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Crystal data for $[Ni(dmpe)_2](PF_6)_2$.

Identification code	bc226
Empirical formula	$C_{13}H_{35}F_{12}NNiO_2P_6$
Formula mass	709.95
Crystal size, mm	$0.25 \times 0.23 \times 0.21$
Crystal color, habit	yellow block
Crystal system	Monoclinic
Space group	$P2_1/c$
a, Å	17.7374(2)
b, Å	9.064
c, Å	17.9013(2)
α, °	90
β, °	96.1870(10)
γ, °	90
Volume, $Å^3$	2861.32(5)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.648
Absorption coefficient, mm^{-1}	1.105
F(000)	1448
Absorption correction[1]	Semi-empirical from equivalents
Range Transmission Coefficients	0.80 and 0.77

1) Blessing, *Acta Cryst.* (1995) A51. 33-38

Table 1. Data collection parameters for $[Ni(dmpe)_2](PF_6)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	150(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	8192
θ range	$1.15 < \theta < 31.24$
θ range, data collection	$1.15 < \theta < 31.24$
Scan type	ω scans
Index ranges	$-24 \le h \le 25$,
	$-13 \le k \le 13$,
	$-16 \le l \le 25$
Reflections collected	25441
Independent reflections	8707 (R(int) = 0.0263)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 2. Structure Solution and Refinement for $[Ni(dmpe)_2](PF_6)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	8707 / 1/ 551
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0373P)^2+1.0395P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0315, wR2 = 0.0744
Reflections observed	7204
R indices (all data)	R1 = 0.0434, wR2 = 0.0805
Goodness-of-fit[4] on F^2	1.047
Largest diff. peak and hole	0.537 and -0.640

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1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $R1 = \frac{\|F_o|-|F_c\|}{|F_o|}$; $wR2 = \sqrt{\frac{w(F_o^2-F_c^2)^2}{w(F_o^2)^2}}$;

4) $GooF = S = \sqrt{\frac{w(F_o^2-F_c^2)^2}{(M-N)}}$ where M is the number of reflections and N is the number of parameters refined.

Table 3. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Ni(dmpe)_2](PF_6)_2$.

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

	x	y	z	Ueq
Ni	2494(1)	5119(1)	2357(1)	18(1)
P(1)	1775(1)	4641(1)	1296(1)	22(1)
P(2)	3201(1)	3246(1)	2054(1)	23(1)
P(3)	3188(1)	5534(1)	3444(1)	23(1)
P(4)	1813(1)	7053(1)	2630(1)	23(1)
C(1)	755(1)	4536(3)	1296(1)	42(1)
C(2)	1921(2)	5827(2)	510(1)	43(1)
C(3)	2030(1)	2806(2)	975(1)	34(1)
C(4)	2889(1)	2702(2)	1081(1)	35(1)
C(5)	3091(1)	1570(2)	2577(1)	40(1)
C(6)	4213(1)	3491(3)	2046(1)	41(1)
C(7)	3428(1)	4038(2)	4097(1)	32(1)
C(8)	4091(1)	6439(3)	3373(1)	39(1)
C(9)	2679(1)	6861(2)	3971(1)	34(1)
C(10)	2345(1)	8029(2)	3414(1)	36(1)
C(11)	922(1)	6636(2)	2995(1)	35(1)
C(12)	1576(1)	8468(2)	1927(1)	30(1)
P(5)	3958(1)	8138(1)	1125(1)	29(1)
F(1)	4703(1)	7282(2)	1461(1)	60(1)
F(2)	3199(1)	8959(1)	791(1)	52(1)
F(3)	4486(5)	8890(20)	568(10)	66(4)
F(4)	3773(6)	6860(20)	530(9)	55(4)
F(5)	3475(7)	7340(30)	1693(8)	62(4)
F(6)	4205(7)	9370(20)	1718(19)	83(8)
F(3A)	4361(14)	9670(30)	866(19)	79(9)
F(4A)	4000(20)	7650(50)	297(10)	79(12)
F(5A)	3643(11)	6730(30)	1380(30)	84(10)
F(6A)	4050(20)	8890(50)	1921(14)	100(20)
F(3B)	4296(9)	8370(20)	358(5)	58(4)
F(4B)	3595(7)	6578(9)	812(12)	64(3)
F(5B)	3525(8)	7900(20)	1868(7)	61(3)
F(6B)	4233(9)	9672(17)	1432(11)	71(5)
P(6)	1119(1)	2252(1)	3669(1)	26(1)
F(7)	1486(1)	2913(2)	2962(1)	49(1)
F(8)	754(1)	1608(1)	4382(1)	42(1)
F(9)	865(1)	802(1)	3202(1)	45(1)
F(10)	330(1)	3022(1)	3382(1)	43(1)
F(11)	1375(1)	3703(1)	4145(1)	43(1)
F(12)	1911(1)	1487(1)	3962(1)	37(1)

C(13)	5192(4)	-432(11)	4963(6)	77(3)
N(1)	4485(3)	305(7)	4719(3)	59(1)
O(1)	4152(4)	-113(6)	4137(3)	117(2)
O(2)	4318(3)	1317(5)	5123(3)	105(2)
C(14)	-67(3)	9537(5)	-280(3)	125(5)
N(2)	-90(2)	10734(4)	210(2)	151(5)
O(3)	402(2)	10808(4)	729(2)	86(2)
O(4)	-631(2)	11567(5)	78(3)	92(2)

Table 4. Bond lengths (Å) for $[Ni(dmpe)_2](PF_6)_2$.

Ni-P(2)	2.2127(4)	Ni-P(1)	2.2133(4)
Ni-P(4)	2.2134(4)	Ni-P(3)	2.2197(4)
P(1)-C(1)	1.8110(19)	P(1)-C(2)	1.812(2)
P(1)-C(3)	1.8324(18)	P(2)-C(5)	1.806(2)
P(2)-C(6)	1.811(2)	P(2)-C(4)	1.8367(19)
P(3)-C(7)	1.8107(18)	P(3)-C(8)	1.8174(19)
P(3)-C(9)	1.8271(18)	P(4)-C(11)	1.8132(19)
P(4)-C(12)	1.8141(17)	P(4)-C(10)	1.8326(19)
C(3)-C(4)	1.518(3)	C(9)-C(10)	1.528(3)
P(5)-F(5A)	1.489(15)	P(5)-F(6B)	1.554(16)
P(5)-F(4A)	1.557(15)	P(5)-F(3B)	1.570(7)
P(5)-F(6A)	1.571(19)	P(5)-F(6)	1.572(17)
P(5)-F(5)	1.572(9)	P(5)-F(4)	1.582(7)
P(5)-F(1)	1.5925(13)	P(5)-F(3)	1.594(7)
P(5)-F(2)	1.5982(12)	P(5)-F(5B)	1.620(10)
P(6)-F(9)	1.5959(12)	P(6)-F(10)	1.5981(11)
P(6)-F(7)	1.6005(12)	P(6)-F(8)	1.6032(12)
P(6)-F(12)	1.6033(11)	P(6)-F(11)	1.6059(12)
C(13)-N(1)	1.447(8)	N(1)-O(1)	1.201(8)
N(1)-O(2)	1.224(8)	C(14)-N(2)	1.3978
N(2)-O(3)	1.2065	N(2)-O(4)	1.2237

Table 5. Bond angles (°) for $[Ni(dmpe)_2](PF_6)_2$.

P(2)-Ni-P(1)	85.933(16)	P(2)-Ni-P(4)	177.613(18)
P(1)-Ni-P(4)	93.826(16)	P(2)-Ni-P(3)	93.998(16)
P(1)-Ni-P(3)	177.701(18)	P(4)-Ni-P(3)	86.338(16)
C(1)-P(1)-C(2)	104.96(12)	C(1)-P(1)-C(3)	103.50(10)
C(2)-P(1)-C(3)	103.51(10)	C(1)-P(1)-Ni	119.56(8)
C(2)-P(1)-Ni	115.65(7)	C(3)-P(1)-Ni	107.89(6)
C(5)-P(2)-C(6)	105.62(11)	C(5)-P(2)-C(4)	103.18(10)
C(6)-P(2)-C(4)	102.89(10)	C(5)-P(2)-Ni	115.01(7)
C(6)-P(2)-Ni	119.75(8)	C(4)-P(2)-Ni	108.53(6)
C(7)-P(3)-C(8)	103.61(10)	C(7)-P(3)-C(9)	104.77(9)
C(8)-P(3)-C(9)	103.15(11)	C(7)-P(3)-Ni	120.59(6)
C(8)-P(3)-Ni	115.13(7)	C(9)-P(3)-Ni	107.84(6)
C(11)-P(4)-C(12)	104.59(9)	C(11)-P(4)-C(10)	102.79(10)
C(12)-P(4)-C(10)	104.57(9)	C(11)-P(4)-Ni	115.61(7)
C(12)-P(4)-Ni	119.84(6)	C(10)-P(4)-Ni	107.64(6)
C(4)-C(3)-P(1)	107.25(13)	C(3)-C(4)-P(2)	107.28(13)
C(10)-C(9)-P(3)	107.27(13)	C(9)-C(10)-P(4)	107.26(12)
F(5A)-P(5)-F(6B)	141(2)	F(5A)-P(5)-F(4A)	95.9(12)
F(6B)-P(5)-F(4A)	123(2)	F(5A)-P(5)-F(3B)	125.2(19)
F(6B)-P(5)-F(3B)	93.1(8)	F(4A)-P(5)-F(3B)	31.4(18)
F(5A)-P(5)-F(6A)	95.8(15)	F(6B)-P(5)-F(6A)	45(2)
F(4A)-P(5)-F(6A)	167.5(16)	F(3B)-P(5)-F(6A)	136.2(19)
F(5A)-P(5)-F(6)	119.5(18)	F(6B)-P(5)-F(6)	21.6(13)
F(4A)-P(5)-F(6)	144.0(17)	F(3B)-P(5)-F(6)	112.9(7)
F(6A)-P(5)-F(6)	23.8(17)	F(5A)-P(5)-F(5)	32.7(16)
F(6B)-P(5)-F(5)	110.7(9)	F(4A)-P(5)-F(5)	124.5(18)
F(3B)-P(5)-F(5)	155.8(5)	F(6A)-P(5)-F(5)	67.9(17)
F(6)-P(5)-F(5)	91.3(7)	F(5A)-P(5)-F(4)	61.5(18)
F(6B)-P(5)-F(4)	157.8(9)	F(4A)-P(5)-F(4)	34.5(16)
F(3B)-P(5)-F(4)	65.1(4)	F(6A)-P(5)-F(4)	157.1(17)
F(6)-P(5)-F(4)	175.8(5)	F(5)-P(5)-F(4)	90.7(4)
F(5A)-P(5)-F(1)	77.8(7)	F(6B)-P(5)-F(1)	95.0(6)
F(4A)-P(5)-F(1)	95.9(6)	F(3B)-P(5)-F(1)	91.0(3)
F(6A)-P(5)-F(1)	82.3(10)	F(6)-P(5)-F(1)	86.2(7)
F(5)-P(5)-F(1)	91.2(6)	F(4)-P(5)-F(1)	90.2(3)
F(5A)-P(5)-F(3)	145.8(17)	F(6B)-P(5)-F(3)	69.7(9)
F(4A)-P(5)-F(3)	55.9(17)	F(3B)-P(5)-F(3)	24.5(4)
F(6A)-P(5)-F(3)	111.7(18)	F(6)-P(5)-F(3)	88.6(7)
F(5)-P(5)-F(3)	177.0(7)	F(4)-P(5)-F(3)	89.2(4)
F(1)-P(5)-F(3)	85.8(3)	F(5A)-P(5)-F(2)	100.7(7)
F(6B)-P(5)-F(2)	86.3(6)	F(4A)-P(5)-F(2)	84.0(7)
F(3B)-P(5)-F(2)	89.7(3)	F(6A)-P(5)-F(2)	98.1(10)

