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Single crystal X-ray data were collected at 23 °C using an orange crystal of dimensions 0.38 x 0.62 x 0.28 mm on a Siemens P3 diffractometer equipped with a molybdenum tube [$\lambda(K\alpha_1) = 0.70926 \text{ \AA}$; $\lambda(K\alpha_2) = 0.71354 \text{ \AA}$] and a graphite monochromator. The compound crystallized in the centrosymmetric space group $P2_1/c$ with two independent molecules ($Z = 8$) in a cell of dimensions $a = 19.456(4) \text{ \AA}$, $b = 10.485(2) \text{ \AA}$, $c = 29.174(6) \text{ \AA}$, $\beta = 94.75(3)^\circ$, and $V = 5931(2) \text{ \AA}^3$. A total of 9224 independent reflections were gathered ($R_{\text{int}} = 0.017$), the octants collected being $+h$, $-k$, $\pm l$, using the Wyckoff scan method. Three standard reflections were measured after every 100 reflections collected. The structure was solved by direct methods and refined by full-matrix least-squares techniques using structure solution programs from the SHELXTL system. *reference* All nonhydrogen atoms were refined anisotropically. Hydrogen atoms were placed in fixed calculated positions ($C-H = 0.96 \text{ \AA}$). In the molecule containing Ni(2), the three carbons attached to P(8) were each disordered between two positions. The percent occupancies of C(33), C(35), and C(37) were constrained to be identical and refined to 54.4%, while those of C(33b), C(35b), and C(37b), also constrained to be identical, refined to 43.6%. A methyl group, C(32), was disordered between two positions with percent occupancies of 42.9 and 57.1%. Two of the four BF_4 anions were each disordered between two positions which refined to percent occupancies of 62.2 and 37.8 % for B(3) and B(3b) and 44.0 and 56.0% for B(4) and B(4b). Within each of these pairs of disordered anions, the thermal parameters of the boron atoms were constrained to be identical as were the thermal parameters of the attached F atoms. All BF_4 anions except that containing B(1) were constrained to fit an idealized tetrahedral geometry. The structure has been refined to conventional R factor values of $R = 0.0672$ and $R_w = 0.0878$ on the basis of 4845 observed reflections with $I > 3\sigma(I)$ in the 2θ range 4 to 50° , giving a data to parameter ratio of 8.1 : 1. The maximum and minimum residual densities remaining were 0.99 and -0.65 e\AA^{-3} , respectively. The data were corrected for absorption using semi-empirical techniques.

Reference: Sheldrick, G. M.; *SHELXTL Crystallographic System*, Version 4.2/Iris (1991), Siemens Analytical X-ray Insts. Inc., Madison, WI.

STRUCTURE DETERMINATION SUMMARYCrystal Data

Empirical Formula	$C_{19} H_{42} B_2 F_8 Ni O P_4$
Color; Habit	orange prism
Crystal Size (mm)	0.38 x 0.62 x 0.28
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a} = 19.456(4) \text{ \AA}$ $\underline{b} = 10.485(2) \text{ \AA}$ $\underline{c} = 29.174(6) \text{ \AA}$ $\beta = 94.75(3)^\circ$
Volume	$5931(2) \text{ \AA}^3$
Z	8
Formula Weight	642.7
Density(calc.)	1.440 Mg/m^3
Absorption Coefficient	0.932 mm^{-1}
F(000)	2672

Data Collection

Diffractionmeter Used	Siemens P3
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$)
Temperature (K)	296
Monochromator	Highly oriented graphite crystal
2θ Range	4.0 to 50.0 $^\circ$
Scan Type	Wyckoff
Scan Speed	Variable; 4.00 to 30.00 $^\circ$ /min. in ω
Scan Range (ω)	2.00 $^\circ$
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$0 \leq h \leq 16$, $-12 \leq k \leq 0$ $-34 \leq l \leq 34$
Reflections Collected	9557
Independent Reflections	9224 ($R_{\text{int}} = 1.70\%$)
Observed Reflections	4845 ($F > 6.0\sigma(F)$)
Absorption Correction	N/A

