Table 34. Structure Solution and Refinement for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	7396 / 0/ 606
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0313P)^2+4.6821P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0560, wR2 = 0.1074
Reflections observed	4221
R indices (all data)	R1 = 0.1062, wR2 = 0.1349
Goodness-of-fit[4] on F^2	1.144
Largest diff. peak and hole	0.469 and -0.318

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

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 35. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

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

	x	y	z	Ueq
P(1)	-0.29842(4)	0.41653(9)	0.44183(6)	0.0215(2)
P(2)	-0.30388(4)	0.08441(9)	0.44311(5)	0.0210(2)
P(3)	-0.19976(4)	0.07600(9)	0.30938(6)	0.0216(2)
P(4)	-0.19800(4)	0.40854(9)	0.30785(6)	0.0218(2)
C(1)	-0.3735(2)	0.5014(5)	0.3881(3)	0.0345(9)
C(2)	-0.2488(2)	0.5687(4)	0.4875(3)	0.0304(8)
C(3)	-0.3309(2)	0.3281(4)	0.5275(2)	0.0291(8)
C(4)	-0.36373(19)	0.1831(4)	0.4969(3)	0.0294(8)
C(5)	-0.3554(2)	-0.0594(5)	0.3902(3)	0.0349(9)
C(6)	-0.2525(2)	-0.0136(5)	0.5233(3)	0.0343(9)
C(7)	-0.2551(2)	-0.0180(4)	0.2312(2)	0.0306(8)
C(8)	-0.1508(2)	-0.0710(5)	0.3621(3)	0.0363(9)
C(9)	-0.1381(2)	0.1657(4)	0.2526(3)	0.0320(8)
C(10)	-0.1685(2)	0.3117(4)	0.2226(2)	0.0303(8)
C(11)	-0.2438(2)	0.5647(4)	0.2605(3)	0.0326(8)
C(12)	-0.1212(2)	0.4884(5)	0.3603(3)	0.0327(8)
NiA	-0.2629(4)	0.24594(19)	0.3614(4)	0.0146(8)
N(1')	-0.3516(5)	0.2498(10)	0.2607(8)	0.021(2)
C(13')	-0.4088(10)	0.2496(19)	0.2183(12)	0.023(4)
N(1A)	-0.3554(5)	0.2788(12)	0.2212(9)	0.052(3)
C(13A)	-0.4038(9)	0.2741(16)	0.1968(9)	0.033(3)
C(14A)	-0.4734(3)	0.2617(9)	0.1637(4)	0.0605(17)
NiB	-0.2398(3)	0.24508(13)	0.3867(4)	0.0188(9)
N(1#)	-0.1487(5)	0.2455(10)	0.4933(8)	0.038(2)
C(13#)	-0.0981(9)	0.2449(17)	0.5315(8)	0.027(3)
N(1B)	-0.1450(7)	0.2817(17)	0.5319(10)	0.042(3)
C(13B)	-0.0894(14)	0.262(3)	0.5573(10)	0.032(4)
C(14B)	-0.0275(3)	0.2408(8)	0.5852(4)	0.0549(15)
P(5)	0.43047(5)	0.24941(10)	0.37580(7)	0.0302(3)
F(1)	0.50094(13)	0.2048(4)	0.34924(17)	0.0719(9)
F(2)	0.35986(16)	0.2941(4)	0.4023(2)	0.0907(11)
F(3)	0.4522(9)	0.4048(13)	0.3759(15)	0.157(8)
F(4)	0.3978(4)	0.2561(13)	0.2830(5)	0.062(4)
F(5)	0.4026(5)	0.0816(8)	0.3716(10)	0.087(4)
F(6)	0.4564(5)	0.224(3)	0.4652(5)	0.103(6)
F(3')	0.4298(8)	0.3976(16)	0.3284(11)	0.122(6)
F(4')	0.3965(5)	0.176(3)	0.3030(11)	0.152(9)
F(5')	0.4373(9)	0.1146(13)	0.4323(12)	0.120(7)
F(6')	0.4725(5)	0.3347(19)	0.4525(8)	0.097(5)

P(6)	0.06959(5)	0.24338(10)	0.37426(7)	0.0293(2)
F(7)	0.14098(15)	0.2880(5)	0.3496(2)	0.0919(12)
F(8)	-0.00179(12)	0.1971(4)	0.39919(16)	0.0622(8)
F(9)	0.0885(5)	0.0831(7)	0.3561(9)	0.109(5)
F(10)	0.0547(5)	0.4065(7)	0.3961(9)	0.119(4)
F(11)	0.1050(3)	0.2270(12)	0.4651(4)	0.068(3)
F(12)	0.0366(4)	0.2702(17)	0.2867(4)	0.109(5)
F(9')	0.0515(9)	0.126(2)	0.3028(9)	0.094(7)
F(10')	0.0812(10)	0.347(3)	0.4452(12)	0.136(13)
F(11')	0.0972(6)	0.116(3)	0.4324(15)	0.115(10)
F(12')	0.0342(9)	0.3600(19)	0.3155(16)	0.118(10)

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Table 36. Bond lengths (Å) for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

P(1)-C(2)	1.809(4)	P(1)-C(1)	1.814(4)
P(1)-C(3)	1.831(4)	P(1)-NiB	2.2170(16)
P(1)-NiA	2.224(2)	P(2)-C(6)	1.810(4)
P(2)-C(5)	1.817(4)	P(2)-C(4)	1.821(4)
P(2)-NiB	2.2271(16)	P(2)-NiA	2.229(2)
P(3)-C(7)	1.810(4)	P(3)-C(8)	1.812(4)
P(3)-C(9)	1.838(4)	P(3)-NiB	2.2193(17)
P(3)-NiA	2.236(2)	P(4)-C(11)	1.810(4)
P(4)-C(12)	1.813(4)	P(4)-C(10)	1.834(4)
P(4)-NiB	2.2167(18)	P(4)-NiA	2.225(2)
C(3)-C(4)	1.527(6)	C(9)-C(10)	1.515(6)
NiA-N(1')	2.278(19)	N(1')-C(13')	1.26(2)
C(13')-C(14A)	1.48(2)	N(1A)-C(13A)	0.998(19)
C(13A)-C(14A)	1.429(19)	NiB-N(1#)	2.372(18)
N(1#)-C(13#)	1.123(19)	C(13#)-C(14B)	1.568(17)
N(1B)-C(13B)	1.15(3)	C(13B)-C(14B)	1.28(3)
P(5)-F(4')	1.474(9)	P(5)-F(3)	1.474(10)
P(5)-F(6)	1.532(8)	P(5)-F(5')	1.540(9)
P(5)-F(3')	1.559(10)	P(5)-F(1)	1.580(3)
P(5)-F(2)	1.583(3)	P(5)-F(4)	1.602(8)
P(5)-F(5)	1.619(8)	P(5)-F(6')	1.632(8)
P(6)-F(10')	1.506(11)	P(6)-F(9)	1.542(5)
P(6)-F(12)	1.542(6)	P(6)-F(12')	1.549(14)
P(6)-F(10)	1.562(6)	P(6)-F(11')	1.564(11)
P(6)-F(7)	1.585(3)	P(6)-F(8)	1.591(3)
P(6)-F(11)	1.596(6)	P(6)-F(9')	1.605(10)

Table 37. Bond angles (°) for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

