ORGANOMETALLICS
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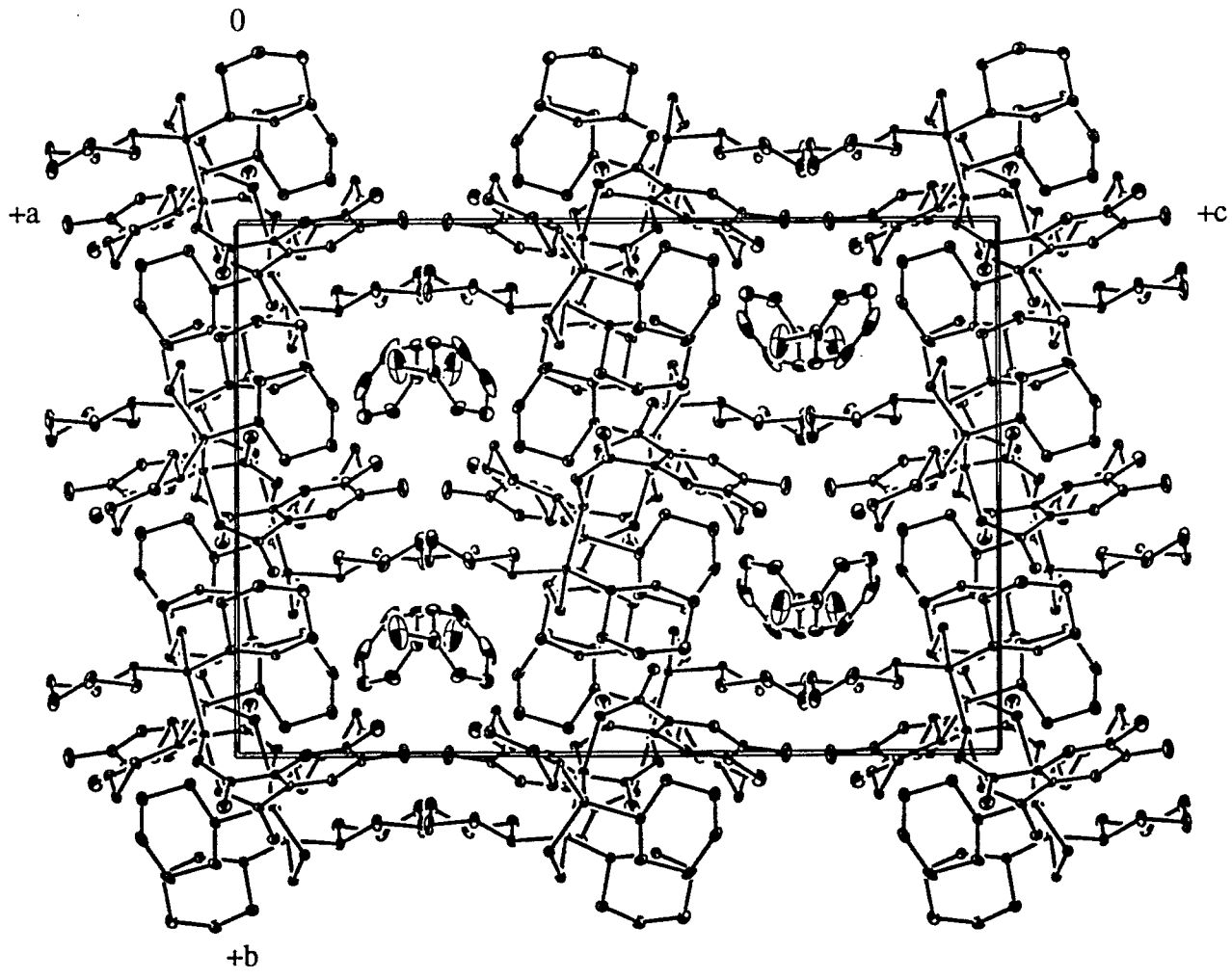
L933-1

Sample: MAD2

Compound: $C_{40}H_{56}ClF_2NiO_4P_2$

Ni(OCO-4,5-$F_2C_6H_2$COO-2)(dcpe) (7).



L9332

Experimental

Data Collection

A yellow prismatic crystal of $C_{40}H_{56}ClF_2NiO_4P_2$ having approximate dimensions of 0.10 x 0.14 x 0.12 mm was mounted on a quartz fibre. All measurements were made on a Rigaku AFC6R diffractometer with graphite monochromated Cu-Kα radiation and a 12kW rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $84.27 < 2\theta < 100.42°$ corresponded to a primitive orthorhombic cell with dimensions:

a = 21.214(4) Å

b = 16.131(5) Å

c = 22.869(3) Å

V = 7825(2) Å^3

For Z = 8 and F.W. = 794.98, the calculated density is 1.35 g/cm^3. The systematic absences of:

0kl: k $\neq$ 2n

h0l: l $\neq$ 2n

hk0: h $\neq$ 2n

uniquely determine the space group to be:

Pbca (#61)

The data were collected at a temperature of 23 $\pm$ 1°C using the ω-2θ scan technique to a maximum 2θ value of 120.1°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.30° with a take-off angle of 6.0°. Scans of $(1.00 + 0.30 \tan \theta)°$ were made at a speed of 8.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 4 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 0.5 mm, the crystal to detector distance was 400 mm, and the detector aperture was 7.0 x 7.0 mm (horizontal x vertical).

Data Reduction

A total of 6431 reflections was collected. The intensities of three representative reflections were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Cu-Kα radiation is 25.2 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.88 to 1.00. The data were corrected for Lorentz and polarization effects.

L933-3

Structure Solution and Refinement

The structure was solved by and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in calculated positions but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 3271 observed reflections ($I > 3.00\sigma(I)$) and 452 variable parameters and converged (largest parameter shift was 0.03 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.050$$

$$R_w = \sqrt{(\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2)} = 0.047$$

The standard deviation of an observation of unit weight[4] was 1.99. The weighting scheme was based on counting statistics and included a factor (p = 0.007) to downweight the intense reflections. Plots of $\Sigma w(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.67 and -0.87 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) ~~ORIENT~~: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould. R.O., Smits, J.M.M. and Smykalla. C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(2) DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(|Fo| - |Fc|)^2$

where w = $\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$

$\sigma^2(Fo^2) = \frac{S^2(C+R^2B)+(pFo^2)^2}{Lp^2}$

S = Scan rate

C = Total Integrated Peak Count

R = Ratio of Scan Time to background counting time

B = Total Background Count

Lp = Lorentz-polarization factor

p = p-factor

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

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = number of variables

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

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

(7) 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).