Solution and Refinement

System Used	Siemens SHELXTL IRIS
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0008F^2$
Number of Parameters Refined	601
Final R Indices (obs. data)	R = 6.72 %, wR = 8.78 %
R Indices (all data)	R = 12.11 %, wR = 9.84 %
Goodness-of-Fit	2.09
Largest and Mean Δ/σ	0.244, 0.010
Data-to-Parameter Ratio	8.1:1
Largest Difference Peak	0.99 eÅ ⁻³
Largest Difference Hole	-0.65 eÅ ⁻³

Table 4s. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
Ni(1)	4274(1)	2305(1)	1266(1)	35(1)
P(1)	4245(1)	2386(3)	522(1)	46(1)
P(2)	3538(1)	644(2)	1160(1)	44(1)
P(3)	5419(1)	2025(3)	1244(1)	47(1)
P(4)	3834(1)	4285(2)	1226(1)	43(1)
C(1)	4301(5)	2186(9)	1876(4)	47(4)
O(1)	4325(4)	2095(8)	2258(2)	73(3)
Ni(2)	931(1)	2265(1)	3635(1)	41(1)
P(5)	1615(2)	1203(3)	4117(1)	64(1)
P(6)	1284(1)	4018(3)	4040(1)	58(1)
P(7)	1654(2)	1700(3)	3101(1)	62(1)
P(8)	111(2)	951(3)	3856(1)	67(1)
C(20)	323(6)	3086(11)	3265(4)	69(5)
O(2)	-72(5)	3591(10)	3021(3)	111(4)
C(2)	3252(6)	575(10)	547(3)	64(4)
C(3)	3847(6)	958(10)	272(3)	60(4)
C(4)	3947(6)	-892(9)	1287(4)	69(5)
C(5)	4164(7)	-1069(10)	1796(4)	84(5)
C(6)	2757(5)	666(11)	1459(3)	62(4)
C(7)	2263(6)	-441(12)	1351(4)	86(6)
C(8)	5107(5)	2497(11)	343(3)	63(4)
C(9)	5581(6)	1647(12)	649(3)	66(5)
C(10)	5934(6)	3437(11)	1396(4)	73(5)
C(11)	5952(6)	3836(13)	1889(4)	86(6)
C(12)	5809(6)	718(11)	1587(4)	69(5)
C(13)	6574(6)	505(14)	1510(4)	98(6)
C(14)	3923(6)	4854(10)	647(3)	60(4)
C(15)	3755(6)	3753(10)	306(3)	64(4)
C(16)	2938(6)	4351(11)	1312(4)	72(5)
C(17)	2579(7)	5640(13)	1267(5)	110(7)
C(18)	4229(6)	5554(9)	1574(3)	63(4)
C(19)	4141(7)	5441(11)	2083(3)	83(5)
C(21)	2077(6)	3583(15)	4365(4)	90(6)
C(22)	2029(7)	2251(14)	4552(4)	99(7)
C(23)	1491(7)	5474(11)	3743(5)	86(6)
C(24)	888(8)	6165(14)	3484(6)	130(9)
C(25)	707(6)	4491(12)	4456(4)	80(5)
C(26)	935(7)	5653(14)	4768(5)	127(8)
C(27)	2257(10)	628(22)	3378(6)	212(14)
C(28)	2282(8)	452(16)	3816(5)	124(8)
C(29)	1396(7)	827(12)	2594(4)	87(6)
C(30)	974(9)	1514(19)	2249(6)	155(10)
C(31)	2124(7)	3053(16)	2908(5)	129(8)
C(32)	2863(21)	2503(42)	2715(16)	114(5)
C(32B)	2610(16)	2993(31)	2545(10)	114(5)
C(33)	510(12)	-377(24)	4168(9)	83(3)
C(33B)	466(16)	298(33)	4409(11)	83(3)
C(34)	1140(7)	-2(16)	4393(6)	133(8)
C(35)	-481(15)	227(28)	3433(9)	97(4)
C(35B)	-32(20)	-418(33)	3438(11)	97(4)
C(36)	-409(12)	-18(21)	3034(6)	240(16)
C(37)	-433(15)	1547(27)	4280(11)	100(4)
C(37B)	-681(19)	1564(36)	3974(14)	100(4)
C(38)	-880(11)	2403(20)	4144(9)	248(17)

