H37'	0.7721(7)	0.5018(7)	0.7888(6)	0.083
C38'	0.7782(8)	0.4765(7)	0.8991(6)	0.065(3)
H38'	0.7701(8)	0.4231(7)	0.8944(6)	0.086
C39'	0.7884(7)	0.5088(5)	0.9649(6)	0.052(2)
H39'	0.7864(7)	0.4764(5)	1.0052(6)	0.069
C40'	0.8022(6)	0.5906(6)	0.9789(5)	0.046(2)
C41'	0.8150(6)	0.6207(5)	1.0510(5)	0.044(2)
C42'	0.8336(5)	0.7015(6)	1.0594(5)	0.040(2)
C44'	0.8091(7)	0.5700(5)	1.1153(5)	0.043(2)
C45'	0.7260(6)	0.5467(5)	1.1326(5)	0.040(2)
C46'	0.7178(6)	0.4911(5)	1.1883(5)	0.046(2)
H46'	0.6612(6)	0.4766(5)	1.2000(5)	0.061

C47'	0.7935(6)	0.4595(6)	1.2242(5)	0.047(2)
H47'	0.7870(6)	0.4216(6)	1.2593(5)	0.062
C48'	0.8821(7)	0.4805(6)	1.2118(5)	0.050(2)
C49'	0.9606(8)	0.4500(7)	1.2506(6)	0.061(3)
H49'	0.9550(8)	0.4122(7)	1.2860(6)	0.081
C50'	1.0448(8)	0.4729(7)	1.2391(6)	0.065(3)
H50'	1.0961(8)	0.4512(7)	1.2651(6)	0.086
C51'	1.0510(6)	0.5333(8)	1.1839(6)	0.066(3)
H51'	1.1080(6)	0.5507(8)	1.1757(6)	0.088
C52'	0.9797(6)	0.5642(6)	1.1453(5)	0.044(2)
H52'	0.9872(6)	0.6025(6)	1.1109(5)	0.058
C53'	0.8892(6)	0.5390(6)	1.1560(5)	0.044(2)
H31	0.2824	0.3863	1.1343	0.100
H54	0.4625	0.5248	1.0996	0.100
H31'	0.9314	0.6880	1.2767	0.100
H54'	0.6020	0.5616	1.1123	0.100

$U_{eq}=1/3[U_{11}(aa^*)^2+U_{22}(bb^*)^2+U_{33}(cc^*)^2+2U_{12}aa^*bb^*cos\gamma+2U_{13}aa^*cc^*cos\beta+2U_{23}bb^*cc^*cos\alpha]$

Table 3. Refined Thermal Parameters (U's) for Compound 836

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni	0.0398(6)	0.0446(7)	0.0383(6)	-0.0005(5)	0.0022(5)	-0.0006(6)
O20	0.066(4)	0.042(4)	0.039(3)	0.001(3)	-0.005(3)	0.000(3)
O31	0.045(3)	0.066(5)	0.054(4)	-0.002(3)	0.005(3)	0.000(3)
O43	0.051(4)	0.051(4)	0.040(3)	0.001(3)	0.006(3)	0.000(3)
O54	0.041(3)	0.044(4)	0.055(4)	0.009(3)	0.002(3)	0.002(3)
N1	0.047(4)	0.039(4)	0.039(4)	0.001(4)	-0.001(3)	-0.007(4)
N8	0.042(4)	0.055(5)	0.040(4)	-0.017(4)	0.003(3)	-0.010(4)
C2	0.038(4)	0.040(5)	0.063(6)	-0.008(5)	0.003(4)	0.010(4)
C3	0.080(8)	0.060(7)	0.045(6)	-0.014(5)	0.009(5)	-0.022(6)
C4	0.122(10)	0.037(6)	0.039(5)	-0.015(4)	-0.003(6)	-0.002(6)
C5	0.061(6)	0.107(11)	0.045(6)	-0.020(6)	0.000(5)	-0.020(6)