(8) 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).

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

L9335

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{40}H_{55}ClF_2NiO_4P_2$
Formula Weight	794.98
Crystal Colour, Habit	yellow, prism
Crystal Dimensions	0.10 x 0.14 x 0.12 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (84.3 - 100.4°)
Omega Scan Peak Width at Half-height	0.30°
Lattice Parameters	a = 21.214(4) Å b = 16.131(5) Å c = 22.869(3) Å V = 7825(2) Å^3
Space Group	Pbca (#61)
Z value	8
D_{calc}	1.349 g/cm^3
F_{000}	3368.00
μ(CuKα)	25.16 cm^{-1}

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B. Intensity Measurements

Diffractometer	Rigaku AFC6R
Radiation	CuKα ($\lambda = 1.54178$ Å) graphite monochromated
Take-off Angle	6.0°
Detector Aperture	7.0 mm horizontal 7.0 mm vertical
Crystal to Detector Distance	400 mm
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	8.0°/min (in ω) (up to 4 scans)
Scan Width	$(1.00 + 0.30 \tan\theta)°$
$2\theta_{max}$	120.1°
No. of Reflections Measured	Total: 6431
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8838 - 1.0000)

h, k, l : -18 → 0 ; 0 → 74; 0 → 76

L933-7

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$
p-factor	0.007
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	3271
No. Variables	452
Reflection/Parameter Ratio	7.24
Residuals: R; Rw	0.050 ; 0.047
Goodness of Fit Indicator	1.99
Max Shift/Error in Final Cycle	0.03
Maximum peak in Final Diff. Map	0.67 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.87 $e^-/\AA^3$

L9338

Table 1. Atomic Coordinates and Isotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	x	y	z	B_{eq}
Ni(1)	0.19889(4)	0.03590(6)	0.04518(4)	2.08(2)
Cl(1)	0.2465(2)	0.2281(3)	0.7870(1)	17.9(2)
P(1)	0.29126(7)	0.09149(10)	0.04509(7)	2.08(3)
P(2)	0.16207(7)	0.1557(1)	0.06791(7)	2.00(3)
F(1)	0.0543(2)	0.0467(3)	-0.1844(2)	6.1(1)
F(2)	0.1705(2)	0.0002(3)	-0.2199(2)	6.5(1)
O(1)	0.2339(2)	-0.0687(3)	0.0237(2)	2.61(10)
O(2)	0.2567(2)	-0.1568(3)	-0.0469(2)	3.4(1)
O(3)	0.1179(2)	-0.0129(3)	0.0540(2)	3.0(1)
O(4)	0.0453(2)	-0.0984(3)	0.0191(2)	4.5(1)
C(1)	0.1771(3)	-0.0595(4)	-0.0667(3)	2.6(1)
C(2)	0.1162(3)	-0.0380(4)	-0.0492(3)	2.5(1)
C(3)	0.0740(3)	-0.0040(4)	-0.0892(3)	3.3(2)
C(4)	0.0934(4)	0.0099(5)	-0.1452(3)	3.9(2)
C(5)	0.1531(4)	-0.0120(5)	-0.1630(3)	3.9(2)
C(6)	0.1946(3)	-0.0487(4)	-0.1252(3)	3.2(2)
C(7)	0.2258(3)	-0.0987(4)	-0.0273(3)	2.2(1)
C(8)	0.0911(3)	-0.0525(4)	0.0124(3)	2.9(2)
C(9)	0.2881(3)	0.1844(4)	0.0901(2)	2.2(1)
C(10)	0.2268(3)	0.2311(4)	0.0753(3)	2.3(1)
C(11)	0.1100(3)	0.1954(4)	0.0102(3)	2.1(1)
C(12)	0.1416(3)	0.1867(4)	-0.0497(3)	2.4(1)
C(13)	0.0968(3)	0.2172(4)	-0.0983(3)	3.3(2)
C(14)	0.0784(3)	0.3059(5)	-0.0861(3)	4.3(2)

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Table 1. Atomic Coordinates and Isotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	x	y	z	B_{eq}
C(15)	0.0458(3)	0.3153(5)	-0.0271(3)	3.9(2)
C(16)	0.0887(3)	0.2851(4)	0.0211(3)	3.0(2)
C(17)	0.1196(3)	0.1625(4)	0.1381(3)	2.8(2)
C(18)	0.0528(3)	0.1280(4)	0.1364(3)	3.7(2)
C(19)	0.0208(3)	0.1393(6)	0.1954(3)	5.3(2)
C(20)	0.0574(4)	0.0984(6)	0.2436(3)	6.1(3)
C(21)	0.1237(4)	0.1318(6)	0.2466(3)	6.0(2)
C(22)	0.1571(3)	0.1240(5)	0.1874(3)	4.0(2)
C(23)	0.3188(3)	0.1238(4)	-0.0287(3)	2.6(2)
C(24)	0.3479(3)	0.0519(4)	-0.0624(3)	3.0(2)
C(25)	0.3635(3)	0.0792(5)	-0.1254(3)	4.0(2)
C(26)	0.4059(3)	0.1546(5)	-0.1263(3)	4.1(2)
C(27)	0.3775(3)	0.2257(5)	-0.0919(3)	4.1(2)
C(28)	0.3620(3)	0.2010(4)	-0.0293(3)	3.2(2)
C(29)	0.3501(3)	0.0216(4)	0.0774(2)	2.1(1)
C(30)	0.4155(3)	0.0607(4)	0.0860(3)	2.7(1)
C(31)	0.4612(3)	-0.0021(4)	0.1109(3)	3.1(2)
C(32)	0.4378(3)	-0.0382(4)	0.1680(3)	3.3(2)
C(33)	0.3730(3)	-0.0770(4)	0.1597(3)	3.0(2)
C(34)	0.3259(3)	-0.0148(4)	0.1351(3)	2.6(1)
C(35)	0.3102(5)	0.2142(8)	0.7398(4)	6.5(3)
C(36)	0.3107(6)	0.1476(6)	0.7077(5)	6.9(3)
C(37)	0.3602(8)	0.1369(7)	0.6713(5)	8.8(4)
C(38)	0.4089(7)	0.194(1)	0.6692(6)	11.5(7)