B(1)	5759(8)	-2653(16)	933(5)	65(6)
F(1)	5506(5)	-3782(8)	739(3)	121(4)
F(2)	6376(4)	-2455(9)	792(3)	132(5)
F(3)	5352(5)	-1680(9)	770(3)	130(4)
F(4)	5772(5)	-2724(9)	1398(3)	142(5)
B(2)	1130(4)	2355(7)	726(2)	99(8)
F(5)	766(4)	3058(10)	401(3)	192(6)
F(6)	1712(4)	1916(11)	556(3)	203(7)
F(7)	1301(6)	3088(12)	1101(3)	247(9)
F(8)	743(6)	1358(11)	848(5)	306(12)
B(3)	7826(5)	2232(10)	2452(3)	152(6)
F(9)	7273(6)	2556(17)	2681(5)	165(2)
F(10)	7883(9)	945(9)	2439(5)	165(2)
F(11)	7741(9)	2695(14)	2017(3)	165(2)
F(12)	8405(6)	2732(15)	2671(5)	165(2)
B(3B)	7799(8)	2482(15)	2524(5)	152(6)
F(9B)	7440(12)	3569(20)	2583(8)	165(2)
F(10B)	7359(12)	1477(21)	2490(8)	165(2)
F(11B)	8129(12)	2573(24)	2134(7)	165(2)
F(12B)	8268(12)	2308(23)	2889(7)	165(2)
B(4)	2847(6)	-1901(12)	4827(4)	100(4)
F(13)	2466(9)	-978(18)	5011(6)	152(2)
F(14)	2461(9)	-2497(19)	4483(6)	152(2)
F(15)	3407(8)	-1366(18)	4656(6)	152(2)
F(16)	3056(11)	-2757(17)	5157(6)	152(2)
B(4B)	2825(5)	-2287(9)	4883(3)	100(4)
F(13B)	2241(6)	-2165(16)	5101(5)	152(2)
F(14B)	2752(8)	-3257(12)	4577(5)	152(2)
F(15B)	2949(8)	-1185(11)	4661(5)	152(2)
F(16B)	3365(7)	-2538(14)	5195(5)	152(2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 5s. Bond lengths (Å)

Ni(1)-P(1)	2.168 (3)	Ni(1)-P(2)	2.260 (3)
Ni(1)-P(3)	2.253 (3)	Ni(1)-P(4)	2.245 (3)
Ni(1)-C(1)	1.780 (11)	P(1)-C(3)	1.811 (11)
P(1)-C(8)	1.801 (11)	P(1)-C(15)	1.806 (11)
P(2)-C(2)	1.832 (10)	P(2)-C(4)	1.820 (10)
P(2)-C(6)	1.812 (11)	P(3)-C(9)	1.832 (10)
P(3)-C(10)	1.822 (12)	P(3)-C(12)	1.824 (11)
P(4)-C(14)	1.812 (10)	P(4)-C(16)	1.783 (11)
P(4)-C(18)	1.807 (10)	C(1)-O(1)	1.115 (13)
Ni(2)-P(5)	2.163 (3)	Ni(2)-P(6)	2.261 (3)
Ni(2)-P(7)	2.263 (3)	Ni(2)-P(8)	2.242 (3)
Ni(2)-C(20)	1.760 (12)	P(5)-C(22)	1.815 (14)
P(5)-C(28)	1.807 (16)	P(5)-C(34)	1.796 (17)
P(6)-C(21)	1.801 (12)	P(6)-C(23)	1.817 (13)
P(6)-C(25)	1.790 (12)	P(7)-C(27)	1.770 (21)
P(7)-C(29)	1.776 (13)	P(7)-C(31)	1.802 (16)
P(8)-C(33)	1.805 (25)	P(8)-C(33B)	1.835 (31)
P(8)-C(35)	1.785 (27)	P(8)-C(35B)	1.888 (34)
P(8)-C(37)	1.805 (31)	P(8)-C(37B)	1.731 (38)
C(20)-O(2)	1.133 (15)	C(2)-C(3)	1.515 (16)
C(4)-C(5)	1.521 (16)	C(6)-C(7)	1.523 (16)
C(8)-C(9)	1.520 (15)	C(10)-C(11)	1.494 (17)
C(12)-C(13)	1.540 (16)	C(14)-C(15)	1.541 (14)
C(16)-C(17)	1.522 (17)	C(18)-C(19)	1.514 (14)
C(21)-C(22)	1.505 (21)	C(23)-C(24)	1.524 (20)
C(25)-C(26)	1.562 (19)	C(27)-C(28)	1.289 (24)
C(29)-C(30)	1.439 (21)	C(31)-C(32)	1.689 (47)
C(31)-C(32B)	1.479 (34)	C(33)-C(34)	1.398 (28)
C(33B)-C(34)	1.353 (34)	C(35)-C(36)	1.212 (32)
C(35B)-C(36)	1.402 (38)	C(37)-C(38)	1.290 (35)
C(37B)-C(38)	1.095 (45)	B(1)-F(1)	1.386 (18)
B(1)-F(2)	1.315 (18)	B(1)-F(3)	1.353 (18)
B(1)-F(4)	1.357 (15)	B(2)-F(5)	1.354 (11)
B(2)-F(6)	1.353 (11)	B(2)-F(7)	1.355 (13)
B(2)-F(8)	1.355 (14)	B(3)-F(9)	1.356 (17)
B(3)-F(10)	1.355 (14)	B(3)-F(11)	1.355 (15)
B(3)-F(12)	1.355 (15)	B(3B)-F(9B)	1.355 (27)
B(3B)-F(10B)	1.356 (28)	B(3B)-F(11B)	1.355 (27)
B(3B)-F(12B)	1.355 (26)	B(4)-F(13)	1.355 (23)
B(4)-F(14)	1.355 (21)	B(4)-F(15)	1.356 (22)
B(4)-F(16)	1.355 (21)	B(4B)-F(13B)	1.355 (16)
B(4B)-F(14B)	1.354 (16)	B(4B)-F(15B)	1.356 (16)
B(4B)-F(16B)	1.357 (16)		