C6	0.063(6)	0.077(7)	0.038(5)	0.003(6)	0.006(4)	-0.014(7)
C7	0.040(5)	0.076(8)	0.043(5)	-0.001(5)	-0.003(4)	-0.017(5)
C9	0.055(6)	0.033(5)	0.061(6)	0.008(5)	0.020(5)	-0.016(4)
C10	0.035(5)	0.060(6)	0.051(6)	-0.009(5)	0.003(4)	-0.006(5)
C11	0.051(6)	0.046(6)	0.062(6)	-0.001(5)	0.007(5)	0.006(5)
C12	0.048(5)	0.040(5)	0.052(6)	0.015(4)	-0.007(4)	0.004(4)
C13	0.056(6)	0.063(7)	0.058(7)	-0.006(5)	-0.011(5)	-0.004(5)
C14	0.068(7)	0.054(7)	0.090(9)	0.048(7)	0.014(7)	0.006(6)
C15	0.072(7)	0.061(8)	0.074(8)	0.027(7)	0.014(6)	-0.005(6)
C16	0.054(6)	0.080(8)	0.041(5)	0.005(5)	0.003(5)	-0.018(6)
C17	0.048(5)	0.057(6)	0.041(5)	0.009(5)	0.008(4)	-0.013(5)
C18	0.045(5)	0.047(6)	0.051(6)	0.013(5)	-0.005(4)	-0.002(4)
C19	0.037(5)	0.048(6)	0.048(5)	0.008(4)	0.001(4)	-0.016(4)
C21	0.067(6)	0.052(7)	0.041(5)	0.015(4)	0.013(5)	0.011(5)
C22	0.066(6)	0.030(5)	0.042(5)	0.005(4)	0.006(4)	-0.003(4)
C23	0.053(6)	0.074(8)	0.058(6)	0.003(6)	0.003(5)	-0.003(5)
C24	0.067(7)	0.068(7)	0.058(6)	-0.014(6)	0.026(6)	-0.010(6)
C25	0.077(7)	0.063(7)	0.045(5)	0.004(6)	-0.011(5)	-0.017(7)
C26	0.106(10)	0.064(8)	0.041(6)	-0.014(5)	-0.001(6)	-0.010(7)
C27	0.066(7)	0.092(10)	0.057(7)	0.001(7)	-0.002(5)	-0.014(7)
C28	0.068(7)	0.080(9)	0.063(7)	0.024(6)	0.001(6)	-0.027(6)
C29	0.075(7)	0.053(6)	0.039(5)	0.010(5)	0.005(4)	-0.015(6)
C30	0.058(6)	0.069(7)	0.040(5)	0.018(5)	0.009(5)	-0.010(5)
C32	0.056(6)	0.049(6)	0.032(5)	0.006(4)	0.004(4)	0.014(5)
C33	0.044(5)	0.046(5)	0.035(5)	0.003(4)	0.000(4)	0.013(4)
C34	0.069(7)	0.062(7)	0.051(6)	0.011(5)	-0.001(5)	0.016(6)
C35	0.048(5)	0.055(6)	0.048(5)	0.023(5)	0.007(4)	0.006(5)
C36	0.071(7)	0.060(7)	0.046(5)	0.006(5)	0.017(5)	0.014(5)

C37	0.075(8)	0.053(7)	0.075(8)	0.013(6)	0.015(7)	0.010(6)
C38	0.038(5)	0.057(7)	0.109(10)	-0.008(7)	-0.023(6)	0.006(5)
C39	0.059(6)	0.045(6)	0.065(7)	-0.003(5)	-0.011(5)	0.004(5)
C40	0.041(5)	0.059(6)	0.041(5)	-0.007(5)	0.003(4)	0.004(4)
C41	0.033(4)	0.047(5)	0.046(5)	0.002(4)	0.000(4)	0.003(4)
C42	0.022(4)	0.033(5)	0.048(5)	-0.004(4)	-0.009(4)	0.006(3)