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Table 1. Atomic Coordinates and Isotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	x	y	z	B_{eq}
C(39)	0.4074(9)	0.259(1)	0.7038(7)	13.3(8)
C(40)	0.3575(9)	0.2710(7)	0.7406(5)	9.7(5)
H(3)	0.0323	0.0094	-0.0777	3.9655
H(6)	0.2347	-0.0667	-0.1385	3.8724
H(9a)	0.2884	0.1695	0.1303	2.6842
H(9b)	0.3234	0.2187	0.0819	2.6842
H(10a)	0.2320	0.2604	0.0396	2.8142
H(10b)	0.2173	0.2692	0.1058	2.8142
H(11)	0.0733	0.1616	0.0098	2.5349
H(12a)	0.1791	0.2189	-0.0503	2.8265
H(12b)	0.1518	0.1301	-0.0564	2.8265
H(13a)	0.1175	0.2140	-0.1351	3.9142
H(13b)	0.0602	0.1834	-0.0990	3.9142
H(14a)	0.0506	0.3242	-0.1160	5.1878
H(14a)	0.0494	0.3266	-0.1179	4.6169
H(15a)	0.0359	0.3720	-0.0208	4.6400
H(15b)	0.0081	0.2835	-0.0270	4.6400
H(16a)	0.0667	0.2876	0.0573	3.6089
H(16b)	0.1247	0.3200	0.0229	3.6089
H(17)	0.1160	0.2198	0.1470	3.3444
H(18a)	0.0294	0.1565	0.1072	4.4018
H(18b)	0.0544	0.0706	0.1271	4.4018
H(19a)	0.0174	0.1969	0.2036	6.3053
H(19b)	-0.0201	0.1156	0.1938	6.3053

L933-11

Table 1. Atomic Coordinates and Isotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	x	y	z	B_{eq}
H(20a)	0.0368	0.1085	0.2798	7.2680
H(20b)	0.0589	0.0404	0.2365	7.2680
H(21a)	0.1222	0.1886	0.2575	7.2090
H(21b)	0.1466	0.1014	0.2751	7.2090
H(22a)	0.1633	0.0669	0.1790	4.8251
H(22b)	0.1967	0.1510	0.1898	4.8251
H(23)	0.2821	0.1391	-0.0498	3.1500
H(24a)	0.3854	0.0346	-0.0434	3.5989
H(24b)	0.3189	0.0070	-0.0636	3.5989
H(25a)	0.3841	0.0349	-0.1449	4.7639
H(25b)	0.3254	0.0921	-0.1452	4.7639
H(26a)	0.4454	0.1404	-0.1096	4.9591
H(26b)	0.4118	0.1717	-0.1657	4.9591
H(27a)	0.4068	0.2703	-0.0911	4.9586
H(27b)	0.3400	0.2432	-0.1107	4.9586
H(28a)	0.3411	0.2457	-0.0104	3.8263
H(28b)	0.3999	0.1886	-0.0090	3.8263
H(29)	0.3552	-0.0234	0.0510	2.5712
H(30a)	0.4308	0.0797	0.0494	3.1895
H(30b)	0.4120	0.1061	0.1123	3.1895
H(31a)	0.4665	-0.0457	0.0835	3.7525
H(31b)	0.5005	0.0244	0.1176	3.7525
H(32a)	0.4664	-0.0795	0.1811	3.9646
H(32b)	0.4351	0.0047	0.1965	3.9646

L933-12

Table 1. Atomic Coordinates and Isotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	x	y	z	B_{eq}
H(33a)	0.3765	-0.1224	0.1334	3.6090
H(33b)	0.3581	-0.0963	0.1965	3.6090
H(34a)	0.3201	0.0287	0.1626	3.0677
H(34b)	0.2869	-0.0420	0.1284	3.0677
H(36)	0.2776	0.1082	0.7097	8.3186
H(37)	0.3617	0.0893	0.6469	10.5424
H(38)	0.4430	0.1868	0.6428	13.8029
H(39)	0.4411	0.2977	0.7034	15.9875
H(40)	0.3560	0.3176	0.7660	11.6822
H(41)	0.1153	0.3393	-0.0863	5.1878