Table 6s. Bond angles (°)

P(1)-Ni(1)-P(2)	86.0(1)	P(1)-Ni(1)-P(3)	85.4(1)
P(2)-Ni(1)-P(3)	120.8(1)	P(1)-Ni(1)-P(4)	86.2(1)
P(2)-Ni(1)-P(4)	118.0(1)	P(3)-Ni(1)-P(4)	119.6(1)
P(1)-Ni(1)-C(1)	178.2(3)	P(2)-Ni(1)-C(1)	92.7(3)
P(3)-Ni(1)-C(1)	94.2(3)	P(4)-Ni(1)-C(1)	95.5(3)
Ni(1)-P(1)-C(3)	110.2(3)	Ni(1)-P(1)-C(8)	110.2(3)
C(3)-P(1)-C(8)	108.3(5)	Ni(1)-P(1)-C(15)	110.4(3)
C(3)-P(1)-C(15)	108.7(5)	C(8)-P(1)-C(15)	108.9(5)
Ni(1)-P(2)-C(2)	107.5(4)	Ni(1)-P(2)-C(4)	113.1(4)
C(2)-P(2)-C(4)	104.8(5)	Ni(1)-P(2)-C(6)	118.2(4)
C(2)-P(2)-C(6)	105.7(5)	C(4)-P(2)-C(6)	106.5(5)
Ni(1)-P(3)-C(9)	107.7(4)	Ni(1)-P(3)-C(10)	114.3(4)
C(9)-P(3)-C(10)	105.8(6)	Ni(1)-P(3)-C(12)	116.7(4)
C(9)-P(3)-C(12)	105.1(5)	C(10)-P(3)-C(12)	106.3(5)
Ni(1)-P(4)-C(14)	106.7(4)	Ni(1)-P(4)-C(16)	113.7(4)
C(14)-P(4)-C(16)	106.8(5)	Ni(1)-P(4)-C(18)	120.6(4)
C(14)-P(4)-C(18)	102.2(5)	C(16)-P(4)-C(18)	105.5(5)
Ni(1)-C(1)-O(1)	178.8(9)	P(5)-Ni(2)-P(6)	86.3(1)
P(5)-Ni(2)-P(7)	85.9(1)	P(6)-Ni(2)-P(7)	113.2(1)
P(5)-Ni(2)-P(8)	84.9(1)	P(6)-Ni(2)-P(8)	122.8(1)
P(7)-Ni(2)-P(8)	122.3(1)	P(5)-Ni(2)-C(20)	175.7(4)
P(6)-Ni(2)-C(20)	94.7(4)	P(7)-Ni(2)-C(20)	97.5(4)
P(8)-Ni(2)-C(20)	91.0(4)	Ni(2)-P(5)-C(22)	110.9(5)
Ni(2)-P(5)-C(28)	109.7(5)	C(22)-P(5)-C(28)	108.0(7)
Ni(2)-P(5)-C(34)	110.0(5)	C(22)-P(5)-C(34)	109.1(7)
C(28)-P(5)-C(34)	109.2(8)	Ni(2)-P(6)-C(21)	106.2(5)
Ni(2)-P(6)-C(23)	120.2(4)	C(21)-P(6)-C(23)	104.5(6)
Ni(2)-P(6)-C(25)	113.5(4)	C(21)-P(6)-C(25)	105.7(6)
C(23)-P(6)-C(25)	105.5(6)	Ni(2)-P(7)-C(27)	106.2(6)
Ni(2)-P(7)-C(29)	124.0(5)	C(27)-P(7)-C(29)	100.5(8)
Ni(2)-P(7)-C(31)	111.7(5)	C(27)-P(7)-C(31)	108.0(8)
C(29)-P(7)-C(31)	105.1(6)	Ni(2)-P(8)-C(33)	109.5(8)