C(2)-P(1)-C(1)	104.8(2)	C(2)-P(1)-C(3)	103.55(19)
C(1)-P(1)-C(3)	102.69(19)	C(2)-P(1)-NiB	114.9(2)
C(1)-P(1)-NiB	122.6(3)	C(3)-P(1)-NiB	106.06(14)
C(2)-P(1)-NiA	125.9(2)	C(1)-P(1)-NiA	107.7(3)
C(3)-P(1)-NiA	109.87(13)	NiB-P(1)-NiA	15.08(3)
C(6)-P(2)-C(5)	103.7(2)	C(6)-P(2)-C(4)	102.7(2)
C(5)-P(2)-C(4)	103.2(2)	C(6)-P(2)-NiB	109.5(3)
C(5)-P(2)-NiB	125.7(2)	C(4)-P(2)-NiB	109.67(12)
C(6)-P(2)-NiA	123.9(3)	C(5)-P(2)-NiA	113.8(2)
C(4)-P(2)-NiA	107.18(14)	NiB-P(2)-NiA	15.03(3)
C(7)-P(3)-C(8)	104.1(2)	C(7)-P(3)-C(9)	102.87(19)
C(8)-P(3)-C(9)	102.85(19)	C(7)-P(3)-NiB	120.9(3)
C(8)-P(3)-NiB	115.9(2)	C(9)-P(3)-NiB	108.06(13)
C(7)-P(3)-NiA	106.5(3)	C(8)-P(3)-NiA	127.8(2)
C(9)-P(3)-NiA	110.12(13)	NiB-P(3)-NiA	15.03(3)
C(11)-P(4)-C(12)	104.2(2)	C(11)-P(4)-C(10)	103.29(19)
C(12)-P(4)-C(10)	103.27(19)	C(11)-P(4)-NiB	125.2(2)
C(12)-P(4)-NiB	109.8(3)	C(10)-P(4)-NiB	108.93(13)
C(11)-P(4)-NiA	114.1(2)	C(12)-P(4)-NiA	124.7(3)
C(10)-P(4)-NiA	104.90(14)	NiB-P(4)-NiA	15.08(3)
C(4)-C(3)-P(1)	107.3(2)	C(3)-C(4)-P(2)	108.0(2)
C(10)-C(9)-P(3)	107.0(2)	C(9)-C(10)-P(4)	108.5(3)
P(1)-NiA-P(4)	91.69(10)	P(1)-NiA-P(2)	85.21(8)
P(4)-NiA-P(2)	163.9(5)	P(1)-NiA-P(3)	162.5(5)
P(4)-NiA-P(3)	85.08(10)	P(2)-NiA-P(3)	93.14(10)
P(1)-NiA-N(1')	99.1(3)	P(4)-NiA-N(1')	97.4(5)
P(2)-NiA-N(1')	98.7(3)	P(3)-NiA-N(1')	98.4(4)
C(13')-N(1')-NiA	166.6(9)	N(1')-C(13')-C(14A)	174.1(11)
N(1A)-C(13A)-C(14A)	177.6(14)	C(13A)-C(14A)-C(13')	17.5(5)
P(4)-NiB-P(1)	92.12(8)	P(4)-NiB-P(3)	85.70(7)
P(1)-NiB-P(3)	167.3(5)	P(4)-NiB-P(2)	165.9(5)
P(1)-NiB-P(2)	85.43(6)	P(3)-NiB-P(2)	93.66(7)
P(4)-NiB-N(1#)	97.8(3)	P(1)-NiB-N(1#)	94.6(4)
P(3)-NiB-N(1#)	98.1(2)	P(2)-NiB-N(1#)	96.2(4)
C(13#)-N(1#)-NiB	166.1(10)	N(1#)-C(13#)-C(14B)	178.9(14)
N(1B)-C(13B)-C(14B)	179(3)	C(13B)-C(14B)-C(13#)	14.9(12)
F(4')-P(5)-F(3)	122.5(10)	F(4')-P(5)-F(6)	142.9(9)
F(3)-P(5)-F(6)	94.6(8)	F(4')-P(5)-F(5')	98.1(9)
F(3)-P(5)-F(5')	139.1(9)	F(6)-P(5)-F(5')	44.9(6)
F(4')-P(5)-F(3')	89.9(9)	F(3)-P(5)-F(3')	32.8(7)
F(6)-P(5)-F(3')	127.1(8)	F(5')-P(5)-F(3')	171.9(8)
F(4')-P(5)-F(1)	89.0(5)	F(3)-P(5)-F(1)	88.4(7)

F(6)-P(5)-F(1)	92.0(4)	F(5')-P(5)-F(1)	87.6(4)
F(3')-P(5)-F(1)	91.6(6)	F(4')-P(5)-F(2)	91.0(5)
F(3)-P(5)-F(2)	91.5(7)	F(6)-P(5)-F(2)	88.0(4)
F(5')-P(5)-F(2)	92.5(4)	F(3')-P(5)-F(2)	88.4(6)
F(1)-P(5)-F(2)	179.93(17)	F(4')-P(5)-F(4)	29.9(10)
F(3)-P(5)-F(4)	92.7(9)	F(6)-P(5)-F(4)	172.4(8)
F(5')-P(5)-F(4)	128.0(8)	F(3')-P(5)-F(4)	60.0(7)
F(1)-P(5)-F(4)	90.1(3)	F(2)-P(5)-F(4)	89.8(3)
F(4')-P(5)-F(5)	54.5(8)	F(3)-P(5)-F(5)	176.4(8)
F(6)-P(5)-F(5)	88.4(7)	F(5')-P(5)-F(5)	44.2(6)
F(3')-P(5)-F(5)	143.9(7)	F(1)-P(5)-F(5)	93.5(4)
F(2)-P(5)-F(5)	86.6(4)	F(4)-P(5)-F(5)	84.2(5)
F(4')-P(5)-F(6')	175.8(6)	F(3)-P(5)-F(6')	54.9(7)
F(6)-P(5)-F(6')	39.8(5)	F(5')-P(5)-F(6')	84.2(7)
F(3')-P(5)-F(6')	87.7(7)	F(1)-P(5)-F(6')	87.5(4)
F(2)-P(5)-F(6')	92.5(4)	F(4)-P(5)-F(6')	147.6(7)
F(5)-P(5)-F(6')	128.2(6)	F(10')-P(6)-F(9)	136.6(12)
F(10')-P(6)-F(12)	130.5(12)	F(9)-P(6)-F(12)	92.7(5)
F(10')-P(6)-F(12')	94.7(12)	F(9)-P(6)-F(12')	128.5(10)
F(12)-P(6)-F(12')	35.8(8)	F(10')-P(6)-F(10)	40.4(11)
F(9)-P(6)-F(10)	176.4(5)	F(12)-P(6)-F(10)	90.1(5)
F(12')-P(6)-F(10)	54.3(8)	F(10')-P(6)-F(11')	88.1(11)
F(9)-P(6)-F(11')	49.4(8)	F(12)-P(6)-F(11')	141.1(10)
F(12')-P(6)-F(11')	173.3(9)	F(10)-P(6)-F(11')	128.1(10)
F(10')-P(6)-F(7)	89.7(5)	F(9)-P(6)-F(7)	86.5(3)
F(12)-P(6)-F(7)	90.0(3)	F(12')-P(6)-F(7)	90.6(6)
F(10)-P(6)-F(7)	91.3(4)	F(11')-P(6)-F(7)	95.4(5)
F(10')-P(6)-F(8)	90.5(5)	F(9)-P(6)-F(8)	93.0(3)
F(12)-P(6)-F(8)	90.3(3)	F(12')-P(6)-F(8)	89.8(6)
F(10)-P(6)-F(8)	89.2(4)	F(11')-P(6)-F(8)	84.1(5)
F(7)-P(6)-F(8)	179.5(2)	F(10')-P(6)-F(11)	46.1(11)
F(9)-P(6)-F(11)	90.6(5)	F(12)-P(6)-F(11)	176.2(5)
F(12')-P(6)-F(11)	140.8(10)	F(10)-P(6)-F(11)	86.5(4)
F(11')-P(6)-F(11)	42.5(9)	F(7)-P(6)-F(11)	88.2(3)
F(8)-P(6)-F(11)	91.5(2)	F(10')-P(6)-F(9')	174.5(8)
F(9)-P(6)-F(9')	42.7(6)	F(12)-P(6)-F(9')	51.2(6)
F(12')-P(6)-F(9')	86.7(10)	F(10)-P(6)-F(9')	140.5(8)
F(11')-P(6)-F(9')	89.9(10)	F(7)-P(6)-F(9')	95.7(5)
F(8)-P(6)-F(9')	84.1(5)	F(11)-P(6)-F(9')	132.4(8)

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Table 38. Anisotropic displacement parameters ($Å^2$) for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