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

L933-13

Table 2. Anisotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	0.0219(5)	0.0283(6)	0.0289(5)	-0.0018(5)	-0.0020(5)	-0.0013(5)
Cl(1)	0.160(3)	0.402(7)	0.118(3)	0.181(4)	0.018(3)	0.054(4)
P(1)	0.0210(8)	0.0319(9)	0.0262(8)	0.0007(7)	-0.0019(8)	-0.0006(8)
P(2)	0.0209(8)	0.0295(9)	0.0257(8)	0.0006(8)	0.0004(7)	-0.0008(8)
F(1)	0.087(3)	0.081(4)	0.062(3)	0.018(3)	-0.038(3)	-0.001(3)
F(2)	0.101(4)	0.115(4)	0.033(2)	0.014(3)	-0.005(3)	0.009(3)
O(1)	0.031(3)	0.031(3)	0.036(2)	0.003(2)	-0.011(2)	-0.006(2)
O(2)	0.044(3)	0.040(3)	0.044(3)	0.015(2)	0.002(3)	-0.003(3)
O(3)	0.032(2)	0.041(3)	0.039(3)	-0.014(2)	0.006(2)	-0.010(2)
O(4)	0.042(3)	0.058(4)	0.070(4)	-0.028(3)	0.007(3)	-0.008(3)
C(1)	0.039(4)	0.030(4)	0.029(3)	-0.005(3)	-0.005(3)	-0.006(3)
C(2)	0.030(3)	0.025(3)	0.039(4)	-0.002(3)	-0.010(3)	-0.006(3)
C(3)	0.033(4)	0.045(5)	0.047(4)	-0.002(4)	-0.011(4)	-0.010(4)
C(4)	0.056(5)	0.053(5)	0.040(4)	0.007(4)	-0.025(4)	-0.002(4)
C(5)	0.070(6)	0.047(5)	0.031(4)	0.002(4)	-0.006(4)	0.001(4)
C(6)	0.046(4)	0.044(4)	0.033(4)	0.004(4)	-0.002(4)	-0.002(3)
C(7)	0.025(3)	0.023(4)	0.038(4)	-0.001(3)	0.003(3)	0.004(3)
C(8)	0.032(4)	0.030(4)	0.049(5)	0.003(3)	0.003(4)	0.000(3)
C(9)	0.021(3)	0.034(4)	0.030(3)	0.005(3)	-0.002(3)	-0.002(3)
C(10)	0.025(3)	0.036(4)	0.028(4)	0.005(3)	-0.002(3)	-0.003(3)
C(11)	0.019(3)	0.029(4)	0.033(4)	-0.002(3)	-0.001(3)	0.001(3)
C(12)	0.027(3)	0.033(4)	0.029(4)	-0.001(3)	-0.002(3)	-0.003(3)
C(13)	0.040(4)	0.045(5)	0.039(4)	-0.003(4)	-0.012(4)	0.004(4)
C(14)	0.061(5)	0.056(5)	0.047(5)	0.019(5)	-0.031(4)	0.009(4)

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Table 2. Anisotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(15)	0.043(4)	0.048(5)	0.056(5)	0.017(4)	-0.009(4)	-0.004(4)
C(16)	0.030(4)	0.040(4)	0.044(4)	0.007(3)	-0.001(3)	-0.001(3)
C(17)	0.036(4)	0.043(4)	0.026(4)	-0.008(4)	0.010(3)	-0.003(3)
C(18)	0.032(4)	0.063(5)	0.044(4)	-0.004(4)	0.009(3)	-0.008(4)
C(19)	0.048(5)	0.099(8)	0.052(5)	-0.032(5)	0.025(4)	-0.025(5)
C(20)	0.072(6)	0.115(8)	0.044(5)	-0.038(6)	0.026(5)	-0.009(6)
C(21)	0.069(6)	0.132(9)	0.027(4)	-0.035(6)	0.002(4)	0.004(5)
C(22)	0.038(4)	0.082(6)	0.033(4)	-0.012(4)	0.002(4)	0.005(4)
C(23)	0.023(3)	0.047(4)	0.029(4)	0.011(3)	-0.001(3)	0.009(3)
C(24)	0.035(4)	0.041(4)	0.038(4)	-0.002(3)	0.001(3)	0.000(3)
C(25)	0.052(5)	0.063(5)	0.036(4)	0.015(4)	0.006(4)	0.004(4)
C(26)	0.046(5)	0.067(6)	0.044(5)	0.021(4)	0.014(4)	0.023(4)
C(27)	0.042(4)	0.050(5)	0.065(5)	0.012(4)	0.010(4)	0.031(4)
C(28)	0.034(4)	0.036(4)	0.051(5)	0.009(3)	0.008(3)	0.012(3)
C(29)	0.019(3)	0.032(4)	0.031(4)	0.002(3)	-0.003(3)	0.003(3)
C(30)	0.024(3)	0.038(4)	0.039(4)	0.000(3)	-0.007(3)	0.004(3)
C(31)	0.024(4)	0.047(4)	0.048(4)	0.004(3)	-0.008(3)	0.005(4)
C(32)	0.033(4)	0.052(5)	0.041(4)	0.011(4)	-0.009(3)	0.002(4)
C(33)	0.045(4)	0.042(5)	0.027(4)	0.008(4)	0.000(3)	0.004(3)
C(34)	0.027(3)	0.036(4)	0.034(3)	0.001(3)	-0.001(3)	0.009(3)
C(35)	0.090(8)	0.106(9)	0.051(6)	0.056(7)	-0.022(6)	0.001(6)
C(36)	0.116(9)	0.070(7)	0.078(7)	-0.011(7)	-0.042(7)	-0.019(6)
C(37)	0.18(2)	0.076(9)	0.073(8)	0.055(10)	-0.004(9)	-0.002(7)
C(38)	0.08(1)	0.26(3)	0.10(1)	0.05(1)	0.002(9)	0.10(1)

L933-15

Table 2. Anisotropic Displacement Parameters for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(39)	0.17(2)	0.21(2)	0.12(2)	-0.11(2)	-0.12(2)	0.12(2)
C(40)	0.25(2)	0.045(6)	0.074(9)	-0.021(10)	-0.10(1)	0.006(6)

The general temperature factor expression:

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

L933-16

Table 3. Interatomic Distances (Å) Involving Non-Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	atom	distance	atom	atom	distance
Ni(1)	P(1)	2.155(2)	Ni(1)	P(2)	2.149(2)
Ni(1)	O(1)	1.907(4)	Ni(1)	O(3)	1.901(4)
Cl(1)	C(35)	1.744(10)	P(1)	C(9)	1.819(6)
P(1)	C(23)	1.860(6)	P(1)	C(29)	1.837(6)
P(2)	C(10)	1.842(6)	P(2)	C(11)	1.837(6)
P(2)	C(17)	1.843(6)	F(1)	C(4)	1.359(7)
F(2)	C(5)	1.368(7)	O(1)	C(7)	1.274(7)
O(2)	C(7)	1.229(7)	O(3)	C(8)	1.278(7)
O(4)	C(8)	1.232(7)	C(1)	C(2)	1.396(8)
C(1)	C(6)	1.398(8)	C(1)	C(7)	1.510(8)
C(2)	C(3)	1.393(8)	C(2)	C(8)	1.524(8)
C(3)	C(4)	1.361(9)	C(4)	C(5)	1.378(9)
C(5)	C(6)	1.368(9)	C(9)	C(10)	1.541(7)
C(11)	C(12)	1.531(8)	C(11)	C(16)	1.538(8)
C(12)	C(13)	1.543(8)	C(13)	C(14)	1.510(9)
C(14)	C(15)	1.523(9)	C(15)	C(16)	1.510(8)
C(17)	C(18)	1.523(8)	C(17)	C(22)	1.512(9)
C(18)	C(19)	1.523(9)	C(19)	C(20)	1.50(1)
C(20)	C(21)	1.51(1)	C(21)	C(22)	1.534(9)
C(23)	C(24)	1.524(8)	C(23)	C(28)	1.546(8)
C(24)	C(25)	1.541(8)	C(25)	C(26)	1.513(10)
C(26)	C(27)	1.516(10)	C(27)	C(28)	1.521(9)
C(29)	C(30)	1.535(7)	C(29)	C(34)	1.535(8)
C(30)	C(31)	1.513(8)	C(31)	C(32)	1.513(9)