Ni(2)-P(8)-C(33B)	104.9(10)	Ni(2)-P(8)-C(35)	119.8(9)
C(33)-P(8)-C(35)	104.3(12)	Ni(2)-P(8)-C(35B)	110.6(11)
C(33B)-P(8)-C(35B)	107.9(15)	Ni(2)-P(8)-C(37)	117.1(9)
C(33)-P(8)-C(37)	99.9(12)	C(35)-P(8)-C(37)	103.9(13)
Ni(2)-P(8)-C(37B)	119.7(13)	C(33B)-P(8)-C(37B)	103.9(17)
C(35B)-P(8)-C(37B)	109.0(17)	Ni(2)-C(20)-O(2)	178.5(10)
P(2)-C(2)-C(3)	108.9(7)	P(1)-C(3)-C(2)	109.0(7)
P(2)-C(4)-C(5)	112.8(8)	P(2)-C(6)-C(7)	115.5(8)
P(1)-C(8)-C(9)	109.0(7)	P(3)-C(9)-C(8)	106.6(8)
P(3)-C(10)-C(11)	115.5(9)	P(3)-C(12)-C(13)	113.1(8)
P(4)-C(14)-C(15)	108.8(7)	P(1)-C(15)-C(14)	107.0(7)
P(4)-C(16)-C(17)	118.0(8)	P(4)-C(18)-C(19)	114.6(8)
P(6)-C(21)-C(22)	110.5(9)	P(5)-C(22)-C(21)	110.3(9)
P(6)-C(23)-C(24)	116.3(10)	P(6)-C(25)-C(26)	116.5(9)
P(7)-C(27)-C(28)	120.8(16)	P(5)-C(28)-C(27)	116.8(14)
P(7)-C(29)-C(30)	115.5(11)	P(7)-C(31)-C(32)	107.6(17)
P(7)-C(31)-C(32B)	124.1(16)	P(8)-C(33)-C(34)	110.1(16)
P(8)-C(33B)-C(34)	110.7(21)	P(5)-C(34)-C(33)	116.9(14)
P(5)-C(34)-C(33B)	112.8(17)	P(8)-C(35)-C(36)	129.4(23)
P(8)-C(35B)-C(36)	110.7(22)	P(8)-C(37)-C(38)	116.6(23)
P(8)-C(37B)-C(38)	137.9(32)	F(1)-B(1)-F(2)	108.1(12)
F(1)-B(1)-F(3)	108.8(11)	F(2)-B(1)-F(3)	107.1(12)
F(1)-B(1)-F(4)	109.7(12)	F(2)-B(1)-F(4)	112.3(12)
F(3)-B(1)-F(4)	110.7(12)	F(5)-B(2)-F(6)	109.5(7)

F(5)-B(2)-F(7) 109.6(8)
F(5)-B(2)-F(8) 109.5(8)
F(7)-B(2)-F(8) 109.2(9)
F(9)-B(3)-F(11) 109.4(11)
F(9)-B(3)-F(12) 109.5(11)
F(11)-B(3)-F(12) 109.6(12)
F(9B)-B(3B)-F(11B) 109.4(18)
F(9B)-B(3B)-F(12B) 109.4(18)
F(11B)-B(3B)-F(12B) 109.5(17)
F(13)-B(4)-F(15) 109.4(14)
F(13)-B(4)-F(16) 109.5(14)
F(15)-B(4)-F(16) 109.3(14)
F(13B)-B(4B)-F(15B) 109.5(12)
F(13B)-B(4B)-F(16B) 109.6(11)
F(15B)-B(4B)-F(16B) 109.2(11)