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}
P(1)	0.0260(4)	0.0169(4)	0.0233(5)	-0.0018(4)	0.0097(4)	0.0009(3)
P(2)	0.0258(4)	0.0173(4)	0.0212(5)	0.0009(3)	0.0084(4)	-0.0035(3)
P(3)	0.0268(4)	0.0159(4)	0.0240(5)	-0.0011(4)	0.0103(4)	0.0017(3)
P(4)	0.0269(4)	0.0155(4)	0.0250(5)	0.0020(4)	0.0107(4)	-0.0013(3)
C(1)	0.036(2)	0.033(2)	0.034(2)	0.0028(18)	0.0038(17)	0.0014(17)
C(2)	0.0303(19)	0.0255(18)	0.037(2)	-0.0079(17)	0.0097(17)	-0.0017(15)
C(3)	0.040(2)	0.0253(17)	0.026(2)	-0.0005(15)	0.0159(17)	0.0042(16)
C(4)	0.0290(19)	0.0290(19)	0.033(2)	0.0064(16)	0.0153(17)	-0.0004(15)
C(5)	0.042(2)	0.031(2)	0.031(2)	-0.0040(17)	0.0015(18)	-0.0170(18)
C(6)	0.033(2)	0.034(2)	0.035(2)	-0.0006(18)	0.0008(17)	0.0014(17)
C(7)	0.034(2)	0.0283(19)	0.029(2)	-0.0026(16)	0.0044(16)	0.0032(16)
C(8)	0.043(2)	0.035(2)	0.032(2)	-0.0025(18)	0.0041(19)	0.0080(18)
C(9)	0.037(2)	0.0308(19)	0.033(2)	-0.0042(17)	0.0208(18)	-0.0006(16)
C(10)	0.038(2)	0.0287(19)	0.027(2)	-0.0002(16)	0.0175(17)	-0.0048(16)
C(11)	0.034(2)	0.0268(19)	0.037(2)	0.0077(18)	0.0075(18)	-0.0004(16)
C(12)	0.034(2)	0.034(2)	0.031(2)	0.0011(18)	0.0046(16)	-0.0008(17)
NiA	0.0154(16)	0.0167(7)	0.0116(14)	0.0002(5)	0.0022(14)	-0.0017(5)
N(1')	0.017(4)	0.023(4)	0.021(6)	-0.001(4)	-0.009(4)	0.005(3)
C(13')	0.020(5)	0.024(6)	0.032(10)	0.007(5)	0.036(7)	-0.014(4)
N(1A)	0.045(5)	0.056(5)	0.051(7)	-0.015(5)	-0.009(5)	0.008(4)
C(13A)	0.033(6)	0.042(7)	0.032(7)	-0.003(5)	0.037(5)	-0.014(5)
C(14A)	0.048(3)	0.084(5)	0.053(4)	0.003(3)	0.019(3)	-0.012(3)
NiB	0.0243(15)	0.0112(5)	0.0231(15)	-0.0014(4)	0.0112(15)	-0.0014(4)
N(1#)	0.025(4)	0.041(5)	0.050(7)	0.005(4)	0.011(5)	-0.001(3)
C(13#)	0.036(7)	0.031(5)	0.017(7)	0.007(5)	0.011(6)	0.002(4)
N(1B)	0.037(6)	0.053(7)	0.035(8)	0.013(6)	0.002(6)	0.002(5)
C(13B)	0.046(9)	0.042(8)	0.006(7)	0.001(7)	-0.007(7)	-0.009(5)
C(14B)	0.045(3)	0.083(5)	0.038(3)	0.000(3)	0.008(3)	-0.008(3)
P(5)	0.0278(5)	0.0358(6)	0.0287(6)	0.0004(4)	0.0097(5)	0.0009(4)
F(1)	0.0308(14)	0.140(3)	0.0463(17)	0.0028(18)	0.0104(12)	0.0188(16)
F(2)	0.057(2)	0.139(3)	0.083(3)	0.000(2)	0.0370(18)	0.036(2)
F(3)	0.150(13)	0.045(7)	0.27(3)	-0.044(10)	0.023(14)	-0.062(8)
F(4)	0.032(4)	0.129(9)	0.028(4)	0.027(5)	0.011(3)	0.031(5)
F(5)	0.105(7)	0.038(4)	0.115(10)	0.018(5)	0.011(7)	-0.013(4)
F(6)	0.050(5)	0.24(2)	0.022(4)	0.007(7)	0.005(3)	-0.006(8)
F(3')	0.122(10)	0.095(10)	0.151(12)	0.087(9)	0.031(8)	0.036(8)
F(4')	0.064(6)	0.25(2)	0.134(13)	-0.148(13)	0.000(8)	-0.058(10)
F(5')	0.154(13)	0.064(6)	0.160(17)	0.065(8)	0.089(12)	0.017(7)
F(6')	0.068(6)	0.155(12)	0.064(7)	-0.062(7)	-0.008(5)	0.001(6)

P(6)	0.0280(5)	0.0323(6)	0.0288(6)	0.0012(4)	0.0085(5)	0.0030(4)
F(7)	0.0496(18)	0.152(3)	0.081(2)	-0.002(2)	0.0346(17)	-0.034(2)
F(8)	0.0339(14)	0.106(2)	0.0484(17)	-0.0020(17)	0.0133(12)	-0.0106(15)
F(9)	0.103(6)	0.044(4)	0.189(13)	-0.056(6)	0.055(7)	0.004(3)
F(10)	0.150(7)	0.039(3)	0.158(11)	-0.028(5)	-0.015(7)	0.031(4)
F(11)	0.038(3)	0.115(7)	0.047(4)	0.034(4)	-0.006(2)	-0.001(4)
F(12)	0.088(6)	0.200(14)	0.029(3)	0.043(5)	-0.025(3)	-0.043(7)
F(9')	0.101(11)	0.127(14)	0.056(9)	-0.056(9)	0.020(7)	-0.018(10)
F(10')	0.115(16)	0.22(3)	0.084(13)	-0.108(16)	0.042(11)	-0.091(17)
F(11')	0.056(7)	0.132(18)	0.15(2)	0.096(17)	-0.001(9)	0.034(9)
F(12')	0.102(11)	0.076(10)	0.18(3)	0.094(13)	0.049(14)	0.042(10)

Table 39. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Ni(dmpe)_2(CH_3CN)](PF_6)_2$.

	x	y	z	Ueq
H(1A)	-0.391(2)	0.577(5)	0.422(3)	0.052(13)
H(1B)	-0.405(2)	0.428(5)	0.370(3)	0.055(13)
H(1C)	-0.3616(19)	0.556(4)	0.344(2)	0.039(11)
H(2A)	-0.2766(19)	0.623(4)	0.518(2)	0.036(11)
H(2B)	-0.238(2)	0.635(5)	0.447(3)	0.049(13)
H(2C)	-0.209(2)	0.533(4)	0.517(2)	0.043(12)
H(3A)	-0.290(2)	0.309(5)	0.563(3)	0.051(13)
H(3B)	-0.3594(18)	0.394(4)	0.546(2)	0.027(10)
H(4A)	-0.3998(19)	0.204(4)	0.465(2)	0.025(10)
H(4B)	-0.375(2)	0.124(5)	0.538(3)	0.043(12)
H(5A)	-0.384(2)	-0.108(5)	0.426(3)	0.046(12)
H(5B)	-0.328(2)	-0.130(5)	0.370(3)	0.046(12)
H(5C)	-0.385(2)	-0.011(5)	0.344(3)	0.056(14)
H(6A)	-0.284(2)	-0.074(5)	0.553(3)	0.056(13)
H(6B)	-0.230(2)	0.055(6)	0.554(3)	0.070(16)
H(6C)	-0.225(2)	-0.075(5)	0.503(3)	0.051(14)
H(7A)	-0.2320(18)	-0.084(4)	0.199(2)	0.028(10)
H(7B)	-0.276(2)	0.052(5)	0.198(3)	0.057(14)
H(7C)	-0.286(2)	-0.079(5)	0.256(3)	0.052(13)
H(8A)	-0.128(2)	-0.123(4)	0.325(2)	0.039(11)
H(8B)	-0.183(2)	-0.152(5)	0.382(3)	0.051(12)
H(8C)	-0.125(2)	-0.027(5)	0.398(3)	0.044(13)
H(9A)	-0.096(2)	0.182(5)	0.294(3)	0.044(12)
H(9B)	-0.131(2)	0.104(5)	0.212(3)	0.048(13)
H(10A)	-0.209(2)	0.302(4)	0.178(2)	0.036(11)
H(10B)	-0.138(2)	0.374(4)	0.198(2)	0.043(12)
H(11A)	-0.219(2)	0.611(4)	0.223(2)	0.040(11)
H(11B)	-0.249(2)	0.633(5)	0.307(3)	0.047(12)
H(11C)	-0.2801(19)	0.533(4)	0.229(2)	0.030(10)
H(12A)	-0.104(2)	0.553(5)	0.323(3)	0.063(15)
H(12B)	-0.090(2)	0.409(6)	0.374(3)	0.075(16)
H(12C)	-0.132(2)	0.545(5)	0.406(3)	0.063(15)
H(14A)	-0.483(3)	0.344(8)	0.140(4)	0.12(3)
H(14B)	-0.504(3)	0.248(5)	0.196(4)	0.063(18)
H(14C)	-0.480(4)	0.184(8)	0.143(4)	0.12(3)
H(14D)	-0.025(3)	0.314(8)	0.628(4)	0.12(3)
H(14E)	0.000(3)	0.277(6)	0.560(3)	0.065(18)
H(14F)	-0.023(4)	0.163(9)	0.618(5)	0.14(3)