F(6)-P(5)-F(2)	94.8(7)	F(5)-P(5)-F(2)	87.7(6)
F(4)-P(5)-F(2)	88.9(3)	F(1)-P(5)-F(2)	178.54(9)
F(3)-P(5)-F(2)	95.4(3)	F(5A)-P(5)-F(5B)	53.7(19)
F(6B)-P(5)-F(5B)	89.2(7)	F(4A)-P(5)-F(5B)	144.8(19)
F(3B)-P(5)-F(5B)	174.1(5)	F(6A)-P(5)-F(5B)	47.6(19)
F(6)-P(5)-F(5B)	70.3(7)	F(5)-P(5)-F(5B)	21.5(5)
F(4)-P(5)-F(5B)	112.0(5)	F(1)-P(5)-F(5B)	94.3(4)
F(3)-P(5)-F(5B)	158.8(5)	F(2)-P(5)-F(5B)	85.0(4)
F(9)-P(6)-F(10)	90.20(7)	F(9)-P(6)-F(7)	90.59(8)
F(10)-P(6)-F(7)	89.94(7)	F(9)-P(6)-F(8)	90.11(7)
F(10)-P(6)-F(8)	90.02(7)	F(7)-P(6)-F(8)	179.30(8)
F(9)-P(6)-F(12)	90.16(6)	F(10)-P(6)-F(12)	179.61(7)
F(7)-P(6)-F(12)	90.21(6)	F(8)-P(6)-F(12)	89.82(6)
F(9)-P(6)-F(11)	179.52(8)	F(10)-P(6)-F(11)	90.06(6)
F(7)-P(6)-F(11)	89.82(8)	F(8)-P(6)-F(11)	89.48(7)
F(12)-P(6)-F(11)	89.58(6)	O(1)-N(1)-O(2)	128.4(7)
O(1)-N(1)-C(13)	116.4(6)	O(2)-N(1)-C(13)	115.1(8)
O(3)-N(2)-O(4)	126.9	O(3)-N(2)-C(14)	117.4
O(4)-N(2)-C(14)	115.7		

Table 6. Anisotropic displacement parameters ($Å^2$) for $[Ni(dmpe)_2](PF_6)_2$.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni	18(1)	18(1)	18(1)	-2(1)	0(1)	2(1)
P(1)	22(1)	22(1)	20(1)	-2(1)	-2(1)	2(1)
P(2)	22(1)	24(1)	24(1)	-2(1)	1(1)	6(1)
P(3)	25(1)	22(1)	20(1)	-1(1)	-3(1)	0(1)
P(4)	28(1)	20(1)	21(1)	0(1)	1(1)	7(1)
C(1)	24(1)	54(1)	45(1)	-12(1)	-4(1)	-1(1)
C(2)	67(2)	34(1)	26(1)	2(1)	-3(1)	-7(1)
C(3)	39(1)	30(1)	31(1)	-10(1)	-7(1)	5(1)
C(4)	38(1)	39(1)	28(1)	-9(1)	1(1)	13(1)
C(5)	61(1)	24(1)	39(1)	0(1)	17(1)	8(1)
C(6)	26(1)	49(1)	50(1)	-2(1)	7(1)	9(1)
C(7)	39(1)	28(1)	28(1)	4(1)	-5(1)	4(1)
C(8)	34(1)	47(1)	34(1)	1(1)	-6(1)	-14(1)
C(9)	46(1)	31(1)	22(1)	-7(1)	-6(1)	9(1)
C(10)	51(1)	24(1)	30(1)	-8(1)	-7(1)	10(1)
C(11)	37(1)	35(1)	34(1)	5(1)	13(1)	11(1)
C(12)	36(1)	25(1)	28(1)	4(1)	2(1)	6(1)
P(5)	34(1)	29(1)	24(1)	-2(1)	2(1)	5(1)
F(1)	50(1)	69(1)	56(1)	-7(1)	-19(1)	21(1)
F(2)	48(1)	47(1)	59(1)	3(1)	1(1)	21(1)
F(3)	61(3)	85(8)	54(7)	21(5)	23(4)	-10(4)
F(4)	46(4)	59(7)	55(6)	-32(5)	-17(3)	17(4)
F(5)	42(3)	106(11)	38(6)	31(5)	3(4)	-17(6)
F(6)	33(3)	76(12)	140(20)	-77(11)	-11(7)	6(5)
F(3A)	75(11)	80(13)	79(15)	24(12)	-9(10)	-42(10)
F(4A)	110(20)	90(20)	33(8)	-24(13)	-18(12)	60(18)
F(5A)	63(9)	57(11)	130(30)	57(14)	9(13)	-2(7)
F(6A)	130(30)	130(30)	39(8)	-50(13)	-30(13)	90(30)
F(3B)	63(6)	85(8)	29(4)	2(4)	18(4)	31(5)
F(4B)	66(4)	27(2)	95(9)	-18(4)	-10(5)	4(2)
F(5B)	59(6)	96(7)	29(4)	15(4)	10(4)	13(5)
F(6B)	54(4)	43(3)	114(15)	-30(5)	7(5)	-10(2)
P(6)	24(1)	26(1)	27(1)	0(1)	4(1)	2(1)
F(7)	47(1)	62(1)	41(1)	19(1)	15(1)	4(1)
F(8)	40(1)	53(1)	34(1)	3(1)	12(1)	-3(1)
F(9)	45(1)	41(1)	49(1)	-18(1)	3(1)	0(1)
F(10)	30(1)	49(1)	48(1)	-3(1)	-5(1)	12(1)
F(11)	45(1)	29(1)	53(1)	-8(1)	-8(1)	1(1)
F(12)	28(1)	34(1)	49(1)	7(1)	2(1)	7(1)

C(13)	56(5)	82(5)	99(7)	51(6)	27(4)	7(3)
N(1)	70(4)	45(2)	67(4)	21(3)	36(3)	13(3)
O(1)	143(5)	109(4)	87(4)	48(3)	-51(3)	-60(4)
O(2)	150(5)	66(3)	115(4)	26(3)	88(4)	40(3)
C(14)	195(9)	167(7)	13(2)	-21(3)	6(3)	-169(8)
N(2)	162(8)	111(6)	209(11)	109(7)	150(8)	77(6)
O(3)	76(3)	100(4)	76(3)	41(3)	-14(2)	-19(3)
O(4)	87(3)	103(4)	90(3)	49(3)	34(3)	47(3)

Table 7. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Ni(dmpe)_2](PF_6)_2$.

	x	y	z	Ueq
H(1A)	547(15)	5510(30)	1325(16)	67(8)
H(1B)	670(14)	3910(30)	1719(16)	56(8)
H(1C)	559(13)	4080(30)	837(14)	44(6)
H(2A)	1567(15)	5510(30)	88(16)	56(7)
H(2B)	2450(20)	5760(50)	440(20)	134(16)
H(2C)	1783(13)	6740(30)	609(14)	47(7)
H(3A)	1814(12)	2030(20)	1341(13)	37(6)
H(3B)	1851(14)	2700(30)	466(15)	55(7)
H(4A)	3103(12)	3460(30)	718(14)	44(6)
H(4B)	3045(13)	1720(30)	1005(14)	48(7)
H(5A)	3353(13)	770(30)	2371(14)	48(7)
H(5B)	2550(15)	1380(30)	2573(15)	61(8)
H(5C)	3346(13)	1690(30)	3034(15)	45(7)
H(6A)	4442(16)	3450(30)	2562(18)	67(8)
H(6B)	4311(16)	4370(30)	1773(17)	69(9)
H(6C)	4387(14)	2670(30)	1793(15)	55(7)
H(7A)	3836(13)	3430(30)	3926(13)	46(6)
H(7B)	2993(13)	3490(30)	4153(13)	40(6)
H(7C)	3586(14)	4450(30)	4546(15)	51(7)
H(8A)	4335(14)	6550(30)	3855(15)	53(7)
H(8B)	3992(14)	7340(30)	3135(15)	56(7)
H(8C)	4411(15)	5820(30)	3149(16)	60(8)
H(9A)	2285(12)	6310(20)	4198(12)	31(5)
H(9B)	2997(14)	7270(30)	4343(14)	50(7)
H(10A)	2753(14)	8530(30)	3197(14)	50(7)
H(10B)	2028(13)	8650(30)	3635(14)	49(7)
H(11A)	729(14)	7550(30)	3136(14)	51(7)
H(11B)	1013(13)	5980(30)	3432(14)	47(7)
H(11C)	579(14)	6180(30)	2615(15)	56(7)
H(12A)	1160(13)	8130(20)	1547(13)	43(6)
H(12B)	2002(12)	8700(20)	1709(12)	32(5)
H(12C)	1402(12)	9340(30)	2159(13)	43(6)
H(13A)	5107	-1499	4979	93
H(13B)	5386	-81	5465	93
H(13C)	5563	-216	4610	93
H(14A)	386	9610	-547	151
H(14B)	-521	9548	-645	151
H(14C)	-51	8615	7	151