F(6)-B(2)-F(7) 109.4(8)
F(6)-B(2)-F(8) 109.5(9)
F(9)-B(3)-F(10) 109.5(12)
F(10)-B(3)-F(11) 109.5(11)
F(10)-B(3)-F(12) 109.4(11)
F(9B)-B(3B)-F(10B) 109.5(17)
F(10B)-B(3B)-F(11B) 109.5(18)
F(10B)-B(3B)-F(12B) 109.5(18)
F(13)-B(4)-F(14) 109.5(14)
F(14)-B(4)-F(15) 109.4(14)
F(14)-B(4)-F(16) 109.7(14)
F(13B)-B(4B)-F(14B) 109.5(11)
F(14B)-B(4B)-F(15B) 109.7(11)
F(14B)-B(4B)-F(16B) 109.3(11)

Table 7s. Anisotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	38(1)	35(1)	32(1)	3(1)	2(1)	1(1)
P(1)	54(2)	54(2)	31(1)	4(1)	1(1)	2(1)
P(2)	55(2)	33(1)	44(2)	-2(1)	4(1)	-4(1)
P(3)	38(2)	60(2)	42(1)	9(1)	6(1)	4(1)
P(4)	50(2)	32(1)	45(1)	6(1)	-3(1)	0(1)
C(1)	45(7)	41(6)	56(7)	3(5)	5(5)	-3(5)
O(1)	109(7)	81(6)	29(4)	4(5)	7(4)	-1(4)
Ni(2)	33(1)	48(1)	43(1)	-1(1)	1(1)	-2(1)
P(5)	46(2)	88(2)	58(2)	11(2)	-1(1)	17(2)
P(6)	38(2)	72(2)	64(2)	-10(1)	12(1)	-28(2)
P(7)	58(2)	81(2)	47(2)	4(2)	14(1)	-9(2)
P(8)	50(2)	79(2)	72(2)	-15(2)	6(2)	13(2)
C(20)	67(9)	65(8)	72(8)	-10(7)	-2(7)	10(7)
O(2)	95(7)	110(8)	120(8)	22(6)	-38(6)	39(6)
C(2)	83(9)	55(7)	52(6)	-4(6)	-8(6)	-20(6)
C(3)	73(8)	68(8)	41(6)	4(6)	8(6)	-7(5)
C(4)	89(9)	33(6)	86(9)	4(6)	8(7)	-4(6)
C(5)	133(12)	38(7)	80(9)	4(7)	2(8)	16(6)
C(6)	55(7)	70(8)	61(7)	-16(6)	9(6)	0(6)
C(7)	75(9)	93(10)	89(9)	-30(8)	-2(7)	5(8)
C(8)	62(8)	86(9)	43(6)	9(6)	9(5)	8(6)
C(9)	60(8)	96(9)	45(6)	6(7)	18(6)	-8(6)
C(10)	51(8)	85(9)	86(9)	5(7)	13(7)	2(8)
C(11)	59(8)	102(11)	95(10)	-24(8)	-11(7)	-19(8)
C(12)	62(8)	80(9)	63(7)	26(7)	-4(6)	13(7)
C(13)	63(10)	126(13)	103(10)	39(9)	-10(7)	-3(9)
C(14)	68(8)	49(7)	62(7)	9(6)	7(6)	19(6)
C(15)	80(9)	63(8)	47(6)	10(7)	-9(6)	3(6)
C(16)	61(8)	59(7)	96(9)	12(6)	4(7)	-5(7)
C(17)	86(11)	108(12)	137(13)	39(9)	8(9)	3(10)
C(18)	98(9)	30(6)	58(7)	-5(6)	-12(6)	-2(5)
C(19)	137(12)	56(8)	52(7)	5(8)	-12(7)	-8(6)
C(21)	57(9)	141(14)	72(9)	-23(9)	-1(7)	-43(9)
C(22)	71(10)	162(15)	60(8)	11(10)	-27(7)	11(9)
C(23)	83(10)	61(9)	122(11)	-25(7)	47(9)	-25(8)
C(24)	147(16)	63(10)	183(18)	-6(11)	22(13)	12(11)
C(25)	68(9)	102(10)	73(8)	-17(7)	32(7)	-39(7)
C(26)	114(12)	153(15)	125(12)	-51(11)	72(10)	-90(11)
C(27)	219(23)	293(30)	136(17)	201(22)	93(17)	60(19)
C(28)	104(12)	150(16)	119(13)	92(11)	19(10)	22(12)
C(29)	102(11)	75(9)	84(9)	-12(8)	15(8)	-27(8)
C(30)	161(18)	189(21)	112(14)	-14(16)	-7(13)	-66(14)
C(31)	113(12)	181(16)	106(11)	-77(12)	84(10)	-78(11)
C(32)	114(8)	114(8)	114(8)	0(1)	9(1)	0(1)
C(32B)	114(8)	114(8)	114(8)	0(1)	9(1)	0(1)
C(33)	83(6)	83(6)	83(6)	0(1)	7(1)	0(1)
C(33B)	83(6)	83(6)	83(6)	0(1)	7(1)	0(1)
C(34)	102(13)	144(15)	153(15)	15(11)	-5(11)	110(12)
C(35)	97(7)	97(7)	97(7)	0(1)	8(1)	0(1)
C(35B)	97(7)	97(7)	97(7)	0(1)	8(1)	0(1)
C(36)	313(31)	274(30)	133(18)	-232(26)	27(20)	-46(19)
C(37)	100(7)	100(7)	100(7)	0(1)	8(1)	0(1)
C(37B)	100(7)	100(7)	100(7)	0(1)	8(1)	0(1)
C(38)	146(20)	237(28)	352(37)	25(19)	-35(21)	-216(28)
B(1)	58(11)	85(11)	51(8)	1(9)	-1(7)	-12(8)