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Table 40. Crystal data for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

Identification code	bc192
Empirical formula	$C_{16}H_{39}B_2F_8NNiP_4$
Formula mass	601.69
Crystal size, mm	$0.12 \times 0.09 \times 0.09$
Crystal color, habit	red parallelepiped
Crystal system	Triclinic
Space group	$P\bar{1}$
a, Å	10.7503(12)
b, Å	14.2268(19)
c, Å	17.8531(15)
α, °	93.236(6)
β, °	92.155(6)
γ, °	92.390(5)
Volume, $Å^3$	2721.6(5)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.468
Absorption coefficient, mm^{-1}	1.009
F(000)	1248
Absorption correction[1]	Multiscan
Range Transmission Coefficients	0.91 and 0.89

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

Table 41. Data collection parameters for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	169(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	6306
θ range	$1.14 < \theta < 27.50$
θ range, data collection	$1.14 < \theta < 27.50$
Scan type	ω scans
Index ranges	$-13 \le h \le 13$, $-18 \le k \le 18$, $0 \le l \le 23$
Reflections collected	35802
Independent reflections	12420 (R(int) = 0.0518)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 42. Structure Solution and Refinement for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	12420 / 60/ 582
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0482P)^2+4.9849P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0528, wR2 = 0.1142
Reflections observed	8652
R indices (all data)	R1 = 0.0899, wR2 = 0.1336
Goodness-of-fit[4] on F^2	1.021
Largest diff. peak and hole	1.244 and -0.859

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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 43. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

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

	x	y	z	Ueq
Ni1	-0.25198(4)	0.25100(3)	1.08016(3)	0.01927(11)
N1	-0.4292(3)	0.2567(2)	1.10828(18)	0.0291(7)
P11	-0.25066(9)	0.13775(7)	1.16010(6)	0.0257(2)
P21	-0.08555(9)	0.31775(7)	1.14156(6)	0.0255(2)
P31	-0.28451(10)	0.37132(7)	1.00895(7)	0.0319(2)
P41	-0.23637(9)	0.15578(7)	0.97543(5)	0.0234(2)
C11	-0.3583(4)	0.0380(3)	1.1334(3)	0.0371(10)
C21	-0.3078(4)	0.1787(4)	1.2510(2)	0.0442(12)
C31	-0.1035(4)	0.0865(3)	1.1844(3)	0.0372(10)
C41	-0.0139(5)	0.1583(4)	1.2258(3)	0.0373(19)
C4'1	0.0208(14)	0.1501(11)	1.1711(9)	0.025(5)
C51	0.0251(5)	0.2370(4)	1.1806(3)	0.0564(15)
C61	0.0239(4)	0.3821(3)	1.0857(2)	0.0365(10)
C71	-0.1077(5)	0.4018(4)	1.2194(3)	0.0560(15)
C81	-0.2756(5)	0.4884(3)	1.0559(3)	0.0572(15)
C91	-0.4430(4)	0.3673(4)	0.9701(3)	0.0469(12)
C101	-0.1924(4)	0.3821(3)	0.9257(3)	0.0423(11)
C111	-0.2110(5)	0.2983(4)	0.8692(3)	0.0461(12)
C121	-0.1600(4)	0.2078(3)	0.8966(2)	0.0359(10)
C131	-0.1393(4)	0.0543(3)	0.9816(3)	0.0355(10)
C141	-0.3828(4)	0.1035(3)	0.9345(2)	0.0395(11)
C151	-0.5287(4)	0.2449(3)	1.1255(2)	0.0314(9)
C161	-0.6552(4)	0.2257(4)	1.1490(3)	0.0482(12)
B12	-0.1477(4)	0.2607(3)	1.4450(3)	0.0336(11)
F12	-0.1064(3)	0.3211(2)	1.39193(17)	0.0628(9)
F22	-0.1507(4)	0.1707(2)	1.4141(2)	0.0826(12)
F32	-0.2640(3)	0.2873(3)	1.46571(19)	0.0706(10)
F42	-0.0661(3)	0.2676(2)	1.50616(16)	0.0618(8)
B22	0.2034(5)	0.2008(4)	0.9460(3)	0.0448(14)
F52	0.3249(3)	0.1956(5)	0.9595(3)	0.155(3)
F62	0.1670(5)	0.2874(2)	0.9225(2)	0.1138(18)
F72	0.1659(3)	0.1337(2)	0.88964(14)	0.0556(8)
F82	0.1377(3)	0.1836(2)	1.00859(14)	0.0487(7)
Ni3	0.28572(4)	0.26080(3)	0.57602(2)	0.02029(12)
N3	0.4806(3)	0.2772(2)	0.59962(18)	0.0290(7)
P13	0.25814(10)	0.24977(7)	0.69781(5)	0.0257(2)
P23	0.23517(9)	0.10678(7)	0.56206(6)	0.0265(2)
P33	0.32262(9)	0.27178(8)	0.45425(5)	0.0263(2)
P43	0.21835(9)	0.40697(7)	0.57918(5)	0.0232(2)

C13	0.2866(4)	0.3511(3)	0.7638(2)	0.0380(10)
C23	0.3679(4)	0.1723(3)	0.7400(2)	0.0398(11)
C33	0.1023(4)	0.2055(3)	0.7205(2)	0.0326(9)
C43	0.0420(4)	0.1337(3)	0.6611(2)	0.0369(10)
C53	0.1333(4)	0.0619(3)	0.6336(2)	0.0358(10)
C63	0.1437(4)	0.0683(3)	0.4777(2)	0.0360(10)
C73	0.3611(4)	0.0247(3)	0.5598(3)	0.0452(12)
C83	0.2019(4)	0.2559(3)	0.3792(2)	0.0359(10)
C93	0.4442(4)	0.1966(3)	0.4212(2)	0.0403(11)
C103	0.3897(4)	0.3891(3)	0.4410(2)	0.0365(10)
C113	0.2964(5)	0.4677(3)	0.4389(2)	0.0412(11)
C123	0.1837(4)	0.4551(3)	0.4883(2)	0.0347(10)
C133	0.0698(4)	0.4253(3)	0.6224(2)	0.0316(9)
C143	0.3268(4)	0.4983(3)	0.6224(2)	0.0319(9)
C153	0.5824(4)	0.2804(3)	0.6197(2)	0.0280(9)
C163	0.7125(4)	0.2822(4)	0.6466(3)	0.0405(11)
B14	0.6296(6)	0.5310(4)	0.7809(3)	0.0506(15)
F14	0.7530(4)	0.5423(4)	0.7663(2)	0.1101(16)
F24	0.5634(4)	0.5935(3)	0.74158(18)	0.0917(13)
F34	0.5902(3)	0.4408(2)	0.7586(2)	0.0884(12)
F44	0.6183(4)	0.5480(2)	0.85686(16)	0.0762(11)
B24	0.3289(5)	-0.0168(4)	0.2808(3)	0.0453(13)
F54	0.4325(4)	0.0298(3)	0.2612(2)	0.1073(15)
F64	0.3204(5)	-0.1046(3)	0.24816(19)	0.1030(15)
F74	0.3418(5)	-0.0310(3)	0.3577(2)	0.1109(16)
F84	0.2315(5)	0.0308(5)	0.2727(5)	0.213(4)

Table 44. Bond lengths (Å) for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