L933-17

Table 3. Interatomic Distances (Å) Involving Non-Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	distance	atom	atom	distance
C(32)	C(33)	1.522(9)	C(33)	C(34)	1.523(8)
C(35)	C(36)	1.30(1)	C(35)	C(40)	1.36(1)
C(36)	C(37)	1.35(1)	C(37)	C(38)	1.39(2)
C(38)	C(39)	1.31(2)	C(39)	C(40)	1.36(2)

L933-18

Table 4. Interatomic Distances (Å) Involving Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	atom	distance	atom	atom	distance
C(3)	H(3)	0.95	C(6)	H(6)	0.95
C(9)	H(9a)	0.95	C(9)	H(9b)	0.95
C(10)	H(10a)	0.95	C(10)	H(10b)	0.95
C(11)	H(11)	0.95	C(12)	H(12a)	0.95
C(12)	H(12b)	0.95	C(13)	H(13a)	0.95
C(13)	H(13b)	0.95	C(14)	H(14a)	0.95
C(14)	H(14a)	1.01	C(14)	H(41)	0.95
C(15)	H(15a)	0.95	C(15)	H(15b)	0.95
C(16)	H(16a)	0.95	C(16)	H(16b)	0.95
C(17)	H(17)	0.95	C(18)	H(18a)	0.95
C(18)	H(18b)	0.95	C(19)	H(19a)	0.95
C(19)	H(19b)	0.95	C(20)	H(20a)	0.95
C(20)	H(20b)	0.95	C(21)	H(21a)	0.95
C(21)	H(21b)	0.95	C(22)	H(22a)	0.95
C(22)	H(22b)	0.95	C(23)	H(23)	0.95
C(24)	H(24a)	0.95	C(24)	H(24b)	0.95
C(25)	H(25a)	0.95	C(25)	H(25b)	0.95
C(26)	H(26a)	0.95	C(26)	H(26b)	0.95
C(27)	H(27a)	0.95	C(27)	H(27b)	0.95
C(28)	H(28a)	0.95	C(28)	H(28b)	0.95
C(29)	H(29)	0.95	C(30)	H(30a)	0.95
C(30)	H(30b)	0.95	C(31)	H(31a)	0.95
C(31)	H(31b)	0.95	C(32)	H(32a)	0.95
C(32)	H(32b)	0.95	C(33)	H(33a)	0.95

L933-19

Table 4. Interatomic Distances (Å) Involving Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	distance	atom	atom	distance
C(33)	H(33b)	0.95	C(34)	H(34a)	0.95
C(34)	H(34b)	0.95	C(36)	H(36)	0.95
C(37)	H(37)	0.95	C(38)	H(38)	0.95
C(39)	H(39)	0.95	C(40)	H(40)	0.95

L933-20

Table 5. Interatomic Angles (°) Involving Non-Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ni(1)	P(2)	87.50(7)	P(1)	Ni(1)	O(1)	90.8(1)
P(1)	Ni(1)	O(3)	174.0(1)	P(2)	Ni(1)	O(1)	178.1(1)
P(2)	Ni(1)	O(3)	91.0(1)	O(1)	Ni(1)	O(3)	90.7(2)
Ni(1)	P(1)	C(9)	108.0(2)	Ni(1)	P(1)	C(23)	113.8(2)
Ni(1)	P(1)	C(29)	111.3(2)	C(9)	P(1)	C(23)	107.1(3)
C(9)	P(1)	C(29)	107.6(3)	C(23)	P(1)	C(29)	108.8(3)
Ni(1)	P(2)	C(10)	110.2(2)	Ni(1)	P(2)	C(11)	111.0(2)
Ni(1)	P(2)	C(17)	116.2(2)	C(10)	P(2)	C(11)	106.6(3)
C(10)	P(2)	C(17)	104.2(3)	C(11)	P(2)	C(17)	108.2(3)
Ni(1)	O(1)	C(7)	121.3(4)	Ni(1)	O(3)	C(8)	122.0(4)
C(2)	C(1)	C(6)	119.2(6)	C(2)	C(1)	C(7)	124.5(6)
C(6)	C(1)	C(7)	116.2(6)	C(1)	C(2)	C(3)	120.2(6)
C(1)	C(2)	C(8)	123.4(6)	C(3)	C(2)	C(8)	116.4(6)
C(2)	C(3)	C(4)	119.2(7)	F(1)	C(4)	C(3)	120.5(7)
F(1)	C(4)	C(5)	118.6(7)	C(3)	C(4)	C(5)	120.9(7)
F(2)	C(5)	C(4)	119.6(7)	F(2)	C(5)	C(6)	119.4(7)
C(4)	C(5)	C(6)	121.0(7)	C(1)	C(6)	C(5)	119.3(6)
O(1)	C(7)	O(2)	123.6(6)	O(1)	C(7)	C(1)	118.6(5)
O(2)	C(7)	C(1)	117.8(6)	O(3)	C(8)	O(4)	123.9(6)
O(3)	C(8)	C(2)	117.1(6)	O(4)	C(8)	C(2)	118.9(6)
P(1)	C(9)	C(10)	108.0(4)	P(2)	C(10)	C(9)	109.1(4)
P(2)	C(11)	C(12)	110.3(4)	P(2)	C(11)	C(16)	112.8(4)
C(12)	C(11)	C(16)	111.2(5)	C(11)	C(12)	C(13)	110.1(5)
C(12)	C(13)	C(14)	109.2(5)	C(13)	C(14)	C(15)	112.0(6)