F(1)	155(8)	102(6)	106(6)	-49(6)	12(5)	5(5)
F(2)	66(6)	195(10)	140(8)	-17(6)	37(5)	9(6)
F(3)	141(8)	140(8)	105(6)	73(7)	-3(5)	-25(6)
F(4)	182(9)	191(10)	53(4)	-45(8)	7(5)	11(5)
B(2)	132(18)	102(14)	60(9)	60(13)	-12(11)	-11(10)
F(5)	176(10)	260(14)	147(9)	121(10)	60(8)	74(9)
F(6)	189(11)	308(15)	121(8)	166(11)	60(7)	68(9)
F(7)	200(13)	312(19)	225(15)	77(14)	-4(11)	-88(13)
F(8)	173(13)	308(21)	428(27)	-64(14)	-38(14)	164(20)
B(3)	152(10)	152(10)	152(10)	0(1)	13(1)	0(1)
F(9)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
F(10)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
F(11)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
F(12)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
B(3B)	152(10)	152(10)	152(10)	0(1)	13(1)	0(1)
F(9B)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
F(10B)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
F(11B)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
F(12B)	165(3)	165(3)	165(3)	0(1)	14(1)	0(1)
B(4)	100(6)	100(6)	100(6)	0(1)	8(1)	0(1)
F(13)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
F(14)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
F(15)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
F(16)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
B(4B)	100(6)	100(6)	100(6)	0(1)	8(1)	0(1)
F(13B)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
F(14B)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
F(15B)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)
F(16B)	152(3)	152(3)	152(3)	0(1)	13(1)	0(1)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2(h^2 a^2 U_{11} + \dots + 2hka*b*U_{12})$$