Ni1-N1	1.992(3)	Ni1-P11	2.2120(11)	Ni1-P21	2.2131(11)
Ni1-P31	2.2206(12)	Ni1-P41	2.2617(11)	N1-C151	1.133(5)
P11-C31	1.818(4)	P11-C11	1.823(4)	P11-C21	1.830(4)
P21-C71	1.811(4)	P21-C61	1.821(4)	P21-C51	1.834(5)
P31-C91	1.813(5)	P31-C81	1.820(5)	P31-C101	1.826(5)
P41-C131	1.822(4)	P41-C141	1.822(4)	P41-C121	1.833(4)
C31-C41	1.516(7)	C31-C4'1	1.614(16)	C41-C51	1.472(8)
C4'1-C51	1.237(16)	C101-C111	1.520(7)	C111-C121	1.519(7)
C151-C161	1.458(6)	B12-F22	1.364(5)	B12-F42	1.371(5)
B12-F32	1.380(5)	B12-F12	1.387(5)	B22-F52	1.325(6)
B22-F82	1.373(5)	B22-F72	1.384(6)	B22-F62	1.390(7)
Ni3-N3	2.122(3)	Ni3-P13	2.2189(11)	Ni3-P43	2.2287(11)
Ni3-P23	2.2333(11)	Ni3-P33	2.2373(11)	N3-C153	1.137(5)
P13-C13	1.818(4)	P13-C23	1.819(4)	P13-C33	1.833(4)
P23-C63	1.812(4)	P23-C73	1.824(4)	P23-C53	1.838(4)
P33-C93	1.818(4)	P33-C103	1.822(4)	P33-C83	1.827(4)
P43-C133	1.822(4)	P43-C143	1.826(4)	P43-C123	1.828(4)
C33-C43	1.535(6)	C43-C53	1.521(6)	C103-C113	1.534(7)
C113-C123	1.535(6)	C153-C163	1.460(6)	B14-F14	1.366(7)
B14-F34	1.367(6)	B14-F24	1.370(6)	B14-F44	1.375(6)
B24-F84	1.279(7)	B24-F54	1.339(6)	B24-F64	1.346(6)
B24-F74	1.402(6)				

Table 45. Bond angles (°) for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

N1-Ni1-P11	82.55(10)	N1-Ni1-P21	127.74(10)
P11-Ni1-P21	88.76(4)	N1-Ni1-P31	87.70(10)
P11-Ni1-P31	169.91(4)	P21-Ni1-P31	95.19(4)
N1-Ni1-P41	110.35(10)	P11-Ni1-P41	96.20(4)
P21-Ni1-P41	121.81(4)	P31-Ni1-P41	89.61(4)
C151-N1-Ni1	169.0(3)	C31-P11-C11	105.4(2)
C31-P11-C21	103.6(2)	C11-P11-C21	102.0(2)
C31-P11-Ni1	118.79(14)	C11-P11-Ni1	114.09(15)
C21-P11-Ni1	111.13(17)	C71-P21-C61	102.2(2)
C71-P21-C51	103.5(3)	C61-P21-C51	97.2(2)
C71-P21-Ni1	118.64(18)	C61-P21-Ni1	116.26(15)
C51-P21-Ni1	115.96(18)	C91-P31-C81	100.5(2)
C91-P31-C101	102.5(2)	C81-P31-C101	105.0(3)
C91-P31-Ni1	111.46(16)	C81-P31-Ni1	116.8(2)
C101-P31-Ni1	118.23(16)	C131-P41-C141	102.7(2)
C131-P41-C121	97.2(2)	C141-P41-C121	104.4(2)
C131-P41-Ni1	117.81(15)	C141-P41-Ni1	115.66(15)
C121-P41-Ni1	116.43(15)	C41-C31-C4'1	39.4(6)
C41-C31-P11	111.4(3)	C4'1-C31-P11	116.1(6)
C51-C41-C31	113.9(5)	C51-C4'1-C31	122.4(11)
C4'1-C51-C41	45.0(8)	C4'1-C51-P21	126.6(8)
C41-C51-P21	122.6(4)	C111-C101-P31	113.5(3)
C121-C111-C101	113.8(4)	C111-C121-P41	117.2(3)
N1-C151-C161	177.4(5)	F22-B12-F42	108.9(4)
F22-B12-F32	111.9(4)	F42-B12-F32	110.1(4)
F22-B12-F12	108.5(4)	F42-B12-F12	109.3(4)
F32-B12-F12	108.0(4)	F52-B22-F82	111.4(5)
F52-B22-F72	108.6(4)	F82-B22-F72	108.4(4)
F52-B22-F62	114.6(5)	F82-B22-F62	106.4(4)
F72-B22-F62	107.1(5)	N3-Ni3-P13	88.99(9)
N3-Ni3-P43	105.02(10)	P13-Ni3-P43	91.89(4)
N3-Ni3-P23	108.13(10)	P13-Ni3-P23	87.21(4)
P43-Ni3-P23	146.81(4)	N3-Ni3-P33	88.50(9)
P13-Ni3-P33	177.47(5)	P43-Ni3-P33	89.09(4)
P23-Ni3-P33	93.25(4)	C153-N3-Ni3	171.9(3)
C13-P13-C23	97.8(2)	C13-P13-C33	103.1(2)
C23-P13-C33	106.4(2)	C13-P13-Ni3	121.11(15)
C23-P13-Ni3	111.94(15)	C33-P13-Ni3	114.38(14)
C63-P23-C73	101.8(2)	C63-P23-C53	100.0(2)
C73-P23-C53	103.6(2)	C63-P23-Ni3	115.98(15)
C73-P23-Ni3	118.11(17)	C53-P23-Ni3	114.88(14)
C93-P33-C103	102.1(2)	C93-P33-C83	103.3(2)

C103-P33-C83	103.0(2)	C93-P33-Ni3	113.66(16)
C103-P33-Ni3	108.59(14)	C83-P33-Ni3	123.77(14)
C133-P43-C143	105.86(19)	C133-P43-C123	99.0(2)
C143-P43-C123	101.04(19)	C133-P43-Ni3	116.65(14)
C143-P43-Ni3	115.66(14)	C123-P43-Ni3	116.20(15)
C43-C33-P13	113.9(3)	C53-C43-C33	112.2(4)
C43-C53-P23	112.8(3)	C113-C103-P33	115.4(3)
C103-C113-C123	115.3(3)	C113-C123-P43	115.0(3)
N3-C153-C163	178.4(5)	F14-B14-F34	108.4(5)
F14-B14-F24	109.2(5)	F34-B14-F24	109.9(5)
F14-B14-F44	107.6(5)	F34-B14-F44	111.1(5)
F24-B14-F44	110.6(5)	F84-B24-F54	112.6(6)
F84-B24-F64	115.0(6)	F54-B24-F64	110.9(5)
F84-B24-F74	106.0(6)	F54-B24-F74	107.6(5)
F64-B24-F74	104.0(5)		

Table 46. Anisotropic displacement parameters ($Å^2$) for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