C44	0.050(5)	0.033(5)	0.047(5)	-0.004(4)	-0.004(4)	0.010(4)
C45	0.058(6)	0.037(5)	0.050(6)	-0.008(5)	0.002(5)	-0.018(5)
C46	0.088(9)	0.079(9)	0.061(7)	0.013(7)	-0.006(7)	-0.015(8)
C47	0.085(9)	0.080(9)	0.062(7)	-0.004(7)	-0.009(7)	0.016(7)
C48	0.107(10)	0.052(7)	0.056(6)	-0.021(5)	0.046(7)	-0.012(7)
C49	0.109(12)	0.074(9)	0.099(11)	-0.008(8)	0.018(10)	0.013(9)
C50	0.112(13)	0.114(13)	0.095(11)	-0.039(10)	0.048(10)	0.005(11)
C51	0.067(8)	0.072(9)	0.118(12)	-0.022(8)	0.033(8)	-0.001(7)
C52	0.060(7)	0.064(7)	0.077(8)	-0.035(6)	0.012(6)	-0.001(6)
C53	0.057(6)	0.037(5)	0.076(7)	-0.013(5)	0.020(5)	-0.006(5)
Ni'	0.0424(6)	0.0452(7)	0.0389(6)	0.0019(6)	-0.0002(5)	-0.0015(6)
O20'	0.055(4)	0.048(4)	0.055(4)	0.002(3)	-0.003(3)	-0.004(3)
O31'	0.098(6)	0.045(4)	0.045(4)	0.001(3)	0.010(4)	0.014(4)
O43'	0.065(4)	0.042(4)	0.031(3)	0.001(3)	0.011(3)	-0.010(3)
O54'	0.044(4)	0.050(4)	0.054(4)	-0.003(3)	0.003(3)	-0.011(3)
N1'	0.039(4)	0.048(4)	0.050(4)	0.013(4)	0.004(3)	-0.004(4)
N8'	0.043(4)	0.037(4)	0.051(5)	0.001(4)	0.001(4)	0.001(4)
C2'	0.051(5)	0.038(5)	0.054(5)	0.001(4)	0.017(5)	0.012(4)
C3'	0.044(5)	0.063(7)	0.066(7)	-0.013(6)	-0.001(5)	0.000(5)
C4'	0.057(6)	0.067(7)	0.066(7)	0.003(6)	0.010(5)	-0.008(5)
C5'	0.045(6)	0.068(7)	0.064(7)	0.008(6)	0.007(5)	-0.003(5)
C6'	0.050(6)	0.048(6)	0.080(8)	0.012(6)	0.007(5)	-0.010(5)
C7'	0.047(5)	0.038(5)	0.053(6)	0.004(4)	-0.001(5)	0.011(4)
C9'	0.038(5)	0.054(6)	0.060(6)	-0.014(5)	0.001(4)	-0.009(4)
C10'	0.062(6)	0.043(6)	0.031(4)	-0.002(4)	-0.008(4)	-0.005(4)
C11'	0.056(6)	0.068(7)	0.066(7)	-0.007(6)	-0.009(5)	-0.008(6)
C12'	0.069(7)	0.062(7)	0.036(5)	-0.019(5)	0.001(5)	-0.005(5)
C13'	0.069(7)	0.107(9)	0.040(5)	-0.001(7)	-0.018(5)	-0.022(8)
C14'	0.060(7)	0.120(11)	0.049(6)	-0.021(7)	-0.006(5)	-0.010(7)
C15'	0.081(8)	0.100(11)	0.045(6)	-0.021(7)	0.003(6)	-0.011(8)
C16'	0.079(8)	0.070(8)	0.059(7)	0.023(6)	0.003(6)	-0.001(6)
C17'	0.058(6)	0.064(7)	0.058(6)	-0.001(6)	0.007(5)	0.013(6)
C18'	0.047(5)	0.051(6)	0.045(5)	-0.015(4)	-0.003(4)	0.003(4)
C19'	0.054(5)	0.051(5)	0.035(4)	0.001(5)	0.003(4)	0.004(5)