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Table 8. Crystal data for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

Identification code	bc227
Empirical formula	$C_{20}H_{50}B_2F_8NiOP_4$
Formula mass	662.81
Crystal size, mm	$0.72 \times 0.17 \times 0.08$
Crystal color, habit	yellow parallelepiped
Crystal system	Orthorhombic
Space group	*Pccn*
a, Å	17.7301(2)
b, Å	10.91290(10)
c, Å	15.77990(10)
α, °	90
β, °	90
γ, °	90
Volume, $Å^3$	3053.20(5)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.442
Absorption coefficient, mm^{-1}	0.908
F(000)	1392
Absorption correction[1]	Semi-empirical from equivalents
Range Transmission Coefficients	0.9309 and 0.5610

1) Blessing, *Acta Cryst.* (1995) A51. 33-38.

Table 9. Data collection parameters for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

Diffractometer	Siemens SMART CCD
Temperature, K	162(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	8192
θ range	$2.19 < \theta < 28.28$
θ range, data collection	$2.19 < \theta < 28.28$
Scan type	ω scan
Index ranges	$-20 \le h \le 23$,
	$-14 \le k \le 14$,
	$-21 \le l \le 16$
Reflections collected	22340
Independent reflections	3798 (R(int) = 0.0548)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 10. Structure Solution and Refinement for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	3798 / 0/ 265
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0398P)^2+1.4490P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0316, wR2 = 0.0671
Reflections observed	3145
R indices (all data)	R1 = 0.0438, wR2 = 0.0731
Goodness-of-fit[4] on F^2	0.914
Largest diff. peak and hole	0.562 and -0.320

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1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $R1 = \frac{\|F_o| - |F_c\|}{|F_o|}$; $wR2 = \sqrt{\frac{w(F_o^2 - F_c^2)^2}{w(F_o^2)^2}}$;

4) $GooF = S = \sqrt{\frac{w(F_o^2 - F_c^2)^2}{(M-N)}}$ where M is the number of reflections and N is the number of parameters refined.

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Table 11. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

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

	x	y	z	Ueq
Ni	0.5000	0.5000	0.5000	0.01247(8)
P(1)	0.46361(2)	0.30778(3)	0.47297(2)	0.01449(9)
P(2)	0.37826(2)	0.53317(3)	0.52673(2)	0.01501(9)
C(1)	0.51104(11)	0.19901(14)	0.54327(10)	0.0219(3)
C(2)	0.50543(12)	0.23612(18)	0.63659(11)	0.0294(4)
C(3)	0.47257(10)	0.24611(15)	0.36563(9)	0.0194(3)
C(4)	0.43085(11)	0.12479(16)	0.35183(12)	0.0272(4)
C(5)	0.36225(10)	0.28847(14)	0.49713(10)	0.0212(3)
C(6)	0.33658(10)	0.38703(14)	0.55967(10)	0.0211(3)
C(7)	0.34174(10)	0.64138(14)	0.60494(9)	0.0186(3)
C(8)	0.36129(11)	0.60434(16)	0.69629(10)	0.0241(3)
C(9)	0.33129(10)	0.57387(16)	0.42673(10)	0.0237(3)
C(10)	0.24563(12)	0.5597(2)	0.42557(13)	0.0361(4)
B	0.36307(12)	0.50604(16)	0.18569(13)	0.0250(4)
F(1)	0.31647(7)	0.59906(11)	0.21318(8)	0.0458(3)
F(2)	0.32360(9)	0.39505(12)	0.18319(9)	0.0577(4)
F(3)	0.38820(8)	0.53136(12)	0.10370(7)	0.0446(3)
F(4)	0.42359(7)	0.49455(10)	0.24034(7)	0.0357(3)
O	0.2500	0.2500	0.30825(15)	0.0484(6)

Table 12. Bond lengths (Å) for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

Ni-P(2)	2.2290(4)	Ni-P(2a)	2.2290(4)	Ni-P(1a)	2.2358(3)
Ni-P(1)	2.2358(3)	P(1)-C(1)	1.8295(16)	P(1)-C(3)	1.8294(15)
P(1)-C(5)	1.8490(18)	P(2)-C(7)	1.8267(15)	P(2)-C(6)	1.8329(16)
P(2)-C(9)	1.8387(16)	C(1)-C(2)	1.531(2)	C(3)-C(4)	1.532(2)
C(5)-C(6)	1.529(2)	C(7)-C(8)	1.537(2)	C(9)-C(10)	1.527(3)
B-F(1)	1.379(2)	B-F(4)	1.382(2)	B-F(3)	1.396(2)
B-F(2)	1.399(2)				

Symmetry transformations used to generate equivalent atoms:
a: -x+1,-y+1,-z+1

Table 13. Bond angles (°) for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

P(2)-Ni-P(2a)	180.0	P(2)-Ni-P(1a)	95.222(14)
P(2a)-Ni-P(1a)	84.778(14)	P(2)-Ni-P(1)	84.778(14)
P(2a)-Ni-P(1)	95.222(14)	P(1a)-Ni-P(1)	180.0
C(1)-P(1)-C(3)	106.42(8)	C(1)-P(1)-C(5)	104.35(8)
C(3)-P(1)-C(5)	103.50(7)	C(1)-P(1)-Ni	111.12(5)
C(3)-P(1)-Ni	119.78(5)	C(5)-P(1)-Ni	110.37(5)
C(7)-P(2)-C(6)	103.18(7)	C(7)-P(2)-C(9)	105.26(7)
C(6)-P(2)-C(9)	105.72(8)	C(7)-P(2)-Ni	125.18(6)
C(6)-P(2)-Ni	107.62(6)	C(9)-P(2)-Ni	108.39(6)
C(2)-C(1)-P(1)	112.45(12)	C(4)-C(3)-P(1)	114.05(12)
C(6)-C(5)-P(1)	110.01(11)	C(5)-C(6)-P(2)	108.00(11)
C(8)-C(7)-P(2)	112.57(11)	C(10)-C(9)-P(2)	115.87(13)
F(1)-B-F(4)	109.61(15)	F(1)-B-F(3)	109.70(15)
F(4)-B-F(3)	110.38(17)	F(1)-B-F(2)	110.27(18)
F(4)-B-F(2)	109.10(15)	F(3)-B-F(2)	107.75(16)

Symmetry transformations used to generate equivalent atoms:
a: -x+1,-y+1,-z+1

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Table 14. Anisotropic displacement parameters ($Å^2$) for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni	0.01307(15)	0.01168(12)	0.01266(13)	-0.00103(8)	0.00018(9)	0.00002(9)
P(1)	0.0170(2)	0.01235(16)	0.01410(17)	-0.00082(13)	-0.00034(14)	-0.00058(13)
P(2)	0.0145(2)	0.01638(17)	0.01411(17)	-0.00132(13)	0.00038(14)	0.00072(14)
C(1)	0.0280(10)	0.0173(7)	0.0205(7)	0.0042(5)	-0.0048(6)	-0.0009(6)
C(2)	0.0344(11)	0.0348(10)	0.0189(8)	0.0052(7)	-0.0032(8)	-0.0030(8)
C(3)	0.0212(9)	0.0207(7)	0.0164(7)	-0.0044(5)	-0.0012(6)	-0.0014(6)
C(4)	0.0272(10)	0.0245(8)	0.0300(9)	-0.0113(7)	-0.0025(7)	-0.0035(7)
C(5)	0.0191(8)	0.0197(7)	0.0247(8)	-0.0035(6)	0.0022(6)	-0.0038(6)
C(6)	0.0190(8)	0.0210(7)	0.0232(7)	-0.0014(6)	0.0058(6)	-0.0029(6)
C(7)	0.0169(8)	0.0210(7)	0.0177(7)	-0.0016(5)	0.0002(6)	0.0039(6)
C(8)	0.0264(10)	0.0292(8)	0.0166(7)	-0.0020(6)	0.0001(6)	0.0018(7)
C(9)	0.0225(9)	0.0321(8)	0.0163(7)	-0.0013(6)	-0.0024(6)	0.0016(7)
C(10)	0.0223(10)	0.0560(13)	0.0300(10)	0.0013(9)	-0.0088(8)	0.0005(9)
B	0.0251(11)	0.0226(8)	0.0272(9)	0.0025(7)	-0.0005(8)	-0.0013(7)
F(1)	0.0396(7)	0.0485(7)	0.0493(7)	0.0001(6)	0.0011(6)	0.0193(6)
F(2)	0.0648(10)	0.0430(7)	0.0651(9)	0.0042(6)	-0.0055(7)	-0.0298(7)
F(3)	0.0557(8)	0.0520(7)	0.0262(6)	0.0057(5)	0.0037(5)	0.0006(6)
F(4)	0.0293(6)	0.0447(6)	0.0331(6)	0.0004(4)	-0.0065(5)	0.0059(5)
O	0.0495(15)	0.0634(16)	0.0322(11)	0.000	0.000	-0.0068(12)