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}
Ni1	0.0179(2)	0.0187(2)	0.0212(2)	0.00207(18)	-0.00043(18)	0.00018(18)
N1	0.0210(17)	0.0329(19)	0.0340(19)	0.0042(15)	0.0034(14)	0.0047(14)
P11	0.0247(5)	0.0294(5)	0.0238(5)	0.0086(4)	0.0006(4)	-0.0001(4)
P21	0.0216(5)	0.0269(5)	0.0272(5)	-0.0031(4)	-0.0011(4)	-0.0024(4)
P31	0.0289(6)	0.0232(5)	0.0444(6)	0.0121(5)	-0.0047(5)	0.0011(4)
P41	0.0222(5)	0.0258(5)	0.0217(5)	-0.0010(4)	0.0010(4)	-0.0027(4)
C11	0.034(2)	0.030(2)	0.048(3)	0.015(2)	0.007(2)	-0.0051(18)
C21	0.038(3)	0.069(3)	0.027(2)	0.009(2)	0.0077(19)	0.004(2)
C31	0.038(2)	0.036(2)	0.039(2)	0.0176(19)	-0.0001(19)	0.0051(19)
C41	0.030(3)	0.051(4)	0.031(4)	0.007(3)	-0.005(2)	0.007(3)
C51	0.032(3)	0.060(4)	0.077(4)	0.025(3)	-0.027(2)	-0.006(2)
C61	0.030(2)	0.036(2)	0.042(2)	0.0002(19)	-0.0008(19)	-0.0114(19)
C71	0.052(3)	0.070(4)	0.042(3)	-0.030(3)	0.007(2)	-0.009(3)
C81	0.055(3)	0.026(3)	0.090(4)	0.001(3)	-0.011(3)	0.010(2)
C91	0.032(2)	0.048(3)	0.063(3)	0.028(2)	-0.010(2)	0.006(2)
C101	0.037(2)	0.042(3)	0.049(3)	0.026(2)	-0.007(2)	-0.008(2)
C111	0.044(3)	0.061(3)	0.035(2)	0.021(2)	-0.001(2)	-0.006(2)
C121	0.033(2)	0.052(3)	0.023(2)	0.0041(19)	0.0059(17)	-0.003(2)
C131	0.033(2)	0.030(2)	0.044(3)	-0.0055(19)	0.0099(19)	0.0040(18)
C141	0.031(2)	0.047(3)	0.038(2)	-0.009(2)	-0.0018(19)	-0.010(2)
C151	0.025(2)	0.036(2)	0.033(2)	0.0017(18)	0.0007(17)	0.0021(17)
C161	0.025(2)	0.064(3)	0.056(3)	0.000(3)	0.011(2)	-0.002(2)
B12	0.036(3)	0.032(3)	0.032(3)	0.001(2)	-0.004(2)	-0.002(2)
F12	0.066(2)	0.060(2)	0.067(2)	0.0268(16)	0.0201(16)	0.0113(16)
F22	0.127(3)	0.0358(18)	0.080(2)	-0.0103(16)	-0.038(2)	-0.0006(19)
F32	0.0405(17)	0.100(3)	0.075(2)	0.0276(19)	0.0126(16)	0.0094(17)
F42	0.0536(18)	0.084(2)	0.0443(17)	-0.0095(15)	-0.0200(14)	-0.0011(16)
B22	0.046(3)	0.045(3)	0.043(3)	-0.009(2)	0.020(3)	-0.009(3)
F52	0.030(2)	0.261(7)	0.158(5)	-0.107(5)	0.013(2)	-0.022(3)
F62	0.215(5)	0.038(2)	0.093(3)	0.0103(19)	0.083(3)	-0.004(3)
F72	0.083(2)	0.0497(18)	0.0341(15)	-0.0031(13)	0.0000(14)	0.0135(16)
F82	0.0579(18)	0.0527(17)	0.0358(14)	0.0020(12)	0.0125(13)	-0.0026(14)
Ni3	0.0219(2)	0.0205(2)	0.0184(2)	0.00269(18)	0.00086(18)	-0.00075(18)
N3	0.0276(19)	0.0348(19)	0.0243(17)	0.0011(14)	0.0009(14)	-0.0010(15)
P13	0.0305(5)	0.0272(5)	0.0199(5)	0.0060(4)	0.0017(4)	0.0011(4)
P23	0.0262(5)	0.0209(5)	0.0324(5)	0.0004(4)	0.0056(4)	-0.0001(4)
P33	0.0242(5)	0.0347(6)	0.0193(5)	0.0009(4)	0.0016(4)	-0.0061(4)
P43	0.0260(5)	0.0205(5)	0.0230(5)	0.0037(4)	-0.0034(4)	-0.0008(4)
C13	0.050(3)	0.041(3)	0.022(2)	0.0011(18)	-0.0047(19)	-0.004(2)

C23	0.038(2)	0.050(3)	0.033(2)	0.017(2)	-0.0019(19)	0.008(2)
C33	0.034(2)	0.035(2)	0.030(2)	0.0079(18)	0.0122(18)	0.0015(18)
C43	0.033(2)	0.044(3)	0.035(2)	0.0051(19)	0.0121(19)	-0.0064(19)
C53	0.043(3)	0.027(2)	0.037(2)	0.0058(18)	0.007(2)	-0.0074(19)
C63	0.036(2)	0.034(2)	0.036(2)	-0.0049(19)	0.0037(19)	-0.0078(19)
C73	0.046(3)	0.029(2)	0.062(3)	-0.001(2)	0.008(2)	0.014(2)
C83	0.035(2)	0.048(3)	0.024(2)	0.0032(18)	-0.0051(17)	-0.007(2)
C93	0.030(2)	0.053(3)	0.035(2)	-0.012(2)	0.0062(19)	-0.005(2)
C103	0.037(2)	0.047(3)	0.025(2)	0.0105(19)	0.0003(18)	-0.015(2)
C113	0.057(3)	0.037(3)	0.029(2)	0.0123(19)	-0.004(2)	-0.009(2)
C123	0.044(3)	0.031(2)	0.029(2)	0.0095(17)	-0.0115(19)	0.0007(19)
C133	0.030(2)	0.029(2)	0.035(2)	-0.0049(17)	-0.0031(17)	0.0068(17)
C143	0.035(2)	0.024(2)	0.035(2)	0.0049(17)	-0.0058(18)	-0.0050(17)
C153	0.029(2)	0.033(2)	0.0221(19)	0.0039(16)	0.0017(16)	-0.0006(17)
C163	0.030(2)	0.053(3)	0.038(2)	0.006(2)	-0.0062(19)	0.000(2)
B14	0.062(4)	0.050(4)	0.040(3)	0.004(3)	-0.004(3)	-0.003(3)
F14	0.066(3)	0.188(5)	0.070(3)	-0.004(3)	0.001(2)	-0.045(3)
F24	0.144(4)	0.082(3)	0.049(2)	0.0094(18)	-0.035(2)	0.028(2)
F34	0.079(3)	0.059(2)	0.122(3)	-0.027(2)	-0.003(2)	-0.0108(19)
F44	0.135(3)	0.063(2)	0.0356(16)	0.0171(15)	0.0115(18)	0.035(2)
B24	0.040(3)	0.045(3)	0.049(3)	-0.010(3)	0.006(3)	0.000(3)
F54	0.092(3)	0.115(3)	0.114(3)	0.001(3)	0.051(3)	-0.040(3)
F64	0.198(5)	0.058(2)	0.049(2)	-0.0081(17)	0.000(2)	-0.021(3)
F74	0.163(4)	0.107(3)	0.057(2)	-0.027(2)	0.028(3)	-0.041(3)
F84	0.084(4)	0.155(6)	0.413(12)	0.102(7)	-0.005(5)	0.063(4)

Table 47. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $[Ni(dmpp)_2(CH_3CN)](BF_4)_2$.

	x	y	z	Ueq
H1A1	-0.3259	0.0011	1.0910	0.045
H1B1	-0.4398	0.0612	1.1188	0.045
H1C1	-0.3672	-0.0018	1.1761	0.045
H2A1	-0.3545	0.1270	1.2728	0.053
H2B1	-0.3625	0.2312	1.2441	0.053
H2C1	-0.2370	0.1999	1.2849	0.053
H3A1	-0.1190	0.0329	1.2164	0.045
H3B1	-0.0654	0.0619	1.1380	0.045
H4A1	-0.0539	0.1841	1.2711	0.045
H4B1	0.0611	0.1260	1.2427	0.045
H5A1	0.0697	0.2092	1.1377	0.068
H5B1	0.0876	0.2763	1.2118	0.068
H6A1	-0.0153	0.4377	1.0672	0.044
H6B1	0.0476	0.3412	1.0431	0.044
H6C1	0.0984	0.4020	1.1169	0.044
H7A1	-0.0276	0.4336	1.2352	0.067
H7B1	-0.1412	0.3687	1.2614	0.067
H7C1	-0.1663	0.4486	1.2037	0.067
H8A1	-0.3120	0.5334	1.0227	0.069
H8B1	-0.1882	0.5075	1.0682	0.069
H8C1	-0.3217	0.4875	1.1022	0.069
H9A1	-0.4461	0.4025	0.9245	0.056
H9B1	-0.4977	0.3956	1.0070	0.056
H9C1	-0.4709	0.3016	0.9577	0.056
H10A1	-0.2150	0.4399	0.9010	0.051
H10B1	-0.1031	0.3892	0.9416	0.051
H11A1	-0.3013	0.2877	0.8568	0.055
H11B1	-0.1698	0.3136	0.8224	0.055
H12A1	-0.0709	0.2203	0.9112	0.043
H12B1	-0.1643	0.1603	0.8538	0.043
H13A1	-0.1796	0.0078	1.0123	0.043
H13B1	-0.0578	0.0746	1.0047	0.043
H13C1	-0.1284	0.0259	0.9311	0.043
H14A1	-0.4397	0.1535	0.9236	0.047
H14B1	-0.4207	0.0618	0.9700	0.047
H14C1	-0.3670	0.0671	0.8879	0.047
H16A1	-0.7106	0.2716	1.1282	0.058
H16B1	-0.6564	0.2308	1.2039	0.058
H16C1	-0.6837	0.1620	1.1306	0.058
H1A3	0.2357	0.4028	0.7484	0.046