C21'	0.057(6)	0.033(5)	0.050(5)	-0.012(4)	-0.015(5)	0.012(4)
C22'	0.060(6)	0.064(7)	0.045(5)	0.004(5)	0.001(5)	0.010(5)
C23'	0.107(10)	0.063(7)	0.038(5)	-0.013(5)	-0.002(6)	0.016(7)

C24'	0.110(10)	0.055(7)	0.064(7)	-0.008(6)	0.015(7)	-0.024(7)
C25'	0.083(8)	0.079(8)	0.046(6)	-0.002(6)	-0.008(6)	-0.006(7)
C26'	0.088(9)	0.17(2)	0.032(6)	0.003(8)	0.030(6)	-0.021(10)
C27'	0.14(2)	0.16(2)	0.047(7)	-0.027(9)	0.044(8)	-0.008(13)
C28'	0.079(8)	0.079(9)	0.085(8)	-0.010(7)	0.042(7)	-0.012(7)
C29'	0.056(6)	0.083(8)	0.061(6)	-0.003(7)	-0.003(5)	0.001(7)
C30'	0.057(6)	0.047(6)	0.056(6)	0.000(5)	-0.003(5)	0.005(5)
C32'	0.046(5)	0.056(6)	0.033(4)	0.022(5)	-0.006(4)	-0.009(5)
C33'	0.045(5)	0.047(5)	0.034(5)	0.007(4)	-0.004(4)	0.005(4)
C34'	0.036(5)	0.050(6)	0.050(5)	0.010(4)	0.000(4)	-0.007(4)
C35'	0.043(5)	0.064(7)	0.041(5)	-0.012(5)	0.012(4)	0.003(5)
C36'	0.039(5)	0.107(10)	0.035(5)	0.003(6)	0.001(4)	0.007(6)
C37'	0.059(7)	0.069(8)	0.058(7)	-0.008(6)	0.002(5)	-0.004(6)
C38'	0.071(7)	0.071(8)	0.057(6)	-0.023(6)	0.025(6)	0.006(6)
C39'	0.065(6)	0.030(5)	0.061(6)	0.000(4)	0.009(5)	-0.010(4)
C40'	0.035(4)	0.062(6)	0.041(5)	0.005(5)	0.006(4)	-0.001(4)
C41'	0.034(4)	0.040(5)	0.055(6)	0.007(4)	-0.005(4)	0.008(4)
C42'	0.029(4)	0.055(6)	0.034(4)	-0.004(4)	-0.004(4)	0.004(4)
C44'	0.059(6)	0.033(5)	0.036(5)	-0.004(4)	0.006(4)	0.001(4)
C45'	0.031(4)	0.046(5)	0.042(5)	-0.005(4)	0.003(4)	-0.004(4)
C46'	0.043(5)	0.044(5)	0.050(5)	-0.005(4)	0.005(4)	-0.008(4)
C47'	0.049(5)	0.046(5)	0.044(5)	0.002(4)	-0.001(4)	-0.012(4)
C48'	0.066(6)	0.047(6)	0.037(5)	0.006(4)	0.005(5)	-0.011(5)
C49'	0.065(7)	0.063(7)	0.055(6)	0.017(5)	0.003(5)	0.007(6)
C50'	0.069(7)	0.063(7)	0.062(7)	0.009(6)	0.004(6)	0.017(6)
C51'	0.021(4)	0.106(10)	0.072(7)	-0.009(7)	0.006(5)	-0.004(5)
C52'	0.044(5)	0.050(6)	0.037(5)	0.003(4)	0.006(4)	0.007(4)
C53'	0.036(5)	0.058(6)	0.037(5)	-0.011(4)	-0.003(4)	0.002(4)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(a^{*2}U_{11}h^2+b^{*2}U_{22}k^2+c^{*2}U_{33}l^2+ 2b^*c^*U_{23}kl+2a^*c^*U_{13}hl+2a^*b^*U_{12}hk)]$.