Table 15. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Ni(depe)_2](BF_4)_2 \cdot H_2O$.

	x	y	z	Ueq
H(1A)	0.4872(12)	0.1196(19)	0.5343(13)	0.026(5)
H(1B)	0.5616(13)	0.1928(18)	0.5224(13)	0.027(5)
H(2A)	0.5335(14)	0.181(2)	0.6696(15)	0.040(6)
H(2B)	0.4548(14)	0.234(2)	0.6539(14)	0.034(6)
H(2C)	0.5245(12)	0.317(2)	0.6458(13)	0.028(5)
H(3A)	0.4545(13)	0.3082(19)	0.3264(13)	0.032(5)
H(3B)	0.5248(13)	0.2382(19)	0.3536(12)	0.026(5)
H(4A)	0.4431(14)	0.095(2)	0.2962(17)	0.051(7)
H(4B)	0.3758(13)	0.137(2)	0.3528(13)	0.033(6)
H(4C)	0.4433(13)	0.068(2)	0.3939(15)	0.038(6)
H(5A)	0.3359(13)	0.2966(18)	0.4431(13)	0.030(5)
H(5B)	0.3523(13)	0.207(2)	0.5207(13)	0.033(6)
H(6A)	0.3549(11)	0.3702(16)	0.6156(12)	0.018(4)
H(6B)	0.2829(12)	0.3976(17)	0.5649(12)	0.022(5)
H(7A)	0.3602(12)	0.7202(18)	0.5924(13)	0.026(5)
H(7B)	0.2886(12)	0.6448(17)	0.5976(12)	0.021(5)
H(8A)	0.3492(14)	0.669(2)	0.7344(15)	0.042(6)
H(8B)	0.4131(14)	0.5833(19)	0.7019(13)	0.034(5)
H(8C)	0.3330(13)	0.534(2)	0.7142(14)	0.031(5)
H(9A)	0.3452(13)	0.656(2)	0.4175(13)	0.035(6)
H(9B)	0.3535(13)	0.5247(19)	0.3832(14)	0.031(5)
H(10A)	0.2267(13)	0.590(2)	0.3744(15)	0.042(6)
H(10B)	0.2216(16)	0.605(2)	0.4683(18)	0.054(7)
H(10C)	0.2319(17)	0.472(2)	0.4340(17)	0.058(8)
H(1O)	0.2678(18)	0.295(3)	0.2765(17)	0.059(9)

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Table 16. Crystal data for $[Ni(dmpp)_2](BF_4)_2$.

Identification code	bc204
Empirical formula	$C_{14}H_{36}B_2F_8NiP_4$
Formula mass	560.64
Crystal size, mm	$0.41 \times 0.41 \times 0.32$
Crystal color, habit	deep red block
Crystal system	Monoclinic
Space group	$P2_1/n$
a, Å	9.8371(13)
b, Å	16.764(3)
c, Å	14.8801(18)
α, °	90
β, °	101.136(7)
γ, °	90
Volume, $Å^3$	2407.7(6)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.547
Absorption coefficient, mm^{-1}	1.133
F(000)	1160
Absorption correction[1]	Multiscan
Range Transmission Coefficients	0.71 and 0.66

1) Blessing, *Acta Cryst.* (1995) A51. 33-38.

Table 17. Data collection parameters for $[Ni(dmpp)_2](BF_4)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	160(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	7583
θ range	$1.85 < \theta < 30.81$
θ range, data collection	$1.85 < \theta < 30.81$
Scan type	ω scans
Index ranges	$-14 \leq h \leq 13$, $0 \leq k \leq 23$, $0 \leq l \leq 20$
Reflections collected	21377
Independent reflections	7057 (R(int) = 0.0177)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 18. Structure Solution and Refinement for $[Ni(dmpp)_2](BF_4)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	7057 / 0/ 436
Hydrogen atoms	freely refined, isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0308P)^2+1.7342P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0286, wR2 = 0.0672
Reflections observed	6203
R indices (all data)	R1 = 0.0354, wR2 = 0.0716
Goodness-of-fit[4] on F^2	1.034
Largest diff. peak and hole	0.698 and -0.491

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1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $R1 = \frac{\|F_o|-|F_c\|}{|F_o|}$; $wR2 = \sqrt{\frac{w(F_o^2-F_c^2)^2}{w(F_o^2)^2}}$;

4) $GooF = S = \sqrt{\frac{w(F_o^2-F_c^2)^2}{(M-N)}}$ where M is the number of reflections and N is the number of parameters refined.

Table 19. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Ni(dmpp)_2](BF_4)_2$.

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

	x	y	z	Ueq
Ni	0.773159(17)	0.249318(10)	0.082026(11)	0.01452(5)
P(1)	0.68352(4)	0.35415(2)	0.13717(3)	0.01937(8)
P(3)	0.93097(4)	0.15296(2)	0.09820(2)	0.01744(7)
P(4)	0.59782(4)	0.16590(2)	0.07052(3)	0.01815(7)
C(1)	0.5496(2)	0.34917(11)	0.20571(14)	0.0334(4)
C(2)	0.8296(2)	0.38870(14)	0.22201(14)	0.0372(4)
P(2)	0.89782(13)	0.33044(7)	0.01122(9)	0.01903(17)
C(3)	0.6286(4)	0.4399(3)	0.0636(3)	0.0361(10)
C(4)	0.6881(2)	0.44520(13)	-0.02368(16)	0.0372(6)
C(5)	0.8447(2)	0.43501(11)	-0.00243(15)	0.0315(5)
C(6)	1.0844(3)	0.34169(15)	0.04477(18)	0.0277(4)
C(7)	0.8658(3)	0.2962(2)	-0.10783(15)	0.0306(5)
P(2')	0.8671(10)	0.3234(6)	-0.0119(7)	0.0194(14)
C(3')	0.606(3)	0.4314(16)	0.0570(15)	0.004(3)
C(4')	0.7585(16)	0.4725(9)	0.0295(11)	0.027(4)
C(5')	0.7799(15)	0.4174(8)	-0.0457(10)	0.020(3)
C(6')	1.043(2)	0.3560(12)	0.0266(13)	0.025(4)
C(7')	0.852(3)	0.2685(19)	-0.118(2)	0.041(7)
C(8)	1.07526(17)	0.18263(11)	0.18776(12)	0.0283(3)
C(9)	1.00925(19)	0.12091(10)	0.00281(12)	0.0284(3)
C(10)	0.88242(16)	0.05802(9)	0.14315(11)	0.0225(3)
C(11)	0.74911(16)	0.02169(9)	0.08929(11)	0.0232(3)
C(12)	0.62129(16)	0.06318(9)	0.11093(11)	0.0232(3)
C(13)	0.55242(19)	0.15730(11)	-0.05359(11)	0.0299(3)
C(14)	0.43230(17)	0.18818(11)	0.10212(15)	0.0334(4)
B(1)	1.2213(2)	0.47113(12)	0.27074(13)	0.0308(4)
F(1)	1.21409(19)	0.38884(8)	0.27221(11)	0.0672(4)
F(2)	1.09911(14)	0.50043(11)	0.22147(11)	0.0669(4)
F(3)	1.24426(17)	0.50030(9)	0.35992(8)	0.0587(4)
F(4)	1.32844(13)	0.49515(8)	0.22910(9)	0.0495(3)
B(2)	0.7743(2)	0.18299(14)	0.36421(15)	0.0375(4)
F(5)	0.8790(2)	0.15877(10)	0.43159(15)	0.0893(6)
F(6)	0.67966(19)	0.12283(12)	0.34455(13)	0.0886(7)
F(7)	0.8236(2)	0.20345(10)	0.28622(12)	0.0823(6)
F(8)	0.71692(15)	0.25071(8)	0.39523(9)	0.0502(3)

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Table 20. Bond lengths (Å) for $[Ni(dmpp)_2](BF_4)_2$.

Ni-P(1)	2.1952(4)	Ni-P(4)	2.2013(4)
Ni-P(2')	2.202(10)	Ni-P(3)	2.2210(4)
Ni-P(2)	2.2277(12)	P(1)-C(2)	1.8149(19)
P(1)-C(1)	1.8168(17)	P(1)-C(3)	1.824(4)
P(1)-C(3')	1.83(3)	P(3)-C(8)	1.8187(17)
P(3)-C(9)	1.8217(16)	P(3)-C(10)	1.8253(15)
P(4)-C(14)	1.8187(17)	P(4)-C(13)	1.8199(17)
P(4)-C(12)	1.8239(15)	P(2)-C(6)	1.816(3)
P(2)-C(5)	1.829(2)	P(2)-C(7)	1.831(3)
C(3)-C(4)	1.527(5)	C(4)-C(5)	1.522(3)
P(2')-C(6')	1.80(2)	P(2')-C(7')	1.81(3)
P(2')-C(5')	1.818(17)	C(3')-C(4')	1.77(3)
C(4')-C(5')	1.50(2)	C(10)-C(11)	1.525(2)
C(11)-C(12)	1.525(2)	B(1)-F(2)	1.372(2)
B(1)-F(1)	1.382(2)	B(1)-F(4)	1.382(2)
B(1)-F(3)	1.391(2)	B(2)-F(5)	1.354(3)
B(2)-F(6)	1.365(3)	B(2)-F(7)	1.385(3)
B(2)-F(8)	1.386(3)		

Table 21. Bond angles (°) for $[Ni(dmpp)_2](BF_4)_2$.