H1B3	0.3749	0.3713	0.7643	0.046
H1C3	0.2645	0.3340	0.8141	0.046
H2A3	0.3267	0.1372	0.7784	0.048
H2B3	0.4391	0.2100	0.7630	0.048
H2C3	0.3970	0.1279	0.7011	0.048
H3A3	0.1079	0.1758	0.7692	0.039
H3B3	0.0476	0.2595	0.7264	0.039
H4A3	-0.0296	0.1004	0.6828	0.044
H4B3	0.0100	0.1675	0.6179	0.044
H5A3	0.0861	0.0047	0.6123	0.043
H5B3	0.1854	0.0435	0.6768	0.043
H6A3	0.1349	-0.0007	0.4741	0.043
H6B3	0.1856	0.0901	0.4337	0.043
H6C3	0.0610	0.0947	0.4798	0.043
H7A3	0.3259	-0.0399	0.5524	0.054
H7B3	0.4099	0.0316	0.6074	0.054
H7C3	0.4152	0.0385	0.5184	0.054
H8A3	0.1325	0.2960	0.3911	0.043
H8B3	0.1719	0.1898	0.3746	0.043
H8C3	0.2367	0.2735	0.3317	0.043
H9A3	0.4101	0.1318	0.4123	0.048
H9B3	0.5126	0.1981	0.4592	0.048
H9C3	0.4756	0.2193	0.3744	0.048
H10A3	0.4524	0.4056	0.4821	0.044
H10B3	0.4339	0.3870	0.3933	0.044
H11A3	0.2655	0.4722	0.3863	0.049
H11B3	0.3410	0.5282	0.4547	0.049
H12A3	0.1204	0.4128	0.4604	0.042
H12B3	0.1466	0.5170	0.4971	0.042
H13A3	0.0710	0.3988	0.6719	0.038
H13B3	0.0024	0.3939	0.5906	0.038
H13C3	0.0561	0.4929	0.6280	0.038
H14A3	0.2856	0.5585	0.6260	0.038
H14B3	0.3999	0.5044	0.5916	0.038
H14C3	0.3530	0.4810	0.6728	0.038
H16A3	0.7418	0.3475	0.6594	0.049
H16B3	0.7634	0.2549	0.6072	0.049
H16C3	0.7197	0.2455	0.6912	0.049

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Table 48. Crystal data for $Ni(dmpp)_2$.

Identification code	bc237
Empirical formula	$C_{14}H_{36}NiP_4$
Formula mass	387.02
Crystal size, mm	$0.15 \times 0.05 \times 0.03$
Crystal color, habit	pale yellow needle
Crystal system	monoclinic
Space group	*C*2/*c*
a, Å	17.5777(17)
b, Å	9.5357(11)
c, Å	14.7122(16)
α, °	90
β, °	123.458(5)
γ, °	90
Volume, $Å^3$	2057.4(4)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.249
Absorption coefficient, mm^{-1}	1.243
F(000)	832
Absorption correction	Semi-empirical from equivalents[1]
Range Transmission Coefficients	0.97 and 0.84

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

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Table 49. Data collection parameters for $Ni(dmpp)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	152(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	4342
θ range	$2.55 < \theta < 31.34$
θ range, data collection	$2.55 < \theta < 31.15$
Scan type	ω scan
Index ranges	$-25 \le h \le 21$, $0 \le k \le 13$, $0 \le l \le 21$
Reflections collected	9312
Independent reflections	3115 (R(int) = 0.0420)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 50. Structure Solution and Refinement for $Ni(dmpp)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	3115 / 0/ 159
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0227P)^2+1.4966P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0442, wR2 = 0.0793
Reflections observed	2575
R indices (all data)	R1 = 0.0638, wR2 = 0.0874
Goodness-of-fit[4] on F^2	1.463
Largest diff. peak and hole	0.452 and -0.399

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

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

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

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

Table 51. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $Ni(dmpp)_2$.

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

	x	y	z	Ueq
Ni	0.0000	0.11088(4)	0.2500	0.01533(10)
P(1)	0.02749(4)	0.23890(6)	0.15115(4)	0.01907(13)
P(2)	0.12201(4)	-0.01256(6)	0.33756(4)	0.01921(13)
C(1)	-0.0587(2)	0.2810(4)	0.0080(2)	0.0391(7)
C(2)	0.0725(2)	0.4174(3)	0.1978(3)	0.0365(6)
C(3)	0.11626(17)	0.1716(3)	0.1322(2)	0.0272(5)
C(4)	0.20340(17)	0.1237(3)	0.2381(2)	0.0331(6)
C(5)	0.19232(18)	-0.0174(3)	0.2793(2)	0.0324(6)
C(6)	0.11953(19)	-0.2027(3)	0.3571(2)	0.0333(6)
C(7)	0.21104(17)	0.0349(3)	0.4789(2)	0.0291(5)

Table 52. Bond lengths (Å) for $Ni(dmpp)_2$.

Ni-P(2)	2.1443(6)	Ni-P(1)	2.1479(6)
P(1)-C(1)	1.837(3)	P(1)-C(2)	1.842(3)
P(1)-C(3)	1.845(2)	P(2)-C(6)	1.840(3)
P(2)-C(7)	1.841(3)	P(2)-C(5)	1.853(3)
C(3)-C(4)	1.533(4)	C(4)-C(5)	1.531(4)

Table 53. Bond angles (°) for $Ni(dmpp)_2$.

P(2)-Ni-P(2a)	113.41(4)	P(2)-Ni-P(1a)	115.41(2)
P(2)-Ni-P(1)	101.24(2)	P(1a)-Ni-P(1)	110.72(4)
C(1)-P(1)-C(2)	97.97(16)	C(1)-P(1)-C(3)	97.73(13)
C(2)-P(1)-C(3)	98.77(13)	C(1)-P(1)-Ni	123.32(10)
C(2)-P(1)-Ni	118.92(10)	C(3)-P(1)-Ni	115.40(8)
C(6)-P(2)-C(7)	98.31(12)	C(6)-P(2)-C(5)	97.30(13)
C(7)-P(2)-C(5)	99.22(13)	C(6)-P(2)-Ni	122.19(9)
C(7)-P(2)-Ni	119.30(9)	C(5)-P(2)-Ni	115.91(8)
C(4)-C(3)-P(1)	113.87(17)	C(5)-C(4)-C(3)	113.0(2)
C(4)-C(5)-P(2)	115.07(18)		

Symmetry transformations used to generate equivalent atoms:
a: -x,y,-z+1/2

Table 54. Anisotropic displacement parameters ($Å^2$) for $Ni(dmpp)_2$.

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	0.01588(17)	0.01363(18)	0.01641(18)	0.000	0.00886(14)	0.000
P(1)	0.0197(3)	0.0183(3)	0.0196(3)	0.0029(2)	0.0111(2)	0.0007(2)
P(2)	0.0196(3)	0.0163(3)	0.0204(3)	0.0022(2)	0.0102(2)	0.0030(2)
C(1)	0.0324(13)	0.0522(19)	0.0274(13)	0.0188(13)	0.0131(11)	0.0037(13)
C(2)	0.0473(16)	0.0257(13)	0.0502(17)	-0.0006(12)	0.0354(15)	-0.0074(12)
C(3)	0.0314(12)	0.0307(13)	0.0287(12)	0.0043(11)	0.0224(10)	0.0035(10)
C(4)	0.0269(12)	0.0411(15)	0.0400(14)	0.0087(13)	0.0239(11)	0.0066(11)
C(5)	0.0319(12)	0.0349(14)	0.0370(14)	0.0106(12)	0.0232(11)	0.0168(11)
C(6)	0.0346(13)	0.0203(12)	0.0356(14)	0.0036(11)	0.0134(12)	0.0036(10)
C(7)	0.0244(11)	0.0243(13)	0.0277(12)	0.0022(10)	0.0076(10)	0.0013(10)

Table 55. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $Ni(dmpp)_2$.

	x	y	z	Ueq
H(1A)	-0.033(2)	0.331(4)	-0.024(3)	0.059(10)
H(1B)	-0.108(2)	0.324(4)	0.000(3)	0.053(10)
H(1C)	-0.084(2)	0.191(4)	-0.034(3)	0.061(11)
H(2A)	0.092(2)	0.453(3)	0.155(2)	0.042(8)
H(2B)	0.122(2)	0.413(3)	0.270(3)	0.044(9)
H(2C)	0.027(2)	0.475(4)	0.194(3)	0.054(10)
H(3A)	0.0876(19)	0.095(3)	0.080(2)	0.034(7)
H(3B)	0.1320(18)	0.237(3)	0.100(2)	0.025(7)
H(4A)	0.2228(18)	0.193(3)	0.295(2)	0.029(7)
H(4B)	0.253(2)	0.110(3)	0.223(2)	0.039(8)
H(5A)	0.250(2)	-0.057(3)	0.331(3)	0.045(9)
H(5B)	0.1620(17)	-0.086(3)	0.220(2)	0.023(7)
H(6A)	0.181(2)	-0.242(3)	0.393(2)	0.038(8)
H(6B)	0.081(2)	-0.247(3)	0.285(2)	0.038(8)
H(6C)	0.089(2)	-0.219(3)	0.395(2)	0.035(8)
H(7A)	0.2649(19)	-0.028(3)	0.508(2)	0.036(8)
H(7B)	0.188(2)	0.022(3)	0.527(2)	0.041(8)
H(7C)	0.226(2)	0.126(3)	0.480(2)	0.039(8)

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Table 56. Crystal data for $Pt(dmpp)_2$.