Table 4. Bond Distances in Compound 836, Å

Ni-O20	1.831(6)	Ni-N8	1.843(8)	Ni-N1	1.858(8)
Ni-O43	1.877(7)	O20-C19	1.327(11)	O31-C22	1.382(11)
O43-C42	1.329(10)	O54-C45	1.375(12)	N1-C9	1.240(12)
N1-C2	1.471(11)	N8-C32	1.294(12)	N8-C7	1.499(13)
C2-C3	1.497(14)	C2-C7	1.507(14)	C3-C4	1.548(14)
C4-C5	1.56(2)	C5-C6	1.51(2)	C6-C7	1.547(12)
C9-C10	1.474(14)	C10-C11	1.392(14)	C10-C19	1.473(14)
C11-C12	1.322(14)	C12-C13	1.42(2)	C12-C17	1.449(14)
C13-C14	1.44(2)	C14-C15	1.37(2)	C15-C16	1.39(2)
C16-C17	1.444(13)	C17-C18	1.399(14)	C18-C19	1.408(13)
C18-C21	1.484(14)	C21-C22	1.384(13)	C21-C30	1.414(14)
C22-C23	1.399(14)	C23-C24	1.38(2)	C24-C25	1.36(2)
C25-C26	1.44(2)	C25-C30	1.46(2)	C26-C27	1.33(2)
C27-C28	1.40(2)	C28-C29	1.410(14)	C29-C30	1.37(2)
C32-C33	1.450(13)	C33-C34	1.364(14)	C33-C42	1.389(12)
C34-C35	1.42(2)	C35-C36	1.405(14)	C35-C40	1.416(13)
C36-C37	1.33(2)	C37-C38	1.44(2)	C38-C39	1.39(2)
C39-C40	1.420(14)	C40-C41	1.448(14)	C41-C42	1.380(12)
C41-C44	1.524(13)	C44-C45	1.391(13)	C44-C53	1.404(14)
C45-C46	1.38(2)	C46-C47	1.42(2)	C47-C48	1.42(2)
C48-C49	1.34(2)	C48-C53	1.41(2)	C49-C50	1.34(2)
C50-C51	1.41(2)	C51-C52	1.33(2)	C52-C53	1.39(2)
Ni'-N8'	1.842(8)	Ni'-O43'	1.848(6)	Ni'-O20'	1.855(7)
Ni'-N1'	1.876(8)	O20'-C19'	1.324(11)	O31'-C22'	1.307(13)
O43'-C42'	1.345(10)	O54'-C45'	1.355(11)	N1'-C9'	1.322(11)
N1'-C2'	1.452(11)	N8'-C32'	1.310(12)	N8'-C7'	1.488(11)
C2'-C7'	1.495(13)	C2'-C3'	1.550(14)	C3'-C4'	1.57(2)
C4'-C5'	1.56(2)	C5'-C6'	1.52(2)	C6'-C7'	1.552(14)
C9'-C10'	1.421(13)	C10'-C11'	1.378(12)	C10'-C19'	1.482(14)
C11'-C12'	1.36(2)	C12'-C17'	1.44(2)	C12'-C13'	1.456(13)
C13'-C14'	1.38(2)	C14'-C15'	1.36(2)	C15'-C16'	1.38(2)
C16'-C17'	1.47(2)	C17'-C18'	1.466(13)	C18'-C19'	1.364(13)
C18'-C21'	1.471(14)	C21'-C22'	1.317(14)	C21'-C30'	1.44(2)
C22'-C23'	1.42(2)	C23'-C24'	1.37(2)	C24'-C25'	1.41(2)
C25'-C26'	1.44(2)	C25'-C30'	1.47(2)	C26'-C27'	1.29(2)
C27'-C28'	1.37(2)	C28'-C29'	1.37(2)	C29'-C30'	1.43(2)
C32'-C33'	1.433(14)	C33'-C34'	1.346(13)	C33'-C42'	1.421(12)
C34'-C35'	1.441(14)	C35'-C36'	1.393(14)	C35'-C40'	1.428(14)
C36'-C37'	1.40(2)	C37'-C38'	1.42(2)	C38'-C39'	1.320(14)
C39'-C40'	1.439(14)	C40'-C41'	1.414(13)	C41'-C42'	1.422(13)
C41'-C44'	1.480(13)	C44'-C45'	1.376(13)	C44'-C53'	1.432(13)

C45'-C46'	1.417(13)	C46'-C47'	1.350(13)	C47'-C48'	1.416(14)
C48'-C49'	1.396(14)	C48'-C53'	1.449(13)	C49'-C50'	1.36(2)