P(1)-Ni-P(4)	99.926(18)	P(1)-Ni-P(2')	91.9(3)
P(4)-Ni-P(2')	136.7(3)	P(1)-Ni-P(3)	149.834(17)
P(4)-Ni-P(3)	93.851(19)	P(2')-Ni-P(3)	96.2(3)
P(1)-Ni-P(2)	89.18(3)	P(4)-Ni-P(2)	147.74(4)
P(2')-Ni-P(2)	11.1(2)	P(3)-Ni-P(2)	93.34(3)
C(2)-P(1)-C(1)	100.77(10)	C(2)-P(1)-C(3)	105.59(17)
C(1)-P(1)-C(3)	102.12(15)	C(2)-P(1)-C(3')	113.8(7)
C(1)-P(1)-C(3')	98.2(8)	C(3)-P(1)-C(3')	8.4(8)
C(2)-P(1)-Ni	101.20(7)	C(1)-P(1)-Ni	124.06(6)
C(3)-P(1)-Ni	120.04(15)	C(3')-P(1)-Ni	118.1(7)
C(8)-P(3)-C(9)	105.31(9)	C(8)-P(3)-C(10)	101.09(8)
C(9)-P(3)-C(10)	102.02(8)	C(8)-P(3)-Ni	108.11(6)
C(9)-P(3)-Ni	121.46(6)	C(10)-P(3)-Ni	116.55(5)
C(14)-P(4)-C(13)	102.83(9)	C(14)-P(4)-C(12)	99.86(8)
C(13)-P(4)-C(12)	104.50(8)	C(14)-P(4)-Ni	125.21(6)
C(13)-P(4)-Ni	99.46(6)	C(12)-P(4)-Ni	121.79(5)
C(6)-P(2)-C(5)	100.53(12)	C(6)-P(2)-C(7)	105.91(12)
C(5)-P(2)-C(7)	101.58(14)	C(6)-P(2)-Ni	123.55(10)
C(5)-P(2)-Ni	117.79(8)	C(7)-P(2)-Ni	105.01(10)
C(4)-C(3)-P(1)	116.0(3)	C(5)-C(4)-C(3)	110.9(2)
C(4)-C(5)-P(2)	112.74(14)	C(6')-P(2')-C(7')	110.1(13)
C(6')-P(2')-C(5')	101.4(9)	C(7')-P(2')-C(5')	104.1(12)
C(6')-P(2')-Ni	117.8(8)	C(7')-P(2')-Ni	107.1(10)
C(5')-P(2')-Ni	115.5(6)	C(4')-C(3')-P(1)	99.3(13)
C(5')-C(4')-C(3')	100.3(13)	C(4')-C(5')-P(2')	117.1(11)
C(11)-C(10)-P(3)	114.51(10)	C(12)-C(11)-C(10)	111.54(12)
C(11)-C(12)-P(4)	114.71(10)	F(2)-B(1)-F(1)	108.90(17)
F(2)-B(1)-F(4)	108.74(16)	F(1)-B(1)-F(4)	110.10(17)
F(2)-B(1)-F(3)	110.38(18)	F(1)-B(1)-F(3)	109.59(16)
F(4)-B(1)-F(3)	109.12(16)	F(5)-B(2)-F(6)	109.1(2)
F(5)-B(2)-F(7)	110.8(2)	F(6)-B(2)-F(7)	109.77(19)
F(5)-B(2)-F(8)	107.43(18)	F(6)-B(2)-F(8)	111.85(18)
F(7)-B(2)-F(8)	107.90(19)		

Table 22. Anisotropic displacement parameters ($Å^2$) for $[Ni(dmpp)_2](BF_4)_2$.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ni	0.01420(8)	0.01322(8)	0.01657(8)	0.00026(6)	0.00401(6)	0.00085(6)
P(1)	0.02040(17)	0.01607(15)	0.02229(17)	-0.00221(12)	0.00570(13)	0.00217(12)
P(3)	0.01596(15)	0.01657(15)	0.01995(16)	-0.00054(12)	0.00387(12)	0.00252(12)
P(4)	0.01540(15)	0.01741(15)	0.02136(16)	-0.00028(12)	0.00283(12)	-0.00095(12)
C(1)	0.0342(9)	0.0323(9)	0.0390(9)	-0.0056(7)	0.0204(8)	0.0035(7)
C(2)	0.0362(10)	0.0451(11)	0.0292(9)	-0.0152(8)	0.0037(7)	-0.0084(8)
P(2)	0.0186(4)	0.0193(3)	0.0199(4)	0.0017(3)	0.0055(3)	-0.0019(3)
C(3)	0.033(2)	0.0224(16)	0.056(2)	0.0099(12)	0.0152(15)	0.0088(13)
C(4)	0.0374(11)	0.0352(11)	0.0399(12)	0.0191(9)	0.0097(9)	0.0112(9)
C(5)	0.0341(10)	0.0225(8)	0.0401(11)	0.0092(8)	0.0128(9)	-0.0009(7)
C(6)	0.0192(9)	0.0299(10)	0.0349(11)	-0.0013(9)	0.0079(9)	-0.0054(9)
C(7)	0.0342(12)	0.0368(13)	0.0207(9)	0.0039(9)	0.0053(8)	-0.0047(10)
P(2')	0.015(3)	0.021(2)	0.021(4)	0.005(2)	0.001(2)	-0.005(2)
C(8)	0.0217(7)	0.0299(8)	0.0306(8)	-0.0009(6)	-0.0017(6)	-0.0003(6)
C(9)	0.0312(8)	0.0258(7)	0.0313(8)	-0.0026(6)	0.0143(7)	0.0044(6)
C(10)	0.0246(7)	0.0177(6)	0.0246(7)	0.0034(5)	0.0029(5)	0.0035(5)
C(11)	0.0289(7)	0.0163(6)	0.0247(7)	0.0000(5)	0.0058(6)	-0.0001(5)
C(12)	0.0242(7)	0.0175(6)	0.0284(7)	0.0018(5)	0.0068(6)	-0.0034(5)
C(13)	0.0319(8)	0.0306(8)	0.0231(7)	-0.0013(6)	-0.0048(6)	-0.0032(7)
C(14)	0.0190(7)	0.0317(8)	0.0519(11)	-0.0031(8)	0.0124(7)	-0.0007(6)
B(1)	0.0320(9)	0.0342(9)	0.0259(8)	0.0004(7)	0.0046(7)	-0.0070(7)
F(1)	0.1097(13)	0.0354(7)	0.0622(9)	-0.0014(6)	0.0305(9)	-0.0125(8)
F(2)	0.0341(7)	0.0938(12)	0.0680(10)	0.0191(8)	-0.0019(6)	0.0015(7)
F(3)	0.0847(11)	0.0631(9)	0.0286(6)	-0.0098(6)	0.0113(6)	-0.0179(7)
F(4)	0.0403(7)	0.0636(8)	0.0479(7)	-0.0002(6)	0.0168(5)	-0.0131(6)
B(2)	0.0357(10)	0.0438(11)	0.0356(10)	-0.0087(9)	0.0136(8)	-0.0054(9)
F(5)	0.0829(12)	0.0548(9)	0.1096(15)	-0.0035(9)	-0.0329(11)	0.0191(9)
F(6)	0.0809(12)	0.1060(14)	0.0893(12)	-0.0569(11)	0.0424(10)	-0.0575(11)
F(7)	0.1272(16)	0.0674(10)	0.0746(11)	-0.0044(8)	0.0750(11)	0.0060(10)
F(8)	0.0562(8)	0.0568(8)	0.0423(7)	-0.0034(5)	0.0215(6)	0.0126(6)

Table 23. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Ni(dmpp)_2](BF_4)_2$.

	x	y	z	Ueq
H(1A)	0.552(3)	0.3979(17)	0.2372(18)	0.057(7)
H(1B)	0.569(2)	0.3067(14)	0.2488(16)	0.037(6)
H(1C)	0.463(2)	0.3413(14)	0.1703(16)	0.040(6)
H(2A)	0.809(3)	0.4413(18)	0.246(2)	0.067(8)
H(2B)	0.908(3)	0.3931(15)	0.1968(17)	0.047(7)
H(2C)	0.841(3)	0.3553(16)	0.2670(19)	0.053(7)
H(3A)	0.529(3)	0.4320(14)	0.0429(16)	0.029(6)
H(3B)	0.644(3)	0.4834(17)	0.1017(18)	0.042(7)
H(4A)	0.644(3)	0.4039(17)	-0.072(2)	0.051(8)
H(4B)	0.664(3)	0.4985(17)	-0.0504(19)	0.050(8)
H(5A)	0.889(2)	0.4642(14)	0.0528(16)	0.027(5)
H(5B)	0.888(3)	0.4546(16)	-0.0508(19)	0.045(7)
H(6A)	1.112(3)	0.3787(16)	0.0029(18)	0.044(7)
H(6B)	1.129(3)	0.2937(16)	0.0398(17)	0.036(6)
H(6C)	1.109(2)	0.3634(14)	0.1078(17)	0.032(6)
H(7A)	0.908(4)	0.330(2)	-0.142(2)	0.069(10)
H(7B)	0.777(3)	0.3020(18)	-0.129(2)	0.051(8)
H(7C)	0.900(4)	0.2472(19)	-0.112(2)	0.054(10)
H(3'1)	0.5444	0.4086	0.0025	0.005
H(3'2)	0.5541	0.4710	0.0864	0.005
H(4'1)	0.7442	0.5283	0.0078	0.033
H(4'2)	0.8370	0.4704	0.0823	0.033
H(5'1)	0.8337	0.4463	-0.0851	0.025
H(5'2)	0.6880	0.4052	-0.0836	0.025
H(6'1)	1.1042	0.3095	0.0389	0.030
H(6'2)	1.0496	0.3875	0.0827	0.030
H(6'3)	1.0717	0.3889	-0.0210	0.030
H(7'1)	0.9069	0.2950	-0.1578	0.049
H(7'2)	0.7545	0.2669	-0.1491	0.049
H(7'3)	0.8860	0.2140	-0.1051	0.049
H(8A)	1.134(3)	0.1411(18)	0.199(2)	0.066(8)
H(8B)	1.040(3)	0.1937(17)	0.239(2)	0.061(8)
H(8C)	1.116(3)	0.2289(18)	0.172(2)	0.064(8)
H(9A)	1.075(2)	0.0809(13)	0.0264(15)	0.035(6)
H(9B)	1.056(2)	0.1641(14)	-0.0194(16)	0.042(6)
H(9C)	0.936(2)	0.0996(13)	-0.0460(15)	0.032(5)
H(10A)	0.960(2)	0.0232(12)	0.1443(14)	0.028(5)
H(10B)	0.877(2)	0.0684(12)	0.2057(14)	0.030(5)
H(11A)	0.746(2)	-0.0355(12)	0.1060(13)	0.027(5)
H(11B)	0.749(2)	0.0234(12)	0.0256(14)	0.025(5)