Identification code	bc238
Empirical formula	$C_{14}H_{36}P_4Pt$
Formula mass	523.40
Crystal size, mm	$0.38 \times 0.37 \times 0.21$
Crystal color, habit	colorless rhombic bloc
Crystal system	Monoclinic
Space group	*C*2/*c*
a, Å	17.481(6)
b, Å	9.892(3)
c, Å	14.524(5)
α, °	90
β, °	123.879(7)
γ, °	90
Volume, $Å^3$	2085.3(13)
Z, formula units/cell	4
Density (calculated), $Mg \cdot m^{-3}$	1.667
Absorption coefficient, mm^{-1}	7.025
F(000)	1032
Absorption correction[1]	Semi-empirical from equivalents
Range Transmission Coefficients	0.32 and 0.18

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

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Table 57. Data collection parameters for $Pt(dmpp)_2$.

Diffractometer	Siemens SMART CCD
Temperature, K	160(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	6120
θ range	$2.49 < \theta < 31.14$
θ range, data collection	$2.49 < \theta < 31.14$
Scan type	ω scans
Index ranges	$-24 \le h \le 20$,
	$0 \le k \le 14$,
	$0 \le l \le 21$
Reflections collected	12788
Independent reflections	3155 (R(int) = 0.039)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 58. Structure Solution and Refinement for $Pt(dmpp)_2$.

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	3155 / 0/ 160
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0308P)^2]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0218, wR2 = 0.0508
Reflections observed	3130
R indices (all data)	R1 = 0.0223, wR2 = 0.0510
Goodness-of-fit[4] on F^2	1.113
Extinction coefficient	0.00009(8)
Largest diff. peak and hole	1.432 and -3.053

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

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 59. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $Pt(dmpp)_2$.

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

	x	y	z	Ueq
Pt	0.0000	0.113724(9)	0.2500	0.01414(5)
P(1)	0.02575(4)	0.24079(5)	0.13953(5)	0.01826(10)
P(2)	0.13256(4)	-0.00818(5)	0.34178(5)	0.01693(10)
C(1)	-0.06156(19)	0.2561(3)	-0.0104(2)	0.0370(6)
C(2)	0.0563(2)	0.4201(3)	0.1732(3)	0.0353(6)
C(3)	0.12294(15)	0.1842(2)	0.13307(19)	0.0238(4)
C(4)	0.20971(17)	0.1442(3)	0.2454(2)	0.0257(4)
C(5)	0.20405(17)	0.0030(3)	0.2854(2)	0.0251(4)
C(6)	0.12972(18)	-0.1933(2)	0.3512(2)	0.0266(5)
C(7)	0.22085(16)	0.0309(3)	0.48805(19)	0.0256(4)

Table 60. Bond lengths (Å) for $Pt(dmpp)_2$.

Pt-P(2a)	2.2709(8)	Pt-P(2)	2.2709(8)
Pt-P(1)	2.2721(8)	Pt-P(1a)	2.2723(8)
P(1)-C(2)	1.838(3)	P(1)-C(3)	1.840(2)
P(1)-C(1)	1.841(3)	P(2)-C(6)	1.839(3)
P(2)-C(5)	1.840(2)	P(2)-C(7)	1.841(2)
C(3)-C(4)	1.537(3)	C(4)-C(5)	1.536(4)

Symmetry transformations used to generate equivalent atoms:
a: -x,y,-z+1/2

Table 61. Bond angles (°) for $Pt(dmpp)_2$.

P(2a)-Pt-P(2)	115.85(4)	P(2a)-Pt-P(1)	114.73(3)
P(2)-Pt-P(1)	99.75(3)	P(2a)-Pt-P(1a)	99.74(3)
P(2)-Pt-P(1a)	114.73(3)	P(1)-Pt-P(1a)	112.82(4)
C(2)-P(1)-C(3)	99.68(12)	C(2)-P(1)-C(1)	99.31(15)
C(3)-P(1)-C(1)	98.34(13)	C(2)-P(1)-Pt	119.22(10)
C(3)-P(1)-Pt	114.80(8)	C(1)-P(1)-Pt	121.39(10)
C(6)-P(2)-C(5)	98.42(11)	C(6)-P(2)-C(7)	99.41(12)
C(5)-P(2)-C(7)	99.23(12)	C(6)-P(2)-Pt	120.76(8)
C(5)-P(2)-Pt	115.51(8)	C(7)-P(2)-Pt	119.37(8)
C(4)-C(3)-P(1)	114.64(16)	C(5)-C(4)-C(3)	113.7(2)
C(4)-C(5)-P(2)	115.19(16)		

Symmetry transformations used to generate equivalent atoms:
a: -x,y,-z+1/2

Table 62. Anisotropic displacement parameters ($Å^2$) for $Pt(dmpp)_2$.

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	0.01242(6)	0.01365(7)	0.01546(7)	0.000	0.00722(5)	0.000
P(1)	0.0161(2)	0.0180(2)	0.0186(2)	0.00353(19)	0.00846(19)	-0.00026(17)
P(2)	0.0153(2)	0.0171(2)	0.0178(2)	0.00274(19)	0.0089(2)	0.00292(17)
C(1)	0.0282(12)	0.0490(16)	0.0223(11)	0.0150(12)	0.0068(10)	-0.0015(11)
C(2)	0.0434(15)	0.0193(10)	0.0528(18)	0.0028(12)	0.0328(14)	-0.0025(11)
C(3)	0.0239(9)	0.0289(10)	0.0227(10)	0.0039(9)	0.0155(8)	0.0003(8)
C(4)	0.0183(9)	0.0335(11)	0.0278(12)	0.0051(10)	0.0144(9)	0.0004(9)
C(5)	0.0237(10)	0.0278(10)	0.0291(11)	0.0071(9)	0.0179(9)	0.0088(8)
C(6)	0.0285(11)	0.0180(9)	0.0317(12)	0.0046(9)	0.0157(10)	0.0047(8)
C(7)	0.0206(10)	0.0291(11)	0.0203(10)	0.0022(9)	0.0072(8)	0.0021(8)

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Table 63. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $Pt(dmpp)_2$.

	x	y	z	Ueq
H(1A)	-0.045(3)	0.313(5)	-0.048(4)	0.061(12)
H(1B)	-0.125(3)	0.286(4)	-0.028(3)	0.050(10)
H(1C)	-0.080(2)	0.168(4)	-0.043(3)	0.037(9)
H(2A)	0.076(3)	0.457(4)	0.128(3)	0.049(10)
H(2B)	0.116(3)	0.431(5)	0.252(4)	0.056(11)
H(2C)	0.000(3)	0.469(4)	0.156(3)	0.053(11)
H(3A)	0.100(3)	0.105(3)	0.083(3)	0.027(9)
H(3B)	0.136(2)	0.258(3)	0.094(3)	0.026(7)
H(4A)	0.228(2)	0.217(3)	0.306(3)	0.022(7)
H(4B)	0.264(3)	0.156(4)	0.241(3)	0.034(9)
H(5A)	0.270(2)	-0.031(3)	0.344(3)	0.029(8)
H(5B)	0.173(2)	-0.062(4)	0.217(3)	0.029(7)
H(6A)	0.188(3)	-0.227(4)	0.385(3)	0.042(9)
H(6D)	0.086(2)	-0.232(4)	0.282(3)	0.038(9)
H(6B)	0.095(2)	-0.218(3)	0.389(3)	0.031(8)
H(7D)	0.280(2)	-0.022(4)	0.524(3)	0.043(9)
H(7A)	0.200(2)	0.015(4)	0.533(3)	0.037(9)
H(7B)	0.239(3)	0.123(3)	0.494(4)	0.041(12)