C50'-C51'	1.46(2)	C51'-C52'	1.316(13)	C52'-C53'	1.453(13)

Table 5. Bond Angles in Compound 836, °

O20-Ni-N8	177.3(3)	O20-Ni-N1	95.2(3)	N8-Ni-N1	86.9(3)
O20-Ni-O43	84.0(3)	N8-Ni-O43	93.9(3)	N1-Ni-O43	177.8(3)
C19-O20-Ni	129.1(6)	C42-O43-Ni	128.1(6)	C9-N1-C2	121.2(9)
C9-N1-Ni	126.3(7)	C2-N1-Ni	112.4(6)	C32-N8-C7	120.6(8)
C32-N8-Ni	127.6(7)	C7-N8-Ni	111.7(6)	N1-C2-C3	117.2(8)
N1-C2-C7	104.9(7)	C3-C2-C7	111.8(8)	C2-C3-C4	111.2(9)
C3-C4-C5	109.4(8)	C6-C5-C4	111.9(9)	C5-C6-C7	108.5(10)
N8-C7-C2	106.6(8)	N8-C7-C6	117.6(9)	C2-C7-C6	109.9(8)
N1-C9-C10	127.5(10)	C11-C10-C19	118.6(9)	C11-C10-C9	121.9(9)
C19-C10-C9	119.4(9)	C12-C11-C10	124.0(10)	C11-C12-C13	120.2(10)
C11-C12-C17	118.1(9)	C13-C12-C17	121.1(9)	C12-C13-C14	117.5(11)
C15-C14-C13	122.8(10)	C14-C15-C16	119.3(11)	C15-C16-C17	122.4(11)
C18-C17-C16	122.1(10)	C18-C17-C12	121.2(9)	C16-C17-C12	116.7(9)
C17-C18-C19	119.1(10)	C17-C18-C21	119.5(9)	C19-C18-C21	120.9(9)
O20-C19-C18	120.7(9)	O20-C19-C10	121.2(8)	C18-C19-C10	118.1(9)
C22-C21-C30	119.1(10)	C22-C21-C18	120.7(9)	C30-C21-C18	120.1(9)
O31-C22-C21	122.8(8)	O31-C22-C23	117.3(9)	C21-C22-C23	119.6(9)
C24-C23-C22	122.0(10)	C25-C24-C23	118.8(10)	C24-C25-C26	121.8(11)
C24-C25-C30	121.1(9)	C26-C25-C30	117.0(11)	C27-C26-C25	122.2(11)
C26-C27-C28	121.5(11)	C27-C28-C29	118.2(12)	C30-C29-C28	123.0(11)
C29-C30-C21	124.2(10)	C29-C30-C25	118.0(10)	C21-C30-C25	117.8(10)
N8-C32-C33	124.5(8)	C34-C33-C42	121.5(9)	C34-C33-C32	115.8(9)
C42-C33-C32	122.6(8)	C33-C34-C35	121.3(10)	C36-C35-C40	119.5(10)
C36-C35-C34	121.9(9)	C40-C35-C34	118.0(9)	C37-C36-C35	123.2(10)
C36-C37-C38	118.9(11)	C39-C38-C37	119.2(11)	C38-C39-C40	121.6(11)
C35-C40-C39	117.5(10)	C35-C40-C41	118.9(9)	C39-C40-C41	123.7(9)
C42-C41-C40	120.2(8)	C42-C41-C44	123.8(8)	C40-C41-C44	115.9(8)
O43-C42-C41	117.4(8)	O43-C42-C33	122.9(8)	C41-C42-C33	119.7(8)
C45-C44-C53	117.7(9)	C45-C44-C41	118.6(9)	C53-C44-C41	123.6(8)
O54-C45-C46	114.1(10)	O54-C45-C44	124.2(9)	C46-C45-C44	121.7(11)
C45-C46-C47	121.2(12)	C48-C47-C46	116.7(11)	C49-C48-C53	121.9(14)
C49-C48-C47	117.6(13)	C53-C48-C47	120.3(11)	C50-C49-C48	121(2)
C49-C50-C51	119.2(14)	C52-C51-C50	120(2)	C51-C52-C53	122.0(13)
C52-C53-C44	122.7(10)	C52-C53-C48	115.8(11)	C44-C53-C48	121.1(11)
N8'-Ni'-O43'	94.3(3)	N8'-Ni'-O20'	171.0(3)	O43'-Ni'-O20'	86.9(3)