H(12A)	0.624(2)	0.0654(12)	0.1761(14)	0.025(5)
H(12B)	0.537(2)	0.0358(13)	0.0852(14)	0.033(5)
H(13A)	0.476(3)	0.1215(16)	-0.0694(18)	0.055(7)
H(13B)	0.628(3)	0.1373(14)	-0.0767(16)	0.043(6)
H(13C)	0.532(2)	0.2089(15)	-0.0793(16)	0.045(6)
H(14A)	0.375(2)	0.1467(14)	0.0818(16)	0.040(6)
H(14B)	0.394(3)	0.2362(14)	0.0733(17)	0.043(6)
H(14C)	0.447(2)	0.1912(14)	0.1677(16)	0.038(6)

Table 24. Crystal data for $[Pt(dmpp)_2](PF_6)_2$.

Identification code	bc292
Empirical formula	$C_{15.61}H_{39.73}F_{12}N_{0.27}O_{0.53}P_6Pt$
Formula mass	848.70
Crystal size, mm	$0.24 \times 0.15 \times 0.14$
Crystal color, habit	colorless block
Crystal system	Monoclinic
Space group	$P2_1/c$
a, Å	17.5851(17)
b, Å	9.3130(10)
c, Å	18.412(3)
α, °	90
β, °	94.269(6)
γ, °	90
Volume, $Å^3$	3007.0(6)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.875
Absorption coefficient, mm^{-1}	5.069
F(000)	1662
Absorption correction[1]	multiscan
Range Transmission Coefficients	0.5372 and 0.3759

1) Blessing, *Acta Cryst.* (1995) A51. 33-38.

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Table 25. Data collection parameters for $[Pt(dmpp)_2](PF_6)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	141(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	8192
θ range	$2.22 < \theta < 31.51$
θ range, data collection	$2.22 < \theta < 31.51$
Scan type	ω scans
Index ranges	$-24 \le h \le 25$, $-13 \le k \le 13$, $-26 \le l \le 26$
Reflections collected	39464
Independent reflections	9444 (R(int) = 0.0442)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 26. Structure Solution and Refinement for $[Pt(dmpp)_2](PF_6)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	9444 / 0/ 356
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0351P)^2+5.0718P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0332, wR2 = 0.0771
Reflections observed	8122
R indices (all data)	R1 = 0.0412, wR2 = 0.0805
Goodness-of-fit[4] on F^2	1.047
Extinction coefficient	0.00033(6)
Largest diff. peak and hole	1.238 and -1.274

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1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $R1 = \frac{\|F_o|-|F_c\|}{|F_o|}$; $wR2 = \sqrt{\frac{w(F_o^2-F_c^2)^2}{w(F_o^2)^2}}$;

4) $GooF = S = \sqrt{\frac{w(F_o^2-F_c^2)^2}{(M-N)}}$ where M is the number of reflections and N is the number of parameters refined.

Table 27. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Pt(dmpp)_2](PF_6)_2$.

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

	x	y	z	Ueq
Pt	0.252537(6)	1.014294(12	0.235902(6)	0.01946(5)
P(1)	0.33488(7)	0.83592(12)	0.20474(5)	0.0390(2)
P(2)	0.17423(5)	0.95214(11)	0.13461(5)	0.02842(18)
P(3)	0.17865(7)	1.21545(15)	0.25579(10)	0.0248(3)
P(4)	0.31964(9)	1.05997(13)	0.34664(7)	0.0245(3)
C(1)	0.4357(3)	0.8969(6)	0.2173(3)	0.0397(11)
C(2)	0.3320(3)	0.6691(6)	0.2482(3)	0.0436(12)
C(3)	0.3300(3)	0.7996(6)	0.1081(3)	0.0373(11)
C(4)	0.2600(3)	0.7232(6)	0.0783(3)	0.0376(13)
C(5)	0.1847(3)	0.7603(5)	0.1129(3)	0.0351(10)
C(6)	0.1852(3)	1.0432(5)	0.0512(3)	0.0341(10)
C(7)	0.0739(3)	0.9546(6)	0.1478(3)	0.0376(11)
C(8)	0.1524(3)	1.3233(5)	0.1761(3)	0.0358(10)
C(9)	0.0912(3)	1.1895(5)	0.2983(3)	0.0320(9)
C(10)	0.2312(3)	1.3456(5)	0.3124(3)	0.0352(10)
C(11)	0.2417(4)	1.3059(6)	0.3924(3)	0.0388(12)
C(12)	0.2603(3)	1.1482(5)	0.4093(3)	0.0345(10)
C(13)	0.4044(3)	1.1681(5)	0.3481(3)	0.0364(10)
C(14)	0.3499(3)	0.9013(6)	0.3979(3)	0.0351(10)
P(6)	0.39728(6)	0.31465(10)	0.11103(5)	0.0309(2)
F(7)	0.3708(2)	0.3130(4)	0.19095(16)	0.0697(9)
F(8)	0.4228(2)	0.3144(4)	0.03121(15)	0.0742(10)
F(9)	0.31797(18)	0.3830(4)	0.08443(19)	0.0723(10)
F(10)	0.47610(15)	0.2452(3)	0.13869(16)	0.0564(7)
F(12)	0.36312(16)	0.1588(3)	0.09739(19)	0.0625(8)
F(11)	0.4323(2)	0.4696(3)	0.1265(3)	0.0800(12)
P(5)	0.11507(6)	0.71869(11)	0.36647(6)	0.0340(2)
F(1)	0.0834(8)	0.575(2)	0.3311(14)	0.078(5)
F(2)	0.1401(10)	0.8674(17)	0.3985(16)	0.093(7)
F(3)	0.1472(10)	0.753(3)	0.2915(10)	0.094(6)
F(4)	0.0781(11)	0.683(3)	0.4386(11)	0.084(5)
F(5)	0.03420(17)	0.7825(4)	0.34173(18)	0.0653(8)
F(6)	0.19650(16)	0.6550(3)	0.39217(16)	0.0547(7)
F(1')	0.0920(9)	0.5555(13)	0.3663(14)	0.071(4)
F(2')	0.1480(11)	0.8753(19)	0.3696(13)	0.080(5)
F(3')	0.1345(16)	0.704(3)	0.2849(11)	0.097(7)
F(4')	0.1013(12)	0.729(2)	0.4498(8)	0.065(5)
N(1S)	0.5000	1.0000	1.0000	0.081(5)
C(1S)	0.4493(7)	0.9784(12)	0.9684(7)	0.066(3)

C(2S)	0.3948(9)	0.9537(18)	0.9385(9)	0.102(5)
O(1S)	0.0309(7)	0.0537(15)	0.4967(8)	0.113(4)
C(3S)	0.0606(10)	0.1854(19)	0.4891(10)	0.118(6)
C(1')	0.4039(13)	0.825(3)	0.1603(14)	0.040(5)
C(2')	0.3554(10)	0.6901(19)	0.2768(10)	0.022(4)
C(6')	0.1437(12)	1.139(2)	0.0858(12)	0.034(5)
C(7')	0.0898(13)	0.878(3)	0.1327(13)	0.039(5)
C(3')	0.2584(12)	0.682(2)	0.1513(12)	0.032(4)
C(4')	0.2342(12)	0.7170(19)	0.0749(10)	0.016(3)
C(5')	0.2268(12)	0.891(2)	0.0607(12)	0.034(5)
P(3')	0.1767(5)	1.1875(9)	0.2794(5)	0.0302(19)
P(4')	0.3440(5)	1.0630(7)	0.3323(4)	0.0250(16)
C(8')	0.1832(15)	1.366(3)	0.2364(15)	0.041(6)
C(9')	0.0744(13)	1.148(3)	0.2759(14)	0.032(5)
C(13')	0.4394(13)	1.050(3)	0.3091(14)	0.037(5)
C(14')	0.3380(12)	0.954(2)	0.4151(12)	0.025(4)
C(10')	0.1926(13)	1.223(3)	0.3764(13)	0.036(5)
C(11')	0.2689(14)	1.296(2)	0.3993(13)	0.026(4)
C(12')	0.3371(12)	1.249(2)	0.3601(13)	0.031(5)

Atoms marked with ' are minor component of disordered group.

Table 28. Bond lengths (Å) for $[Pt(dmpp)_2](PF_6)_2$.