Table 8s. H-Atom coordinates ($\times 10^4$) and isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U
H(2A)	2901	1211	484	80
H(2B)	3061	-244	462	80
H(3A)	4170	265	298	80
H(3B)	3705	1092	-47	80
H(4A)	4335	-976	1107	80
H(4B)	3622	-1553	1196	80
H(5A)	4374	-1890	1847	80
H(5B)	4492	-414	1885	80
H(5C)	3774	-996	1975	80
H(6A)	2520	1448	1380	80
H(6B)	2887	686	1783	80
H(7A)	1870	-328	1525	80
H(7B)	2116	-458	1028	80
H(7C)	2488	-1230	1437	80
H(8A)	5268	3359	378	80
H(8B)	5097	2265	24	80
H(9A)	5456	774	587	80
H(9B)	6057	1765	594	80
H(10A)	5773	4134	1203	80
H(10B)	6396	3248	1325	80
H(11A)	6249	4566	1926	80
H(11B)	5497	4064	1965	80
H(11C)	6130	3165	2089	80
H(12A)	5568	-63	1510	80
H(12B)	5781	894	1908	80
H(13A)	6803	-172	1683	80
H(13B)	6588	339	1187	80
H(13C)	6801	1299	1586	80
H(14A)	4368	5221	612	80
H(14B)	3578	5500	584	80
H(15A)	3274	3541	281	80
H(15B)	3885	3977	6	80
H(16A)	2907	4026	1618	80
H(16B)	2702	3762	1102	80
H(17A)	2108	5527	1333	80
H(17B)	2801	6233	1482	80
H(17C)	2593	5965	960	80
H(18A)	4075	6375	1462	80
H(18B)	4716	5496	1544	80
H(19A)	4380	6104	2258	80
H(19B)	3655	5512	2113	80
H(19C)	4302	4625	2196	80
H(21A)	2181	4195	4606	80
H(21B)	2445	3586	4166	80
H(22A)	2471	1924	4666	80
H(22B)	1741	2294	4803	80
H(23A)	1820	5272	3526	80
H(23B)	1711	6048	3965	80
H(24A)	1047	6921	3340	80
H(24B)	672	5609	3254	80
H(24C)	561	6395	3699	80
H(25A)	644	3778	4655	80
H(25B)	267	4680	4296	80
H(26A)	595	5834	4979	80

H(26B)	1368	5467	4936	80
H(26C)	986	6380	4573	80
H(27A)	2701	741	3262	80
H(27B)	2086	-188	3271	80
H(28A)	2309	-423	3913	80
H(28B)	2711	858	3917	80
H(29A)	1144	85	2676	80
H(29B)	1799	542	2455	80
H(30A)	850	996	1984	80
H(30B)	564	1786	2383	80
H(30C)	1226	2248	2160	80
H(31A)	2252	3601	3165	80
H(31B)	1844	3529	2681	80
H(32A)	3132	3198	2611	80
H(32B)	3135	2028	2946	80
H(32C)	2726	1955	2461	80
H(32D)	2805	3817	2495	80
H(32E)	2972	2402	2638	80
H(32F)	2365	2698	2266	80
H(33A)	565	-1090	3968	80
H(33B)	212	-637	4398	80
H(33C)	207	-448	4477	80
H(33D)	420	915	4647	80
H(34A)	1075	279	4700	80
H(34B)	1424	-753	4418	80
H(34C)	1350	-126	4699	80
H(34D)	1172	-791	4229	80
H(35A)	-887	749	3421	80
H(35B)	-606	-575	3562	80
H(35C)	-303	-1068	3569	80
H(35D)	400	-789	3371	80
H(36A)	-811	-407	2880	80
H(36B)	-311	765	2882	80
H(36C)	-23	-586	3026	80
H(36D)	-490	-706	2819	80
H(36E)	-842	344	3102	80
H(36F)	-134	625	2902	80
H(37A)	-160	1848	4547	80
H(37B)	-714	854	4371	80
H(37C)	-841	947	4184	80
H(37D)	-965	1452	3692	80
H(38A)	-1176	2693	4370	80
H(38B)	-597	3097	4056	80
H(38C)	-1155	2096	3878	80
H(38D)	-1368	2396	4171	80
H(38E)	-642	2552	4440	80
H(38F)	-769	3069	3936	80

Table 9s. Extended Hückel Parameters

atom	orbital	H_{ij} (eV)	ζ_1	ζ_2	C_1^a	C_2^a
H	1s	-13.606	1.20			
C	2s	-16.59	1.576			
	2p	-11.26	1.453			
O	2s	-28.48	2.192			
	2p	-13.62	2.018			
P	3s	-16.15	1.816			
	3p	-10.49	1.478			
	3d	-2.11	1.731			
Ni	4s	-7.635	1.473			
	4p	-3.892	1.203			
	3d	-10.00	6.7055	2.8738	0.4212	0.7066

^aCoefficients used in double- ζ expansion of d orbitals. All parameters used are default parameters supplied with CAChe molecular modeling programs. The same trend in bond orders was found using iterative extended Hückel and INDO calculations.