L933-21

Table 5. Interatomic Angles (°) Involving Non-Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(15)	C(16)	110.0(5)	C(11)	C(16)	C(15)	111.2(6)
P(2)	C(17)	C(18)	114.2(5)	P(2)	C(17)	C(22)	111.6(5)
C(18)	C(17)	C(22)	111.0(6)	C(17)	C(18)	C(19)	110.4(6)
C(18)	C(19)	C(20)	111.5(7)	C(19)	C(20)	C(21)	111.0(7)
C(20)	C(21)	C(22)	111.2(6)	C(17)	C(22)	C(21)	112.4(6)
P(1)	C(23)	C(24)	111.9(4)	P(1)	C(23)	C(28)	114.8(4)
C(24)	C(23)	C(28)	111.6(5)	C(23)	C(24)	C(25)	110.0(5)
C(24)	C(25)	C(26)	111.8(6)	C(25)	C(26)	C(27)	111.4(6)
C(26)	C(27)	C(28)	112.1(6)	C(23)	C(28)	C(27)	110.4(6)
P(1)	C(29)	C(30)	114.4(4)	P(1)	C(29)	C(34)	110.7(4)
C(30)	C(29)	C(34)	110.3(5)	C(29)	C(30)	C(31)	110.6(5)
C(30)	C(31)	C(32)	111.8(5)	C(31)	C(32)	C(33)	110.3(5)
C(32)	C(33)	C(34)	111.5(5)	C(29)	C(34)	C(33)	110.6(5)
Cl(1)	C(35)	C(36)	117(1)	Cl(1)	C(35)	C(40)	118(1)
C(36)	C(35)	C(40)	123(1)	C(35)	C(36)	C(37)	117(1)
C(36)	C(37)	C(38)	120(1)	C(37)	C(38)	C(39)	119(1)
C(38)	C(39)	C(40)	120(1)	C(35)	C(40)	C(39)	117(1)

L933-22

Table 6. Interatomic Angles (°) Involving Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(3)	120.3	C(4)	C(3)	H(3)	120.4
C(1)	C(6)	H(6)	120.4	C(5)	C(6)	H(6)	120.3
P(1)	C(9)	H(9a)	109.9	P(1)	C(9)	H(9b)	109.9
C(10)	C(9)	H(9a)	109.9	C(10)	C(9)	H(9b)	109.7
H(9a)	C(9)	H(9b)	109.5	P(2)	C(10)	H(10a)	109.5
P(2)	C(10)	H(10b)	109.6	C(9)	C(10)	H(10a)	109.6
C(9)	C(10)	H(10b)	109.5	H(10a)	C(10)	H(10b)	109.5
P(2)	C(11)	H(11)	107.4	C(12)	C(11)	H(11)	107.4
C(16)	C(11)	H(11)	107.5	C(11)	C(12)	H(12a)	109.3
C(11)	C(12)	H(12b)	109.3	C(13)	C(12)	H(12a)	109.3
C(13)	C(12)	H(12b)	109.3	H(12a)	C(12)	H(12b)	109.5
C(12)	C(13)	H(13a)	109.6	C(12)	C(13)	H(13b)	109.5
C(14)	C(13)	H(13a)	109.5	C(14)	C(13)	H(13b)	109.6
H(13a)	C(13)	H(13b)	109.4	C(13)	C(14)	H(14a)	108.8
C(13)	C(14)	H(14a)	109.8	C(13)	C(14)	H(41)	108.9
C(15)	C(14)	H(14a)	108.9	C(15)	C(14)	H(14a)	109.1
C(15)	C(14)	H(41)	108.8	H(14a)	C(14)	H(14a)	1.3
H(14a)	C(14)	H(41)	109.4	H(14a)	C(14)	H(41)	108.1
C(14)	C(15)	H(15a)	109.4	C(14)	C(15)	H(15b)	109.3
C(16)	C(15)	H(15a)	109.4	C(16)	C(15)	H(15b)	109.3
H(15a)	C(15)	H(15b)	109.5	C(11)	C(16)	H(16a)	109.0
C(11)	C(16)	H(16b)	109.1	C(15)	C(16)	H(16a)	109.1
C(15)	C(16)	H(16b)	109.0	H(16a)	C(16)	H(16b)	109.4
P(2)	C(17)	H(17)	106.5	C(18)	C(17)	H(17)	106.5

L933-23

Table 6. Interatomic Angles (°) Involving Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
C(22)	C(17)	H(17)	106.5	C(17)	C(18)	H(18a)	109.2
C(17)	C(18)	H(18b)	109.3	C(19)	C(18)	H(18a)	109.3
C(19)	C(18)	H(18b)	109.2	H(18a)	C(18)	H(18b)	109.5
C(18)	C(19)	H(19a)	109.0	C(18)	C(19)	H(19b)	108.9
C(20)	C(19)	H(19a)	109.0	C(20)	C(19)	H(19b)	108.9
H(19a)	C(19)	H(19b)	109.5	C(19)	C(20)	H(20a)	109.1
C(19)	C(20)	H(20b)	109.1	C(21)	C(20)	H(20a)	109.0
C(21)	C(20)	H(20b)	109.1	H(20a)	C(20)	H(20b)	109.5
C(20)	C(21)	H(21a)	109.1	C(20)	C(21)	H(21b)	109.0
C(22)	C(21)	H(21a)	109.0	C(22)	C(21)	H(21b)	109.1
H(21a)	C(21)	H(21b)	109.5	C(17)	C(22)	H(22a)	108.7
C(17)	C(22)	H(22b)	108.7	C(21)	C(22)	H(22a)	108.7
C(21)	C(22)	H(22b)	108.7	H(22a)	C(22)	H(22b)	109.5
P(1)	C(23)	H(23)	106.0	C(24)	C(23)	H(23)	105.9
C(28)	C(23)	H(23)	105.8	C(23)	C(24)	H(24a)	109.3
C(23)	C(24)	H(24b)	109.4	C(25)	C(24)	H(24a)	109.4
C(25)	C(24)	H(24b)	109.3	H(24a)	C(24)	H(24b)	109.4
C(24)	C(25)	H(25a)	108.9	C(24)	C(25)	H(25b)	109.0
C(26)	C(25)	H(25a)	109.0	C(26)	C(25)	H(25b)	108.8
H(25a)	C(25)	H(25b)	109.4	C(25)	C(26)	H(26a)	108.9
C(25)	C(26)	H(26b)	109.0	C(27)	C(26)	H(26a)	109.0
C(27)	C(26)	H(26b)	109.0	H(26a)	C(26)	H(26b)	109.5
C(26)	C(27)	H(27a)	108.9	C(26)	C(27)	H(27b)	108.8
C(28)	C(27)	H(27a)	108.8	C(28)	C(27)	H(27b)	108.9