N8'-Ni'-N1'	85.0(3)	O43'-Ni'-N1'	173.3(3)	O20'-Ni'-N1'	94.8(3)
C19'-O20'-Ni'	130.7(6)	C42'-O43'-Ni'	126.2(6)	C9'-N1'-C2'	120.4(8)
C9'-N1'-Ni'	124.5(7)	C2'-N1'-Ni'	114.0(6)	C32'-N8'-C7'	122.0(9)
C32'-N8'-Ni'	126.8(7)	C7'-N8'-Ni'	111.1(7)	N1'-C2'-C7'	104.8(8)
N1'-C2'-C3'	116.6(9)	C7'-C2'-C3'	109.1(8)	C2'-C3'-C4'	108.3(9)
C5'-C4'-C3'	108.5(9)	C6'-C5'-C4'	111.4(9)	C5'-C6'-C7'	108.7(10)

N8'-C7'-C2'	105.1(7)	N8'-C7'-C6'	117.0(9)	C2'-C7'-C6'	113.1(9)
N1'-C9'-C10'	125.9(8)	C11'-C10'-C9'	117.8(9)	C11'-C10'-C19'	119.3(9)
C9'-C10'-C19'	122.8(7)	C12'-C11'-C10'	122.2(11)	C11'-C12'-C17'	119.5(9)
C11'-C12'-C13'	122.1(11)	C17'-C12'-C13'	118.4(10)	C14'-C13'-C12'	119.2(12)
C15'-C14'-C13'	122.6(11)	C14'-C15'-C16'	122.3(12)	C15'-C16'-C17'	118.4(11)
C12'-C17'-C18'	120.0(9)	C12'-C17'-C16'	119.1(10)	C18'-C17'-C16'	120.8(11)
C19'-C18'-C17'	118.0(9)	C19'-C18'-C21'	121.2(8)	C17'-C18'-C21'	120.8(9)
O20'-C19'-C18'	121.2(9)	O20'-C19'-C10'	119.0(8)	C18'-C19'-C10'	119.8(8)
C22'-C21'-C30'	121.4(10)	C22'-C21'-C18'	119.4(10)	C30'-C21'-C18'	119.1(8)
O31'-C22'-C21'	127.6(11)	O31'-C22'-C23'	111.7(10)	C21'-C22'-C23'	120.7(11)
C24'-C23'-C22'	121.4(11)	C23'-C24'-C25'	120.1(12)	C24'-C25'-C26'	128.6(13)
C24'-C25'-C30'	118.4(11)	C26'-C25'-C30'	112.7(12)	C27'-C26'-C25'	128(2)
C26'-C27'-C28'	118.6(14)	C27'-C28'-C29'	121.9(14)	C28'-C29'-C30'	120.4(12)
C29'-C30'-C21'	123.7(10)	C29'-C30'-C25'	118.5(10)	C21'-C30'-C25'	117.7(10)
N8'-C32'-C33'	124.1(8)	C34'-C33'-C42'	122.1(9)	C34'-C33'-C32'	115.8(8)
C42'-C33'-C32'	122.1(8)	C33'-C34'-C35'	121.8(9)	C36'-C35'-C40'	120.6(10)
C36'-C35'-C34'	123.7(10)	C40'-C35'-C34'	115.6(9)	C35'-C36'-C37'	121.6(11)
C36'-C37'-C38'	118.2(10)	C39'-C38'-C37'	119.9(11)	C38'-C39'-C40'	124.9(10)
C41'-C40'-C35'	123.5(9)	C41'-C40'-C39'	121.7(9)	C35'-C40'-C39'	114.8(9)
C40'-C41'-C42'	117.6(9)	C40'-C41'-C44'	121.1(8)	C42'-C41'-C44'	121.4(8)
O43'-C42'-C33'	122.7(8)	O43'-C42'-C41'	118.0(8)	C33'-C42'-C41'	119.3(8)
C45'-C44'-C53'	119.3(8)	C45'-C44'-C41'	119.9(8)	C53'-C44'-C41'	120.5(8)
O54'-C45'-C44'	118.1(8)	O54'-C45'-C46'	120.2(8)	C44'-C45'-C46'	121.6(8)
C47'-C46'-C45'	118.8(9)	C46'-C47'-C48'	124.1(9)	C49'-C48'-C47'	124.3(9)
C49'-C48'-C53'	119.5(9)	C47'-C48'-C53'	116.2(9)	C50'-C49'-C48'	123.0(10)
C49'-C50'-C51'	117.0(10)	C52'-C51'-C50'	122.9(10)	C51'-C52'-C53'	120.7(9)
C44'-C53'-C48'	119.9(9)	C44'-C53'-C52'	123.2(9)	C48'-C53'-C52'	116.9(8)