Pt-P(3')	2.277(8)	Pt-P(1)	2.3042(10)
Pt-P(2)	2.3080(9)	Pt-P(4)	2.3178(11)
Pt-P(3)	2.3243(12)	Pt-P(4')	2.348(7)
P(1)-C(1')	1.52(2)	P(1)-C(2)	1.750(6)
P(1)-C(3)	1.807(5)	P(1)-C(1)	1.860(5)
P(1)-C(2')	1.913(18)	P(1)-C(3')	2.15(2)
P(2)-C(7')	1.63(2)	P(2)-C(6)	1.777(5)
P(2)-C(5')	1.80(2)	P(2)-C(7)	1.798(5)
P(2)-C(5)	1.843(5)	P(2)-C(6')	2.01(2)
P(3)-C(9)	1.792(5)	P(3)-C(10)	1.807(5)
P(3)-C(8)	1.809(5)	P(4)-C(13)	1.797(5)
P(4)-C(12)	1.810(5)	P(4)-C(14)	1.812(5)
C(3)-C(4)	1.491(7)	C(4)-C(5)	1.550(7)
C(10)-C(11)	1.518(7)	C(11)-C(12)	1.532(7)
P(6)-F(8)	1.569(3)	P(6)-F(7)	1.576(3)
P(6)-F(9)	1.577(3)	P(6)-F(10)	1.579(3)
P(6)-F(12)	1.584(3)	P(6)-F(11)	1.586(3)
P(5)-F(2)	1.556(13)	P(5)-F(4)	1.559(17)
P(5)-F(3)	1.563(16)	P(5)-F(2')	1.569(16)
P(5)-F(1)	1.570(11)	P(5)-F(3')	1.571(18)
P(5)-F(1')	1.573(12)	P(5)-F(4')	1.575(16)
P(5)-F(5)	1.577(3)	P(5)-F(6)	1.589(3)
N(1S)-C(1Sa)	1.047(13)	N(1S)-C(1S)	1.047(13)
C(1S)-C(2S)	1.093(17)	O(1S)-C(3S)	1.345(19)
O(1S)-O(1Sb)	1.49(3)	C(3')-C(4')	1.47(3)
C(4')-C(5')	1.64(3)	P(3')-C(10')	1.82(3)
P(3')-C(9')	1.83(2)	P(3')-C(8')	1.85(3)
P(4')-C(13')	1.77(3)	P(4')-C(12')	1.82(2)
P(4')-C(14')	1.84(2)	C(10')-C(11')	1.53(3)
C(11')-C(12')	1.51(3)		

Symmetry transformations used to generate equivalent atoms:
a: -x+1,-y+2,-z+2; b: -x,-y,-z+1
Atoms marked with ' are minor component of disordered group.

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Table 29. Bond angles (°) for $[Pt(dmpp)_2](PF_6)_2$.

P(3')-Pt-P(1)	173.7(2)	P(3')-Pt-P(2)	97.6(2)
P(1)-Pt-P(2)	88.06(4)	P(3')-Pt-P(4)	80.4(2)
P(1)-Pt-P(4)	93.62(5)	P(2)-Pt-P(4)	172.25(5)
P(3')-Pt-P(3)	12.7(2)	P(1)-Pt-P(3)	171.62(5)
P(2)-Pt-P(3)	91.29(4)	P(4)-Pt-P(3)	88.14(5)
P(3')-Pt-P(4')	89.1(3)	P(1)-Pt-P(4')	85.39(19)
P(2)-Pt-P(4')	173.1(2)	P(4)-Pt-P(4')	12.79(19)
P(3)-Pt-P(4')	94.87(18)	C(1')-P(1)-C(2)	103.8(10)
C(1')-P(1)-C(3)	55.7(9)	C(2)-P(1)-C(3)	106.4(3)
C(1')-P(1)-C(1)	45.1(9)	C(2)-P(1)-C(1)	105.9(3)
C(3)-P(1)-C(1)	98.9(2)	C(1')-P(1)-C(2')	102.1(11)
C(2)-P(1)-C(2')	20.5(5)	C(3)-P(1)-C(2')	122.8(6)
C(1)-P(1)-C(2')	90.1(6)	C(1')-P(1)-C(3')	101.9(11)
C(2)-P(1)-C(3')	65.2(6)	C(3)-P(1)-C(3')	56.1(6)
C(1)-P(1)-C(3')	144.9(6)	C(2')-P(1)-C(3')	85.6(8)
C(1')-P(1)-Pt	136.5(9)	C(2)-P(1)-Pt	119.1(2)
C(3)-P(1)-Pt	113.30(17)	C(1)-P(1)-Pt	111.08(17)
C(2')-P(1)-Pt	115.4(6)	C(3')-P(1)-Pt	102.2(6)
C(7')-P(2)-C(6)	109.8(9)	C(7')-P(2)-C(5')	111.6(11)
C(6)-P(2)-C(5')	53.3(7)	C(7')-P(2)-C(7)	27.1(9)
C(6)-P(2)-C(7)	106.3(2)	C(5')-P(2)-C(7)	132.2(7)
C(7')-P(2)-C(5)	72.1(9)	C(6)-P(2)-C(5)	104.8(2)
C(5')-P(2)-C(5)	57.3(7)	C(7)-P(2)-C(5)	99.0(2)
C(7')-P(2)-C(6')	98.2(11)	C(6)-P(2)-C(6')	40.9(7)
C(5')-P(2)-C(6')	94.2(10)	C(7)-P(2)-C(6')	79.5(7)
C(5)-P(2)-C(6')	140.3(7)	C(7')-P(2)-Pt	127.5(9)
C(6)-P(2)-Pt	118.82(16)	C(5')-P(2)-Pt	112.5(7)
C(7)-P(2)-Pt	114.85(18)	C(5)-P(2)-Pt	110.79(16)
C(6')-P(2)-Pt	105.5(6)	C(9)-P(3)-C(10)	104.9(2)
C(9)-P(3)-C(8)	104.7(2)	C(10)-P(3)-C(8)	100.6(2)
C(9)-P(3)-Pt	117.89(17)	C(10)-P(3)-Pt	111.34(16)
C(8)-P(3)-Pt	115.59(17)	C(13)-P(4)-C(12)	104.7(2)
C(13)-P(4)-C(14)	103.8(2)	C(12)-P(4)-C(14)	101.5(2)
C(13)-P(4)-Pt	118.91(18)	C(12)-P(4)-Pt	111.34(16)
C(14)-P(4)-Pt	114.77(18)	C(4)-C(3)-P(1)	115.4(4)
C(3)-C(4)-C(5)	116.7(4)	C(4)-C(5)-P(2)	114.1(3)
C(11)-C(10)-P(3)	114.6(4)	C(10)-C(11)-C(12)	116.1(4)
C(11)-C(12)-P(4)	115.5(4)	F(8)-P(6)-F(7)	179.2(2)
F(8)-P(6)-F(9)	91.03(18)	F(7)-P(6)-F(9)	88.72(19)
F(8)-P(6)-F(10)	89.76(17)	F(7)-P(6)-F(10)	90.49(18)
F(9)-P(6)-F(10)	179.1(2)	F(8)-P(6)-F(12)	89.0(2)
F(7)-P(6)-F(12)	90.24(19)	F(9)-P(6)-F(12)	90.25(19)

F(10)-P(6)-F(12)	89.38(16)	F(8)-P(6)-F(11)	92.0(2)
F(7)-P(6)-F(11)	88.8(2)	F(9)-P(6)-F(11)	90.7(2)
F(10)-P(6)-F(11)	89.7(2)	F(12)-P(6)-F(11)	178.7(2)
F(2)-P(5)-F(4)	89.6(8)	F(2)-P(5)-F(3)	92.3(10)
F(4)-P(5)-F(3)	176.4(10)	F(2)-P(5)-F(2')	20.8(12)
F(4)-P(5)-F(2')	110.2(10)	F(3)-P(5)-F(2')	71.6(9)
F(2)-P(5)-F(1)	174.9(9)	F(4)-P(5)-F(1)	90.8(8)
F(3)-P(5)-F(1)	87.1(8)	F(2')-P(5)-F(1)	157.6(9)
F(2)-P(5)-F(3')	111.4(9)	F(4)-P(5)-F(3')	158.5(9)
F(3)-P(5)-F(3')	19.2(11)	F(2')-P(5)-F(3')	90.6(10)
F(1)-P(5)-F(3')	67.9(9)	F(2)-P(5)-F(1')	157.9(8)
F(4)-P(5)-F(1')	70.7(9)	F(3)-P(5)-F(1')	108.0(8)
F(2')-P(5)-F(1')	173.1(9)	F(1)-P(5)-F(1')	25.0(6)
F(3')-P(5)-F(1')	89.3(9)	F(2)-P(5)-F(4')	68.8(10)
F(4)-P(5)-F(4')	22.6(9)	F(3)-P(5)-F(4')	160.1(8)
F(2')-P(5)-F(4')	89.6(9)	F(1)-P(5)-F(4')	112.3(8)
F(3')-P(5)-F(4')	175.9(10)	F(1')-P(5)-F(4')	90.0(8)
F(2)-P(5)-F(5)	89.8(6)	F(4)-P(5)-F(5)	84.4(7)
F(3)-P(5)-F(5)	92.5(8)	F(2')-P(5)-F(5)	89.0(8)
F(1)-P(5)-F(5)	85.2(7)	F(3')-P(5)-F(5)	90.7(9)
F(1')-P(5)-F(5)	97.8(6)	F(4')-P(5)-F(5)	93.3(6)
F(2)-P(5)-F(6)	89.8(6)	F(4)-P(5)-F(6)	95.2(7)
F(3)-P(5)-F(6)	87.9(8)	F(2')-P(5)-F(6)	90.8(8)
F(1)-P(5)-F(6)	95.2(7)	F(3')-P(5)-F(6)	89.8(9)
F(1')-P(5)-F(6)	82.3(6)	F(4')-P(5)-F(6)	86.1(6)
F(5)-P(5)-F(6)	179.44(18)	C(1Sa)-N(1S)-C(1S)	180.000(6)
N(1S)-C(1S)-C(2S)	176.4(18)	C(3S)-O(1S)-O(1Sb)	155.8(18)
C(4')-C(3')-P(1)	114.6(14)	C(3')-C(4')-C(5')	112.5(16)
C(4')-C(5')-P(2)	103.5(14)	C(10')-P(3')-C(9')	98.7(12)
C(10')-P(3')-C(8')	104.3(12)	C(9')-P(3')-C(8')	105.0(12)
C(10')-P(3')-Pt	115.1(9)	C(9')-P(3')-Pt	116.4(9)
C(8')-P(3')-Pt	115.4(9)	C(13')-P(4')-C(12')	102.6(12)
C(13')-P(4')-C(14')	106.0(11)	C(12')-P(4')-C(14')	106.4(11)
C(13')-P(4')-Pt	114.4(9)	C(12')-P(4')-Pt	110.0(8)
C(14')-P(4')-Pt	116.3(7)	C(11')-C(10')-P(3')	114.8(17)
C(12')-C(11')-C(10')	117.0(19)	C(11')-C(12')-P(4')	118.7(16)

Symmetry transformations used to generate equivalent atoms:
a: -x+1,-y+2,-z+2; b: -x,-y,-z+1
Atoms marked with ' are minor component of disordered group.