2933-24

Table 6. Interatomic Angles (°) Involving Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
H(27a)	C(27)	H(27b)	109.4	C(23)	C(28)	H(28a)	109.3
C(23)	C(28)	H(28b)	109.2	C(27)	C(28)	H(28a)	109.2
C(27)	C(28)	H(28b)	109.3	H(28a)	C(28)	H(28b)	109.4
P(1)	C(29)	H(29)	106.9	C(30)	C(29)	H(29)	107.0
C(34)	C(29)	H(29)	107.0	C(29)	C(30)	H(30a)	109.1
C(29)	C(30)	H(30b)	109.2	C(31)	C(30)	H(30a)	109.2
C(31)	C(30)	H(30b)	109.2	H(30a)	C(30)	H(30b)	109.5
C(30)	C(31)	H(31a)	108.9	C(30)	C(31)	H(31b)	108.8
C(32)	C(31)	H(31a)	108.9	C(32)	C(31)	H(31b)	108.9
H(31a)	C(31)	H(31b)	109.5	C(31)	C(32)	H(32a)	109.3
C(31)	C(32)	H(32b)	109.3	C(33)	C(32)	H(32a)	109.2
C(33)	C(32)	H(32b)	109.3	H(32a)	C(32)	H(32b)	109.5
C(32)	C(33)	H(33a)	109.0	C(32)	C(33)	H(33b)	108.9
C(34)	C(33)	H(33a)	108.9	C(34)	C(33)	H(33b)	109.0
H(33a)	C(33)	H(33b)	109.5	C(29)	C(34)	H(34a)	109.2
C(29)	C(34)	H(34b)	109.2	C(33)	C(34)	H(34a)	109.2
C(33)	C(34)	H(34b)	109.1	H(34a)	C(34)	H(34b)	109.5
C(35)	C(36)	H(36)	121.4	C(37)	C(36)	H(36)	121.3
C(36)	C(37)	H(37)	119.5	C(38)	C(37)	H(37)	119.5
C(37)	C(38)	H(38)	120.2	C(39)	C(38)	H(38)	120.3
C(38)	C(39)	H(39)	120.0	C(40)	C(39)	H(39)	119.8
C(35)	C(40)	H(40)	121.0	C(39)	C(40)	H(40)	121.0

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Table 7. Torsion Angles (°) Involving Non-Hydrogen atoms for $C_{40}H_{56}ClF_2NiO_4P_2$

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ni(1)	P(1)	C(9)	C(10)	-43.2(4)	Ni(1)	P(1)	C(23)	C(24)	-83.3(4)
Ni(1)	P(1)	C(23)	C(28)	148.1(4)	Ni(1)	P(1)	C(29)	C(30)	-172.7(4)
Ni(1)	P(1)	C(29)	C(34)	-47.2(4)	Ni(1)	P(2)	C(10)	C(9)	-24.6(4)
Ni(1)	P(2)	C(11)	C(12)	-48.3(4)	Ni(1)	P(2)	C(11)	C(16)	-173.3(4)
Ni(1)	P(2)	C(17)	C(18)	-77.5(5)	Ni(1)	P(2)	C(17)	C(22)	49.4(5)
Ni(1)	O(1)	C(7)	O(2)	165.4(5)	Ni(1)	O(1)	C(7)	C(1)	-12.6(7)
Ni(1)	O(3)	C(8)	O(4)	165.1(5)	Ni(1)	O(3)	C(8)	C(2)	-17.9(8)
Cl(1)	C(35)	C(36)	C(37)	-179.7(8)	Cl(1)	C(35)	C(40)	C(39)	179(1)
P(1)	Ni(1)	P(2)	C(10)	-1.2(2)	P(1)	Ni(1)	P(2)	C(11)	116.6(2)
P(1)	Ni(1)	P(2)	C(17)	-119.4(2)	P(1)	Ni(1)	O(1)	C(7)	-108.6(4)
P(1)	Ni(1)	O(3)	C(8)	-161(1)	P(1)	C(9)	C(10)	P(2)	41.8(5)
P(1)	C(23)	C(24)	C(25)	174.0(4)	P(1)	C(23)	C(28)	C(27)	-175.7(4)
P(1)	C(29)	C(30)	C(31)	-178.2(4)	P(1)	C(29)	C(34)	C(33)	176.3(4)
P(2)	Ni(1)	P(1)	C(9)	22.5(2)	P(2)	Ni(1)	P(1)	C(23)	-96.2(2)
P(2)	Ni(1)	P(1)	C(29)	140.4(2)	P(2)	Ni(1)	O(1)	C(7)	-80(4)
P(2)	Ni(1)	O(3)	C(8)	122.7(5)	P(2)	C(11)	C(12)	C(13)	178.0(4)
P(2)	C(11)	C(16)	C(15)	-179.8(4)	P(2)	C(17)	C(18)	C(19)	-177.7(5)
P(2)	C(17)	C(22)	C(21)	177.9(5)	F(1)	C(4)	C(3)	C(2)	-176.8(6)
F(1)	C(4)	C(5)	F(2)	-2(1)	F(1)	C(4)	C(5)	C(6)	179.6(6)
F(2)	C(5)	C(4)	C(3)	177.8(7)	F(2)	C(5)	C(6)	C(1)	178.7(6)
O(1)	Ni(1)	P(1)	C(9)	-158.4(2)	O(1)	Ni(1)	P(1)	C(23)	82.9(3)
O(1)	Ni(1)	P(1)	C(29)	-40.5(2)	O(1)	Ni(1)	P(2)	C(10)	-28(4)
O(1)	Ni(1)	P(2)	C(11)	88(4)	O(1)	Ni(1)	P(2)	C(17)	-147(4)
O(1)	Ni(1)	O(3)	C(8)	-56.6(5)	O(1)	C(7)	C(1)	C(2)	-45.9(9)

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Table 7. Torsion Angles (°) Involving Non-Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(1)	C(7)	C(1)	C(6)	137.5(6)	O(2)	C(7)	C(1)	C(2)	135.9(6)
O(2)	C(7)	C(1)	C(6)	-40.7(8)	O(3)	Ni(1)	P(1)	C(9)	-53(1)
O(3)	Ni(1)	P(1)	C(23)	-172(1)	O(3)	Ni(1)	P(1)	C(29)	64(1)
O(3)	Ni(1)	P(2)	C(10)	173.0(2)	O(3)	Ni(1)	P(2)	C(11)	-69.3(2)
O(3)	Ni(1)	P(2)	C(17)	54.8(3)	O(3)	Ni(1)	O(1)	C(7)	77.3(4)
O(3)	C(8)	C(2)	C(1)	64.2(9)	O(3)	C(8)	C(2)	C(3)	-118.1(6)
O(4)	C(8)	C(2)	C(1)	-118.7(7)	O(4)	C(8)	C(2)	C(3)	59.0(9)
C(1)	C(2)	C(3)	C(4)	-1(1)	C(1)	C(6)	C(5)	C(4)	-3(1)
C(2)	C(1)	C(6)	C(5)	4(1)	C(2)	C(3)	C(4)	C(5)	2(1)
C(3)	C(2)	C(1)	C(6)	-1.8(10)	C(3)	C(2)	C(1)	C(7)	-178.3(6)
C(3)	C(4)	C(5)	C(6)	0(1)	C(4)	C(3)	C(2)	C(8)	-179.5(6)
C(5)	C(6)	C(1)	C(7)	-178.7(6)	C(6)	C(1)	C(2)	C(8)	175.8(6)
C(7)	C(1)	C(2)	C(8)	-0.7(10)	C(9)	P(1)	C(23)	C(24)	157.4(4)
C(9)	P(1)	C(23)	C(28)	28.8(5)	C(9)	P(1)	C(29)	C(30)	-54.5(5)
C(9)	P(1)	C(29)	C(34)	71.0(5)	C(9)	C(10)	P(2)	C(11)	-145.1(4)
C(9)	C(10)	P(2)	C(17)	100.7(4)	C(10)	P(2)	C(11)	C(12)	71.6(5)
C(10)	P(2)	C(11)	C(16)	-53.4(5)	C(10)	P(2)	C(17)	C(18)	161.1(5)
C(10)	P(2)	C(17)	C(22)	-71.9(5)	C(10)	C(9)	P(1)	C(23)	79.8(4)
C(10)	C(9)	P(1)	C(29)	-163.4(4)	C(11)	P(2)	C(17)	C(18)	48.0(6)
C(11)	P(2)	C(17)	C(22)	175.0(5)	C(11)	C(12)	C(13)	C(14)	57.3(7)
C(11)	C(16)	C(15)	C(14)	-55.6(8)	C(12)	C(11)	P(2)	C(17)	-176.9(4)
C(12)	C(11)	C(16)	C(15)	55.7(7)	C(12)	C(13)	C(14)	C(15)	-59.1(7)
C(13)	C(12)	C(11)	C(16)	-56.1(6)	C(13)	C(14)	C(15)	C(16)	58.6(8)
C(16)	C(11)	P(2)	C(17)	58.2(5)	C(17)	C(18)	C(19)	C(20)	-57.6(9)

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Table 7. Torsion Angles (°) Involving Non-Hydrogen Atoms for $C_{40}H_{56}ClF_2NiO_4P_2$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(17)	C(22)	C(21)	C(20)	53.3(10)	C(18)	C(17)	C(22)	C(21)	-53.4(8)
C(18)	C(19)	C(20)	C(21)	57.7(10)	C(19)	C(18)	C(17)	C(22)	55.0(8)
C(19)	C(20)	C(21)	C(22)	-54(1)	C(23)	P(1)	C(29)	C(30)	61.2(5)
C(23)	P(1)	C(29)	C(34)	-173.3(4)	C(23)	C(24)	C(25)	C(26)	55.7(7)
C(23)	C(28)	C(27)	C(26)	-54.8(8)	C(24)	C(23)	P(1)	C(29)	41.3(5)
C(24)	C(23)	C(28)	C(27)	55.6(7)	C(24)	C(25)	C(26)	C(27)	-55.5(8)
C(25)	C(24)	C(23)	C(28)	-55.7(7)	C(25)	C(26)	C(27)	C(28)	55.3(8)
C(28)	C(23)	P(1)	C(29)	-87.3(5)	C(29)	C(30)	C(31)	C(32)	-57.0(7)
C(29)	C(34)	C(33)	C(32)	56.5(7)	C(30)	C(29)	C(34)	C(33)	-56.0(7)
C(30)	C(31)	C(32)	C(33)	56.6(8)	C(31)	C(30)	C(29)	C(34)	56.1(7)
C(31)	C(32)	C(33)	C(34)	-56.3(7)	C(35)	C(36)	C(37)	C(38)	0(1)
C(35)	C(40)	C(39)	C(38)	0(2)	C(36)	C(35)	C(40)	C(39)	2(1)
C(36)	C(37)	C(38)	C(39)	1(2)	C(37)	C(36)	C(35)	C(40)	-2(1)
C(37)	C(38)	C(39)	C(40)	-1(2)					