Table 30. Anisotropic displacement parameters ($Å^2$) for $[Pt(dmpp)_2](PF_6)_2$.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt	0.02198(7)	0.01821(6)	0.01834(7)	-0.00148(4)	0.00249(4)	0.00156(4)
P(1)	0.0510(6)	0.0418(6)	0.0244(5)	-0.0001(4)	0.0038(4)	0.0273(5)
P(2)	0.0315(4)	0.0323(5)	0.0210(4)	-0.0040(3)	-0.0007(3)	0.0005(4)
P(3)	0.0259(6)	0.0201(5)	0.0291(7)	-0.0035(5)	0.0057(5)	0.0024(4)
P(4)	0.0223(6)	0.0304(6)	0.0207(5)	-0.0013(4)	0.0010(5)	-0.0012(4)
P(6)	0.0392(5)	0.0282(4)	0.0257(4)	-0.0011(3)	0.0044(4)	0.0048(4)
F(7)	0.103(2)	0.074(2)	0.0366(15)	-0.0028(14)	0.0290(16)	0.0117(19)
F(8)	0.094(2)	0.097(3)	0.0344(15)	0.0135(16)	0.0234(15)	0.036(2)
F(9)	0.0655(19)	0.080(2)	0.071(2)	0.0024(18)	-0.0025(16)	0.0416(17)
F(10)	0.0476(15)	0.0550(17)	0.0638(18)	-0.0118(14)	-0.0156(13)	0.0085(12)
F(12)	0.0534(17)	0.0441(16)	0.089(2)	-0.0220(15)	-0.0008(15)	-0.0066(13)
F(11)	0.097(3)	0.0318(15)	0.116(3)	-0.0100(17)	0.039(2)	-0.0103(16)
P(5)	0.0428(5)	0.0265(5)	0.0320(5)	0.0007(4)	-0.0014(4)	-0.0017(4)
F(1)	0.051(4)	0.050(7)	0.132(13)	-0.046(7)	-0.006(7)	-0.001(4)
F(2)	0.067(8)	0.040(7)	0.161(16)	-0.047(8)	-0.053(9)	0.010(5)
F(3)	0.066(6)	0.165(16)	0.051(8)	0.047(9)	0.007(4)	-0.035(9)
F(4)	0.067(8)	0.135(13)	0.052(9)	0.033(8)	0.025(6)	0.030(7)
F(5)	0.0520(17)	0.066(2)	0.074(2)	-0.0002(16)	-0.0230(15)	0.0077(14)
F(6)	0.0536(16)	0.0474(16)	0.0625(18)	-0.0070(13)	-0.0014(13)	0.0146(12)
F(1')	0.054(5)	0.026(3)	0.132(13)	0.013(6)	-0.007(7)	-0.010(3)
F(2')	0.066(6)	0.027(5)	0.152(15)	0.014(8)	0.032(9)	-0.007(4)
F(3')	0.152(18)	0.108(12)	0.034(5)	-0.001(7)	0.016(9)	0.056(11)
F(4')	0.072(9)	0.093(10)	0.029(3)	-0.006(5)	-0.002(5)	0.045(7)

Atoms marked with ' are minor component of disordered group.

Table 31. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Pt(dmpp)_2](PF_6)_2$.

	x	y	z	Ueq
H(1A)	0.4688	0.8209	0.2040	0.060
H(1B)	0.4477	0.9223	0.2674	0.060
H(1C)	0.4427	0.9791	0.1871	0.060
H(2A)	0.3691	0.6062	0.2294	0.065
H(2B)	0.2821	0.6281	0.2393	0.065
H(2C)	0.3432	0.6815	0.2996	0.065
H(3A)	0.3335	0.8901	0.0825	0.045
H(3B)	0.3741	0.7426	0.0977	0.045
H(4A)	0.2688	0.6208	0.0837	0.045
H(4B)	0.2530	0.7432	0.0265	0.045
H(5A)	0.1822	0.7049	0.1573	0.042
H(5B)	0.1421	0.7313	0.0796	0.042
H(6A)	0.1491	1.0061	0.0142	0.051
H(6B)	0.2360	1.0286	0.0369	0.051
H(6C)	0.1764	1.1440	0.0575	0.051
H(7A)	0.0456	0.9277	0.1032	0.056
H(7B)	0.0592	1.0495	0.1615	0.056
H(7C)	0.0634	0.8880	0.1855	0.056
H(8A)	0.1219	1.4031	0.1897	0.054
H(8B)	0.1236	1.2658	0.1406	0.054
H(8C)	0.1976	1.3582	0.1559	0.054
H(9A)	0.0668	1.2806	0.3040	0.048
H(9B)	0.1019	1.1461	0.3452	0.048
H(9C)	0.0582	1.1280	0.2684	0.048
H(10A)	0.2811	1.3584	0.2941	0.042
H(10B)	0.2048	1.4370	0.3079	0.042
H(11A)	0.1953	1.3305	0.4150	0.047
H(11D)	0.2823	1.3646	0.4151	0.047
H(12A)	0.2127	1.0955	0.4098	0.041
H(12B)	0.2856	1.1425	0.4578	0.041
H(13A)	0.4261	1.1770	0.3973	0.055
H(13B)	0.3917	1.2616	0.3290	0.055
H(13C)	0.4406	1.1234	0.3189	0.055
H(14A)	0.3780	0.9294	0.4423	0.053
H(14B)	0.3817	0.8434	0.3694	0.053
H(14C)	0.3059	0.8469	0.4092	0.053
H(2S1)	0.3854	0.8523	0.9407	0.123
H(2S2)	0.3966	0.9826	0.8886	0.123
H(2S3)	0.3546	1.0045	0.9600	0.123
H(1S)	-0.021(10)	0.030(18)	0.449(11)	0.136

H(3S1)	0.0369	0.2516	0.5204	0.141
H(3S2)	0.0516	0.2161	0.4394	0.141
H(3S3)	0.1145	0.1827	0.5019	0.141
H(1'1)	0.4495	0.8240	0.1924	0.060
H(1'2)	0.4049	0.9058	0.1280	0.060
H(1'3)	0.4009	0.7379	0.1322	0.060
H(2'1)	0.3600	0.5989	0.2532	0.033
H(2'2)	0.3143	0.6864	0.3083	0.033
H(2'3)	0.4021	0.7120	0.3049	0.033
H(6'1)	0.1044	1.1216	0.0478	0.051
H(6'2)	0.1872	1.1809	0.0654	0.051
H(6'3)	0.1250	1.2035	0.1210	0.051
H(7'1)	0.0552	0.9305	0.0997	0.058
H(7'2)	0.0718	0.8804	0.1806	0.058
H(7'3)	0.0930	0.7805	0.1166	0.058
H(3'A)	0.2831	0.5891	0.1527	0.038
H(3'B)	0.2134	0.6746	0.1785	0.038
H(4'A)	0.1853	0.6721	0.0620	0.019
H(4'B)	0.2709	0.6774	0.0435	0.019
H(5'A)	0.1995	0.9106	0.0141	0.041
H(5'B)	0.2767	0.9353	0.0620	0.041
H(8'1)	0.1388	1.4213	0.2452	0.061
H(8'2)	0.1865	1.3546	0.1850	0.061
H(8'3)	0.2279	1.4148	0.2569	0.061
H(9'1)	0.0669	1.0538	0.2954	0.048
H(9'2)	0.0534	1.1516	0.2263	0.048
H(9'3)	0.0494	1.2177	0.3042	0.048
H(13D)	0.4631	1.1428	0.3134	0.055
H(13E)	0.4404	1.0164	0.2599	0.055
H(13F)	0.4667	0.9838	0.3414	0.055
H(14D)	0.3333	0.8548	0.4021	0.037
H(14E)	0.2943	0.9835	0.4398	0.037
H(14F)	0.3834	0.9682	0.4467	0.037
H(10C)	0.1517	1.2839	0.3911	0.043
H(10D)	0.1900	1.1330	0.4024	0.043
H(11B)	0.2626	1.3984	0.3927	0.031
H(11C)	0.2802	1.2786	0.4510	0.031
H(12C)	0.3824	1.2718	0.3913	0.038
H(12D)	0.3386	1.3085	0.3168	0.038

Atoms marked with ' are minor component of disordered group.

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Table 32. Crystal data for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

Identification code	bc191
Empirical formula	$C_{16}H_{38}F_{12}N_2NiP_6$
Formula mass	731.01
Crystal size, mm	$0.23 \times 0.15 \times 0.15$
Crystal color, habit	pale gold block
Crystal system	Monoclinic
Space group	$P2_1/c$
a, Å	19.9406(4)
b, Å	9.0706(2)
c, Å	16.7066(3)
α, °	90
β, °	97.49
γ, °	90
Volume, $Å^3$	2996.03(10)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.621
Absorption coefficient, mm^{-1}	1.054
F(000)	1496
Absorption correction[1]	Multiscan
Range Transmission Coefficients	0.86 and 0.79

1) Blessing, *Acta Cryst.* 1995. A51 33-38

Table 33. Data collection parameters for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	170(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	6530
θ range	$1.03 < \theta < 28.28$
θ range, data collection	$1.03 < \theta < 28.28$
Scan type	ω scans
Index ranges	$-26 \le h \le 26$,
	$-12 \le k \le 11$,
	$-17 \le l \le 22$
Reflections collected	22492
Independent reflections	7396 (R(int) = 0.0467)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed