SUPPORTING INFORMATION

(CM010681C)

Inclusion Ability of 4-Phenylpyridine-Extended Nickel(II) Dibenzoylmethanate, a New Metal-Complex Host

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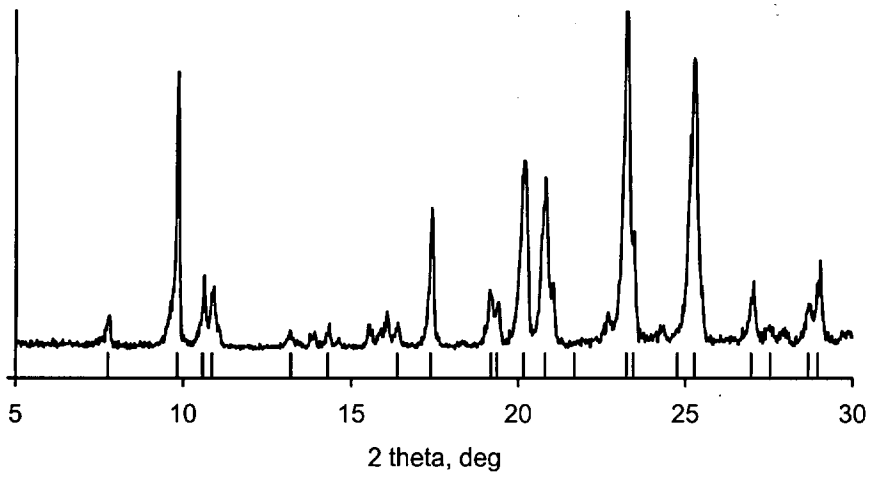

Figure 1S.
Powder diffractogram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(fluorobenzene). Vertical bars show positions of main reflections (>5% of the strongest reflection intensity) calculated from single-crystal XRD results using room temperature unit cell dimensions. Radiation: CoK_α, λ=1.7902 Å.

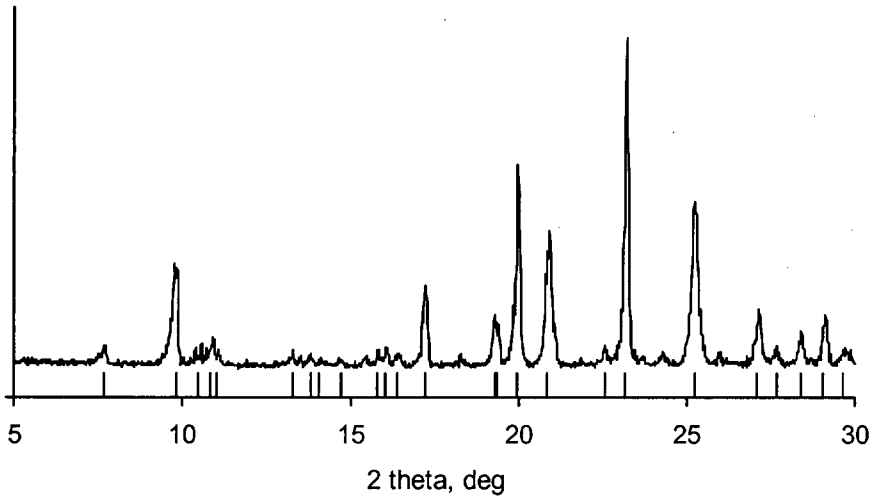

Figure 2S.
Powder diffractogram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(chlorobenzene). Vertical bars show positions of main reflections (>5% of the strongest reflection intensity) calculated from single-crystal XRD results using room temperature unit cell dimensions. Radiation: CoK_α, λ=1.7902 Å.

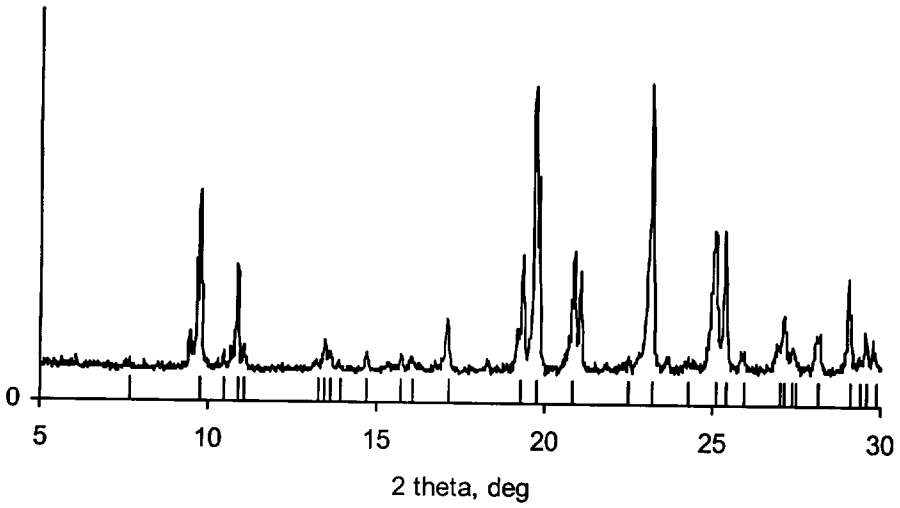

Figure 3S.
Powder diffractogram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(bromobenzene). Vertical bars show positions of main reflections (>5% of the strongest reflection intensity) calculated from single-crystal XRD results using room temperature unit cell dimensions. Radiation: CoK_α, λ=1.7902 Å.

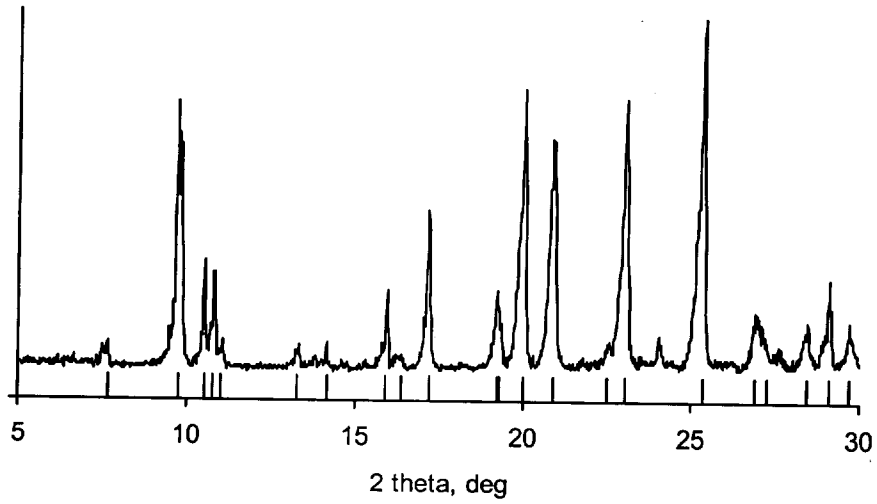

Figure 4S.
Powder diffractogram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(toluene). Vertical bars show positions of main reflections (>5% of the strongest reflection intensity) calculated from single-crystal XRD results using room temperature unit cell dimensions. Radiation: CoK_α, λ=1.7902 Å.

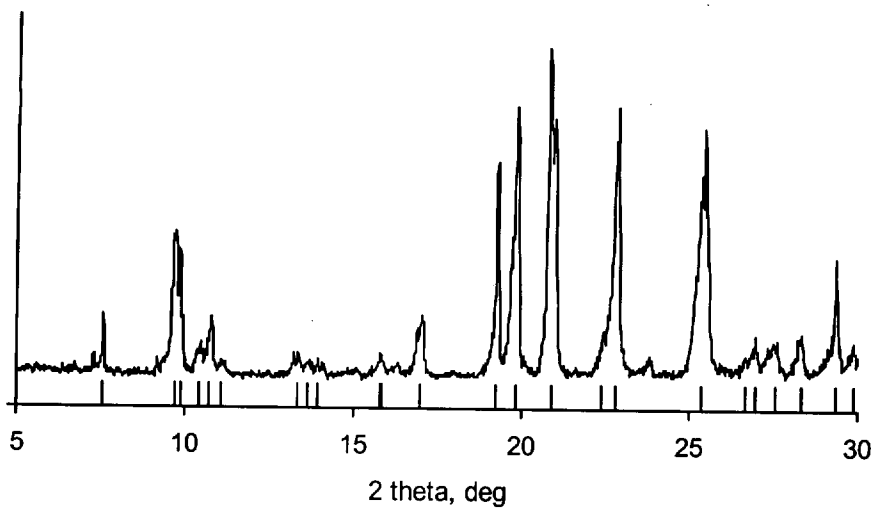

Figure 5S.
Powder diffractogram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(o-xylene). Vertical bars show positions of main reflections (>5% of the strongest reflection intensity) calculated from single-crystal XRD results using room temperature unit cell dimensions. Radiation: CoK_α, λ=1.7902 Å.

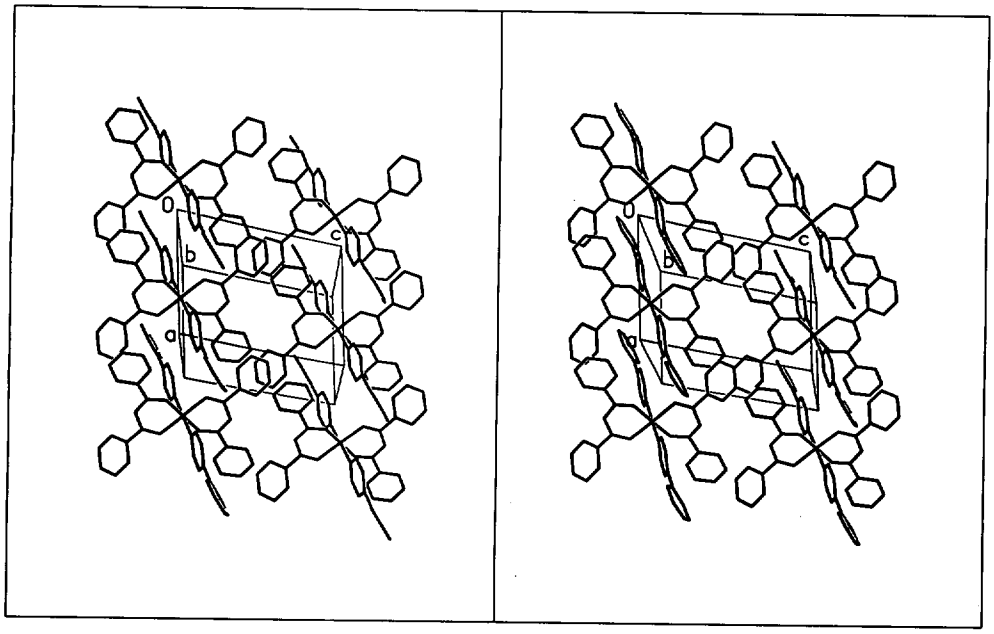

Figure 6S.
Packing stereodiagram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$ (guest-free form of the complex).

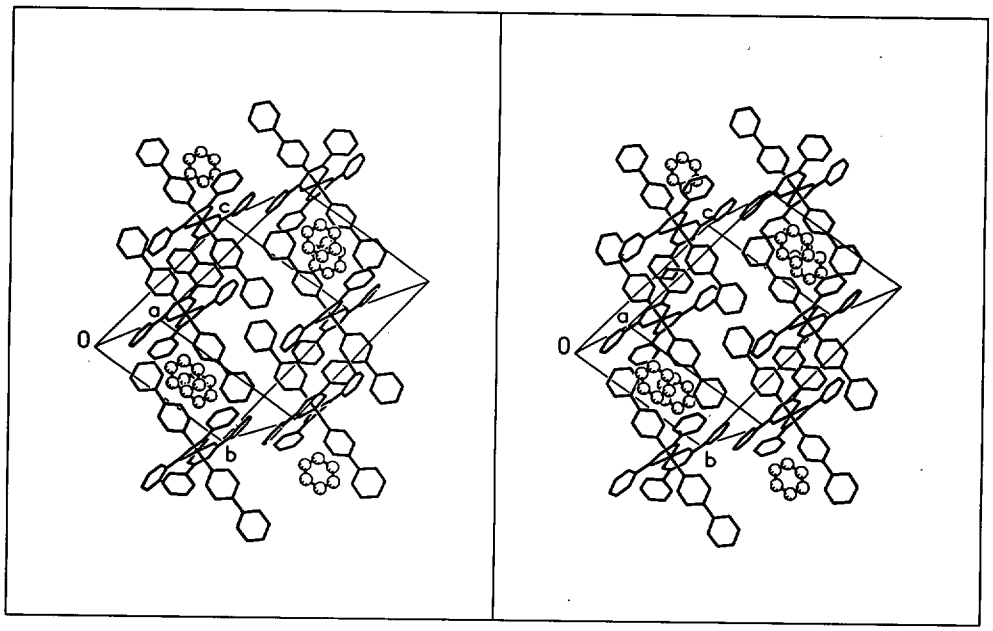

Figure 7S.
Packing stereodiagram of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(benzene) clathrate. Guest molecules are outlined in sticks-and-balls.

Table 1S. Selected Parameters of the $[Ni(4\text{-}PhPy)_2(DBM)_2]$ Molecule in Eight Phases Studied [a),b),c)]

Guest	-	benzene	benzene	fluoro-benzene	chloro-benzene	bromo-benzene	toluene	o-xylene	benzenes [d)]
Phase type (H:G)	guest-free form	(1:4)	(1:1)	(1:1)	(1:1)	(1:1)	(1:1)	(1:1)	average for six (1:1) phases
Phase color	brown	brown	green	green	green	green	green	green	all green
Point symmetry	-1	-1	1	1	1	1	1	1	1
Distances (Å)									
Ni-O1	2.033(1)	2.015(1)	2.032(1)	2.030(2)	2.031(2)	2.029(1)	2.031(2)	2.034(1)	2.031(2)
Ni-O3	2.019(1)	2.002(1)	2.014(1)	2.011(2)	2.012(2)	2.011(1)	2.011(2)	2.011(1)	2.012(2)
Ni-O4			2.023(1)	2.024(2)	2.024(2)	2.028(1)	2.021(2)	2.025(1)	2.024(2)
Ni-O6			2.015(1)	2.012(2)	2.015(2)	2.012(1)	2.010(2)	2.014(1)	2.013(2)
Ni-N7	2.096(1)	2.122(1)	2.130(1)	2.134(2)	2.130(2)	2.131(2)	2.126(2)	2.131(1)	2.130(2)
Ni-N8			2.120(2)	2.116(2)	2.121(2)	2.122(2)	2.123(2)	2.127(2)	2.122(3)
Valent angles (deg)									
O1-Ni-O3	90.32(4)	91.15(4)	90.64(5)	90.72(6)	90.73(6)	90.82(5)	90.77(6)	90.72(5)	90.73(6)
O4-Ni-O6			91.22(5)	91.07(6)	90.95(6)	90.84(5)	91.05(6)	90.92(5)	91.01(6)
O1-Ni-O6{O3'}	{89.68(4)}	{88.85(4)}	89.78(5)	89.88(6)	89.48(6)	89.18(5)	89.39(6)	89.66(5)	89.56(6)
O3-Ni-O4{O1'}			88.37(5)	88.33(6)	88.84(6)	89.17(5)	88.79(6)	88.69(5)	88.70(6)
Line-plane angles (deg)									
(Ni-N7) - Eqt	88.3	89.4	88.6	88.4	88.5	88.2	88.6	89.0	88.6(1)
(Ni-N8) - Eqt			88.9	88.8	88.9	89.1	89.0	89.1	89.0(1)
Plane-plane angles (deg)									
Ring1 - Ring2	0	0	9.5	9.2	10.3	11.1	10.9	12.4	10.6(5)
Eqt - Ph1	+67.9	+9.3	+51.2	+50.7	+49.6	+48.7	+51.0	+52.8	+50.7(6)
Eqt - Ph3	-16.3	+8.1	+10.8	+10.7	+10.5	+9.8	+10.1	+8.5	+10.1(3)
Eqt - Ph4	{-67.9}	{-9.3}	-18.4	-17.9	-16.4	-15.2	-16.1	-12.7	-16.1(8)
Eqt - Ph6	{+16.3}	{-8.1}	+13.3	+13.0	+12.4	+13.0	+12.4	+13.6	+13.0(2)
Eqt - Py7	89.6	84.8	89.4	88.9	86.8	84.8	87.4	86.3	87.3(7)
Eqt - Py8	{89.6}	{84.8}	85.1	84.6	83.7	83.3	83.8	83.3	84.0(3)
α - Py7	+83.2	+71.7	+54.5	+55.2	+54.9	+54.7	+56.0	+56.4	+55.3(3)
α - Ph7	+55.2	-68.8	+83.7	+84.4	+82.8	+81.6	+84.0	+85.3	+83.6(5)
Py7 - Ph7	28.2	39.6	29.4	29.3	27.8	26.9	28.1	28.9	28.4(4)
α - Py8	{-83.2}	{-71.7}	-71.8	-71.9	-73.0	-73.4	-73.0	-74.2	-72.9(4)
α - Ph8	{-55.2}	{+68.8}	+81.2	+81.5	+79.8	+79.2	+80.2	+78.2	+80.0(5)
Py8 - Ph8	{28.2}	{39.6}	27.0	26.6	27.2	27.4	26.8	27.7	27.1(2)

Footnotes to Table 1S:

[a] Atom numbering used in the Table is illustrated in Figure 4.

Definitions of most least-squares planes are shown on Scheme 2;

for example, the planes for the molecule in Figure 4 are as follows:

Ring1 (Ni,O1,C1,C2,C3,O3); Ring2 (Ni,O4,C4,C5,C6,O6); Eqt (Ni,O1,O3,O4,O6);

Ph1 (C11-C16); Ph3 (C31-C36); α (Ni,C2,C5,N7,N8);

Py7 (N7,C71,C72,C73,C74,C75); Ph7 (C76,C77,C78,C79,C7X,C7Y) and so on.

[b] For line-plane and plane-plane angles estimated experimental errors do not exceed 0.1°.

[c] Values for angles involving symmetry generated atoms are given in figure brackets;

for example, the angle O1-Ni-O3', where O3' arises from O3 by centrosymmetry,

corresponds to O1-Ni-O6 in asymmetric molecule.

[d] Benzene, fluorobenzene, chlorobenzene, bromobenzene, toluene, o-xylene.

Table 2S. Refined Occupancy of Guest Orientations in Green $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(Guest) Clathrates[a)]

Guest	Orientation A	Orientation B	Orientation C	Orientation D	Total Occupancy
Benzene					1.003(1)
Fluorobenzene	0.470(5)	0.070(4)	0.440(5)	0.037(3)	1.017(8)
Chlorobenzene	0.316(2)	0.313(2)	0.237(2)	0.139(2)	1.005(5)
Bromobenzene	0.077(1)	0.426(1)	0.366(1)	0.124(1)	0.993(3)
Toluene	0.114(4)	0.418(4)	0.431(4)	0.060(4)	1.023(8)
o-Xylene	0.220(2)	0.557(3)	0.237(3)		1.014(5)

Footnote to Table 2S:
[a)] The positioning of the orientations is shown in Figure 7 in the paper

Table 3S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni	5000	5000	10000	22(1)
O(1)	3469(1)	3991(1)	11473(1)	26(1)
C(1)	3703(2)	3704(1)	12560(1)	24(1)
C(11)	2596(2)	2817(1)	13536(1)	27(1)
C(12)	835(2)	3075(1)	13433(1)	34(1)
C(13)	-212(2)	2243(2)	14297(2)	47(1)
C(14)	494(3)	1143(2)	15253(1)	54(1)
C(15)	2237(3)	877(2)	15365(1)	55(1)
C(16)	3296(2)	1720(1)	14516(1)	41(1)
C(2)	4845(2)	4154(1)	12929(1)	28(1)
O(3)	5809(1)	5671(1)	10984(1)	26(1)
C(3)	5784(1)	5122(1)	12143(1)	24(1)
C(31)	6850(2)	5590(1)	12664(1)	26(1)
C(32)	6930(2)	5156(1)	13916(1)	32(1)
C(33)	7946(2)	5643(2)	14321(1)	41(1)
C(34)	8913(2)	6538(2)	13506(2)	50(1)
C(35)	8869(2)	6959(2)	12267(2)	55(1)
C(36)	7830(2)	6500(2)	11851(1)	42(1)
N(7)	2934(1)	6513(1)	9452(1)	26(1)
C(71)	1411(2)	6292(1)	9371(1)	28(1)
C(72)	-25(2)	7218(1)	9021(1)	27(1)
C(73)	61(2)	8465(1)	8735(1)	26(1)
C(74)	1650(2)	8692(1)	8821(1)	31(1)
C(75)	3030(2)	7708(1)	9176(1)	30(1)
C(76)	-1453(2)	9483(1)	8341(1)	29(1)
C(77)	-2699(2)	9407(1)	7740(1)	35(1)
C(78)	-4076(2)	10382(2)	7318(2)	45(1)
C(79)	-4242(2)	11448(2)	7481(2)	56(1)
C(7X)	-3035(3)	11528(2)	8099(2)	63(1)
C(7Y)	-1658(2)	10552(2)	8523(2)	47(1)

Table 4S. Bond lengths [A] and angles [deg] for [Ni(4-PhPy)2(DBM)2]

Ni-O(3)#1	2.0189(9)
Ni-O(3)	2.0189(9)
Ni-O(1)	2.0325(9)
Ni-O(1)#1	2.0325(9)
Ni-N(7)#1	2.0961(11)
Ni-N(7)	2.0961(11)
O(1)-C(1)	1.2668(14)
C(1)-C(2)	1.4055(16)
C(1)-C(11)	1.4967(16)
C(11)-C(16)	1.3901(19)
C(11)-C(12)	1.3914(18)
C(12)-C(13)	1.386(2)
C(13)-C(14)	1.378(3)
C(14)-C(15)	1.378(3)
C(15)-C(16)	1.394(2)
C(2)-C(3)	1.4004(17)
O(3)-C(3)	1.2700(14)
C(3)-C(31)	1.5023(16)
C(31)-C(36)	1.3860(19)
C(31)-C(32)	1.3974(17)
C(32)-C(33)	1.3893(18)
C(33)-C(34)	1.370(2)
C(34)-C(35)	1.380(3)
C(35)-C(36)	1.388(2)
N(7)-C(75)	1.3411(16)
N(7)-C(71)	1.3428(15)
C(71)-C(72)	1.3770(17)
C(72)-C(73)	1.3983(17)
C(73)-C(74)	1.3985(17)
C(73)-C(76)	1.4791(17)
C(74)-C(75)	1.3819(19)
C(76)-C(7Y)	1.3914(19)
C(76)-C(77)	1.3969(18)
C(77)-C(78)	1.382(2)
C(78)-C(79)	1.377(2)
C(79)-C(7X)	1.387(3)
C(7X)-C(7Y)	1.383(2)
O(3)#1-Ni-O(3)	180.0
O(3)#1-Ni-O(1)	89.68(4)
O(3)-Ni-O(1)	90.32(4)
O(3)#1-Ni-O(1)#1	90.32(4)
O(3)-Ni-O(1)#1	89.68(4)
O(1)-Ni-O(1)#1	180.000(1)
O(3)#1-Ni-N(7)#1	91.19(4)
O(3)-Ni-N(7)#1	88.81(4)
O(1)-Ni-N(7)#1	91.21(4)
O(1)#1-Ni-N(7)#1	88.79(4)
O(3)#1-Ni-N(7)	88.81(4)
O(3)-Ni-N(7)	91.19(4)
O(1)-Ni-N(7)	88.79(4)
O(1)#1-Ni-N(7)	91.21(4)
N(7)#1-Ni-N(7)	180.0
C(1)-O(1)-Ni	122.87(8)
O(1)-C(1)-C(2)	126.96(11)

O(1)-C(1)-C(11)	115.30(10)
C(2)-C(1)-C(11)	117.72(10)
C(16)-C(11)-C(12)	119.38(12)
C(16)-C(11)-C(1)	121.50(12)
C(12)-C(11)-C(1)	119.07(11)
C(13)-C(12)-C(11)	120.34(14)
C(14)-C(13)-C(12)	119.98(16)
C(15)-C(14)-C(13)	120.25(14)
C(14)-C(15)-C(16)	120.22(16)
C(11)-C(16)-C(15)	119.80(15)
C(3)-C(2)-C(1)	125.19(11)
C(3)-O(3)-Ni	124.43(8)
O(3)-C(3)-C(2)	124.86(10)
O(3)-C(3)-C(31)	115.25(10)
C(2)-C(3)-C(31)	119.89(10)
C(36)-C(31)-C(32)	118.02(12)
C(36)-C(31)-C(3)	117.81(11)
C(32)-C(31)-C(3)	124.17(11)
C(33)-C(32)-C(31)	120.48(13)
C(34)-C(33)-C(32)	120.80(14)
C(33)-C(34)-C(35)	119.29(14)
C(34)-C(35)-C(36)	120.44(16)
C(31)-C(36)-C(35)	120.94(14)
C(75)-N(7)-C(71)	117.05(11)
C(75)-N(7)-Ni	123.95(8)
C(71)-N(7)-Ni	119.00(8)
N(7)-C(71)-C(72)	123.60(11)
C(71)-C(72)-C(73)	119.75(11)
C(72)-C(73)-C(74)	116.48(11)
C(72)-C(73)-C(76)	120.97(11)
C(74)-C(73)-C(76)	122.54(11)
C(75)-C(74)-C(73)	120.08(11)
N(7)-C(75)-C(74)	123.05(11)
C(7Y)-C(76)-C(77)	118.17(13)
C(7Y)-C(76)-C(73)	121.53(12)
C(77)-C(76)-C(73)	120.27(11)
C(78)-C(77)-C(76)	120.57(13)
C(79)-C(78)-C(77)	120.61(15)
C(78)-C(79)-C(7X)	119.59(15)
C(7Y)-C(7X)-C(79)	119.90(16)
C(7X)-C(7Y)-C(76)	121.13(15)

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

Table 5S. Anisotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni	23(1)	26(1)	19(1)	-9(1)	-2(1)	-10(1)
O(1)	27(1)	33(1)	21(1)	-10(1)	-2(1)	-13(1)
C(1)	24(1)	26(1)	22(1)	-11(1)	0(1)	-7(1)
C(11)	33(1)	31(1)	22(1)	-14(1)	2(1)	-14(1)
C(12)	31(1)	38(1)	39(1)	-22(1)	6(1)	-13(1)
C(13)	42(1)	61(1)	52(1)	-35(1)	18(1)	-30(1)
C(14)	79(1)	65(1)	34(1)	-24(1)	18(1)	-53(1)
C(15)	86(1)	50(1)	26(1)	-3(1)	-8(1)	-39(1)
C(16)	53(1)	42(1)	27(1)	-7(1)	-9(1)	-21(1)
C(2)	31(1)	38(1)	21(1)	-14(1)	-1(1)	-14(1)
O(3)	30(1)	31(1)	22(1)	-12(1)	-2(1)	-12(1)
C(3)	22(1)	30(1)	24(1)	-16(1)	-1(1)	-5(1)
C(31)	22(1)	36(1)	30(1)	-22(1)	-1(1)	-7(1)
C(32)	29(1)	44(1)	31(1)	-23(1)	-3(1)	-7(1)
C(33)	37(1)	61(1)	42(1)	-36(1)	-9(1)	-5(1)
C(34)	46(1)	70(1)	61(1)	-45(1)	-8(1)	-20(1)
C(35)	58(1)	74(1)	55(1)	-34(1)	3(1)	-43(1)
C(36)	46(1)	58(1)	36(1)	-25(1)	3(1)	-30(1)
N(7)	25(1)	28(1)	24(1)	-11(1)	-2(1)	-10(1)
C(71)	27(1)	27(1)	33(1)	-13(1)	-2(1)	-10(1)
C(72)	25(1)	30(1)	30(1)	-14(1)	-1(1)	-10(1)
C(73)	28(1)	28(1)	24(1)	-11(1)	-2(1)	-8(1)
C(74)	34(1)	28(1)	36(1)	-13(1)	-6(1)	-11(1)
C(75)	29(1)	31(1)	33(1)	-13(1)	-5(1)	-12(1)
C(76)	30(1)	28(1)	29(1)	-12(1)	-3(1)	-7(1)
C(77)	32(1)	36(1)	42(1)	-21(1)	-9(1)	-4(1)
C(78)	37(1)	46(1)	55(1)	-24(1)	-17(1)	0(1)
C(79)	48(1)	42(1)	77(1)	-29(1)	-25(1)	12(1)
C(7X)	67(1)	41(1)	96(2)	-41(1)	-33(1)	11(1)
C(7Y)	50(1)	37(1)	64(1)	-28(1)	-23(1)	0(1)

Table 6S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]

	x	y	z	U(eq)
H(12)	348	3824	12767	41
H(13)	-1416	2430	14230	56
H(14)	-223	568	15836	65
H(15)	2717	116	16023	65
H(16)	4492	1546	14607	49
H(2)	4992	3770	13778	34
H(32)	6285	4522	14493	39
H(33)	7971	5351	15174	49
H(34)	9607	6866	13789	60
H(35)	9555	7567	11697	66
H(36)	7791	6814	10996	50
H(71)	1318	5451	9565	34
H(72)	-1070	7010	8973	33
H(74)	1781	9523	8635	38
H(75)	4096	7886	9227	36
H(77)	-2600	8678	7620	42
H(78)	-4915	10318	6912	54
H(79)	-5177	12124	7172	67
H(7X)	-3155	12252	8229	76
H(7Y)	-838	10613	8946	56

Table 7S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*4(benzene). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni	0	0	10000	28(1)
O(1)	1795(1)	247(1)	10625(1)	33(1)
C(1)	2058(1)	-679(1)	10392(1)	25(1)
C(11)	3508(1)	-219(1)	10912(1)	26(1)
C(12)	4412(2)	1150(2)	11610(1)	36(1)
C(13)	5753(2)	1623(2)	12116(1)	44(1)
C(14)	6209(2)	741(2)	11931(1)	41(1)
C(15)	5325(2)	-616(2)	11235(2)	42(1)
C(16)	3984(1)	-1096(2)	10730(1)	35(1)
C(2)	1108(1)	-2070(1)	9720(1)	30(1)
O(3)	-895(1)	-2021(1)	9314(1)	30(1)
C(3)	-283(1)	-2657(1)	9256(1)	24(1)
C(31)	-1189(1)	-4177(1)	8631(1)	25(1)
C(32)	-804(1)	-5062(1)	8711(1)	31(1)
C(33)	-1708(2)	-6454(2)	8172(1)	38(1)
C(34)	-3001(2)	-6982(2)	7523(1)	40(1)
C(35)	-3393(2)	-6117(2)	7423(1)	41(1)
C(36)	-2498(1)	-4726(1)	7978(1)	32(1)
N(7)	541(1)	12(1)	8502(1)	32(1)
C(71)	1650(1)	1103(1)	8534(1)	33(1)
C(72)	2105(1)	1125(2)	7601(1)	34(1)
C(73)	1417(1)	-17(1)	6571(1)	32(1)
C(74)	247(2)	-1130(2)	6537(1)	36(1)
C(75)	-148(1)	-1072(2)	7503(1)	36(1)
C(76)	1918(2)	-41(2)	5567(1)	34(1)
C(77)	3315(2)	579(2)	5686(1)	42(1)
C(78)	3799(2)	592(2)	4762(2)	51(1)
C(79)	2908(2)	10(2)	3717(2)	55(1)
C(7X)	1522(2)	-613(2)	3584(2)	52(1)
C(7Y)	1029(2)	-653(2)	4499(1)	43(1)
C(1A)	8238(2)	5855(2)	2269(2)	67(1)
C(2A)	7772(3)	5455(3)	1153(2)	79(1)
C(3A)	6406(3)	4777(3)	645(2)	87(1)
C(4A)	5496(2)	4509(2)	1272(2)	74(1)
C(5A)	5977(2)	4935(2)	2399(2)	60(1)
C(6A)	7338(2)	5601(2)	2890(2)	61(1)
C(1B)	5343(2)	4038(2)	4816(2)	54(1)
C(2B)	6338(2)	5395(2)	5402(2)	51(1)
C(3B)	5995(2)	6360(2)	5584(2)	55(1)
C(1C)	-634(2)	4552(2)	5739(2)	51(1)
C(2C)	470(2)	5850(2)	6130(2)	58(1)
C(3C)	1101(2)	6301(2)	5393(2)	54(1)

Table 8S. Bond lengths [A] and angles [deg] for [Ni(4-PhPy)2(DBM)2]*4(benzene).

Ni-O(3)	2.0017(10)
Ni-O(3)#1	2.0017(10)
Ni-O(1)	2.0150(10)
Ni-O(1)#1	2.0150(10)
Ni-N(7)	2.1222(13)
Ni-N(7)#1	2.1222(13)
O(1)-C(1)	1.2613(16)
C(1)-C(2)	1.4083(19)
C(1)-C(11)	1.5085(18)
C(11)-C(16)	1.388(2)
C(11)-C(12)	1.389(2)
C(12)-C(13)	1.386(2)
C(13)-C(14)	1.377(2)
C(14)-C(15)	1.376(2)
C(15)-C(16)	1.384(2)
C(2)-C(3)	1.3955(18)
O(3)-C(3)	1.2674(16)
C(3)-C(31)	1.5061(18)
C(31)-C(32)	1.389(2)
C(31)-C(36)	1.3914(19)
C(32)-C(33)	1.386(2)
C(33)-C(34)	1.381(2)
C(34)-C(35)	1.381(2)
C(35)-C(36)	1.385(2)
N(7)-C(75)	1.3377(18)
N(7)-C(71)	1.3443(18)
C(71)-C(72)	1.379(2)
C(72)-C(73)	1.390(2)
C(73)-C(74)	1.393(2)
C(73)-C(76)	1.482(2)
C(74)-C(75)	1.376(2)
C(76)-C(7Y)	1.391(2)
C(76)-C(77)	1.396(2)
C(77)-C(78)	1.383(2)
C(78)-C(79)	1.374(3)
C(79)-C(7X)	1.382(3)
C(7X)-C(7Y)	1.381(2)
C(1A)-C(2A)	1.353(3)
C(1A)-C(6A)	1.363(3)
C(2A)-C(3A)	1.367(4)
C(3A)-C(4A)	1.379(3)
C(4A)-C(5A)	1.363(3)
C(5A)-C(6A)	1.359(3)
C(1B)-C(2B)	1.379(3)
C(1B)-C(3B)#2	1.380(3)
C(2B)-C(3B)	1.375(3)
C(3B)-C(1B)#2	1.380(3)
C(1C)-C(2C)	1.374(3)
C(1C)-C(3C)#3	1.375(2)
C(2C)-C(3C)	1.377(3)
C(3C)-C(1C)#3	1.375(2)
O(3)-Ni-O(3)#1	180.0
O(3)-Ni-O(1)	91.15(4)

Structure of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*4(benzene) SUPPLEMENTARY

O(3)#1-Ni-O(1)	88.85(4)
O(3)-Ni-O(1)#1	88.85(4)
O(3)#1-Ni-O(1)#1	91.15(4)
O(1)-Ni-O(1)#1	180.0
O(3)-Ni-N(7)	89.77(4)
O(3)#1-Ni-N(7)	90.23(4)
O(1)-Ni-N(7)	89.43(4)
O(1)#1-Ni-N(7)	90.57(4)
O(3)-Ni-N(7)#1	90.23(4)
O(3)#1-Ni-N(7)#1	89.77(4)
O(1)-Ni-N(7)#1	90.57(4)
O(1)#1-Ni-N(7)#1	89.43(4)
N(7)-Ni-N(7)#1	180.0
C(1)-O(1)-Ni	125.63(9)
O(1)-C(1)-C(2)	125.13(13)
O(1)-C(1)-C(11)	115.48(12)
C(2)-C(1)-C(11)	119.37(12)
C(16)-C(11)-C(12)	118.36(13)
C(16)-C(11)-C(1)	123.31(13)
C(12)-C(11)-C(1)	118.33(13)
C(13)-C(12)-C(11)	120.61(15)
C(14)-C(13)-C(12)	120.39(15)
C(15)-C(14)-C(13)	119.51(14)
C(14)-C(15)-C(16)	120.39(15)
C(15)-C(16)-C(11)	120.74(14)
C(3)-C(2)-C(1)	125.86(13)
C(3)-O(3)-Ni	125.42(9)
O(3)-C(3)-C(2)	125.82(12)
O(3)-C(3)-C(31)	114.62(11)
C(2)-C(3)-C(31)	119.56(12)
C(32)-C(31)-C(36)	118.27(12)
C(32)-C(31)-C(3)	123.23(12)
C(36)-C(31)-C(3)	118.44(12)
C(33)-C(32)-C(31)	120.88(13)
C(34)-C(33)-C(32)	120.12(14)
C(35)-C(34)-C(33)	119.69(13)
C(34)-C(35)-C(36)	120.15(14)
C(35)-C(36)-C(31)	120.87(14)
C(75)-N(7)-C(71)	117.01(13)
C(75)-N(7)-Ni	122.27(10)
C(71)-N(7)-Ni	120.62(10)
N(7)-C(71)-C(72)	122.89(14)
C(71)-C(72)-C(73)	120.17(14)
C(72)-C(73)-C(74)	116.57(14)
C(72)-C(73)-C(76)	121.28(13)
C(74)-C(73)-C(76)	122.15(13)
C(75)-C(74)-C(73)	119.88(14)
N(7)-C(75)-C(74)	123.42(14)
C(7Y)-C(76)-C(77)	118.49(15)
C(7Y)-C(76)-C(73)	121.65(14)
C(77)-C(76)-C(73)	119.85(14)
C(78)-C(77)-C(76)	120.52(17)
C(79)-C(78)-C(77)	120.25(18)
C(78)-C(79)-C(7X)	119.94(17)
C(7Y)-C(7X)-C(79)	120.15(17)
C(7X)-C(7Y)-C(76)	120.62(17)
C(2A)-C(1A)-C(6A)	119.6(2)
C(1A)-C(2A)-C(3A)	120.4(2)
C(2A)-C(3A)-C(4A)	120.0(2)

C(5A)-C(4A)-C(3A)	119.3(2)
C(6A)-C(5A)-C(4A)	120.0(2)
C(5A)-C(6A)-C(1A)	120.8(2)
C(2B)-C(1B)-C(3B)#2	120.61(18)
C(3B)-C(2B)-C(1B)	119.69(18)
C(2B)-C(3B)-C(1B)#2	119.70(18)
C(2C)-C(1C)-C(3C)#3	119.67(17)
C(1C)-C(2C)-C(3C)	120.30(17)
C(1C)#3-C(3C)-C(2C)	120.03(17)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+2 #2 -x+1,-y+1,-z+1 #3 -x,-y+1,-z+1

Table 9S. Anisotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*4(benzene).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni	24(1)	21(1)	32(1)	6(1)	1(1)	12(1)
O(1)	27(1)	23(1)	38(1)	5(1)	0(1)	13(1)
C(1)	24(1)	26(1)	24(1)	10(1)	6(1)	12(1)
C(11)	24(1)	30(1)	24(1)	12(1)	6(1)	13(1)
C(12)	30(1)	31(1)	38(1)	8(1)	3(1)	16(1)
C(13)	28(1)	36(1)	45(1)	5(1)	-2(1)	11(1)
C(14)	25(1)	49(1)	40(1)	14(1)	1(1)	18(1)
C(15)	33(1)	44(1)	52(1)	19(1)	6(1)	25(1)
C(16)	28(1)	30(1)	39(1)	10(1)	2(1)	15(1)
C(2)	26(1)	24(1)	37(1)	9(1)	4(1)	15(1)
O(3)	25(1)	23(1)	36(1)	7(1)	2(1)	13(1)
C(3)	27(1)	23(1)	21(1)	9(1)	6(1)	13(1)
C(31)	26(1)	23(1)	23(1)	9(1)	7(1)	13(1)
C(32)	30(1)	27(1)	32(1)	10(1)	4(1)	15(1)
C(33)	41(1)	25(1)	46(1)	13(1)	9(1)	19(1)
C(34)	37(1)	21(1)	46(1)	8(1)	6(1)	10(1)
C(35)	30(1)	29(1)	48(1)	10(1)	-1(1)	11(1)
C(36)	30(1)	26(1)	38(1)	11(1)	4(1)	15(1)
N(7)	27(1)	27(1)	35(1)	9(1)	2(1)	13(1)
C(71)	29(1)	26(1)	34(1)	7(1)	2(1)	13(1)
C(72)	28(1)	29(1)	38(1)	11(1)	5(1)	12(1)
C(73)	30(1)	32(1)	34(1)	12(1)	3(1)	19(1)
C(74)	34(1)	30(1)	30(1)	6(1)	-1(1)	13(1)
C(75)	27(1)	29(1)	36(1)	9(1)	0(1)	8(1)
C(76)	41(1)	28(1)	35(1)	11(1)	9(1)	21(1)
C(77)	43(1)	35(1)	42(1)	15(1)	13(1)	19(1)
C(78)	57(1)	37(1)	56(1)	20(1)	28(1)	22(1)
C(79)	91(2)	44(1)	50(1)	25(1)	39(1)	44(1)
C(7X)	81(1)	56(1)	35(1)	17(1)	15(1)	50(1)
C(7Y)	52(1)	46(1)	37(1)	14(1)	9(1)	35(1)
C(1A)	57(1)	77(2)	78(2)	42(1)	34(1)	37(1)
C(2A)	117(2)	127(2)	85(2)	76(2)	74(2)	104(2)
C(3A)	148(2)	129(2)	43(1)	38(1)	29(2)	115(2)
C(4A)	72(2)	86(2)	65(2)	27(1)	7(1)	47(1)
C(5A)	51(1)	78(2)	64(1)	43(1)	27(1)	35(1)
C(6A)	60(1)	72(1)	47(1)	25(1)	21(1)	32(1)
C(1B)	70(1)	48(1)	55(1)	25(1)	20(1)	36(1)
C(2B)	52(1)	56(1)	46(1)	26(1)	13(1)	26(1)
C(3B)	61(1)	40(1)	49(1)	16(1)	9(1)	20(1)
C(1C)	51(1)	57(1)	42(1)	22(1)	15(1)	26(1)
C(2C)	60(1)	51(1)	35(1)	6(1)	7(1)	19(1)
C(3C)	47(1)	43(1)	48(1)	11(1)	8(1)	14(1)

Table 10S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*4(benzene).

	x	y	z	U(eq)
H(12)	4108	1768	11743	43
H(13)	6361	2562	12593	52
H(14)	7128	1067	12281	49
H(15)	5638	-1227	11099	50
H(16)	3382	-2036	10255	41
H(2)	1445	-2663	9570	36
H(32)	91	-4708	9141	38
H(33)	-1438	-7046	8249	45
H(34)	-3618	-7937	7146	47
H(35)	-4280	-6477	6972	49
H(36)	-2781	-4138	7912	39
H(71)	2143	1894	9230	40
H(72)	2891	1922	7663	41
H(74)	-277	-1927	5849	44
H(75)	-952	-1843	7457	43
H(77)	3938	996	6408	50
H(78)	4751	1005	4849	61
H(79)	3246	34	3086	66
H(7X)	907	-1014	2862	62
H(7Y)	73	-1102	4399	52
H(1A)	9188	6310	2617	80
H(2A)	8398	5647	721	95
H(3A)	6083	4490	-140	105
H(4A)	4544	4033	923	89
H(5A)	5360	4767	2841	72
H(6A)	7666	5892	3675	73
H(1B)	5580	3372	4685	65
H(2B)	7256	5661	5680	61
H(3B)	6677	7296	5984	66
H(1C)	-1072	4245	6249	61
H(2C)	800	6439	6913	69
H(3C)	1860	7201	5667	64

Table 11S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(benzene). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni	4611(1)	1793(1)	2857(1)	22(1)
O(1)	6286(1)	1316(1)	3174(1)	26(1)
C(1)	7283(2)	715(1)	2754(1)	24(1)
C(11)	8389(2)	385(1)	3137(1)	28(1)
C(12)	8681(2)	1103(2)	3508(1)	37(1)
C(13)	9688(2)	811(2)	3873(1)	50(1)
C(14)	10370(2)	-190(2)	3894(1)	57(1)
C(15)	10074(2)	-900(2)	3534(2)	57(1)
C(16)	9095(2)	-617(2)	3145(1)	41(1)
C(2)	7485(2)	358(1)	1944(1)	29(1)
O(3)	5491(1)	1206(1)	1698(1)	25(1)
C(3)	6637(2)	673(1)	1442(1)	23(1)
C(31)	7085(2)	433(1)	507(1)	25(1)
C(32)	8361(2)	7(2)	60(1)	34(1)
C(33)	8717(2)	-117(2)	-820(1)	40(1)
C(34)	7812(2)	174(2)	-1265(1)	39(1)
C(35)	6546(2)	576(2)	-826(1)	41(1)
C(36)	6184(2)	703(2)	53(1)	34(1)
O(4)	2965(1)	2270(1)	2517(1)	26(1)
C(4)	1874(2)	2670(1)	3006(1)	24(1)
C(41)	783(2)	2947(1)	2612(1)	27(1)
C(42)	911(2)	2442(2)	1904(1)	34(1)
C(43)	-50(2)	2690(2)	1502(1)	47(1)
C(44)	-1138(2)	3451(2)	1795(1)	52(1)
C(45)	-1272(2)	3954(2)	2489(1)	49(1)
C(46)	-329(2)	3702(2)	2908(1)	38(1)
C(5)	1600(2)	2867(1)	3876(1)	29(1)
O(6)	3715(1)	2370(1)	4020(1)	24(1)
C(6)	2506(2)	2712(1)	4325(1)	24(1)
C(61)	2047(2)	2957(1)	5260(1)	27(1)
C(62)	846(2)	3578(2)	5638(1)	40(1)
C(63)	486(2)	3782(2)	6500(1)	54(1)
C(64)	1309(2)	3367(2)	6992(1)	53(1)
C(65)	2503(2)	2752(2)	6625(1)	45(1)
C(66)	2871(2)	2547(2)	5761(1)	33(1)
N(7)	5092(1)	3207(1)	2289(1)	24(1)
C(71)	4911(2)	3979(1)	2766(1)	29(1)
C(72)	5214(2)	4902(1)	2418(1)	30(1)
C(73)	5744(2)	5072(1)	1524(1)	26(1)
C(74)	5918(2)	4271(1)	1033(1)	27(1)
C(75)	5586(2)	3372(1)	1428(1)	28(1)
C(76)	6107(2)	6039(1)	1113(1)	27(1)
C(77)	6514(2)	6631(2)	1544(1)	37(1)
C(78)	6892(2)	7514(2)	1135(1)	42(1)
C(79)	6873(2)	7824(2)	293(1)	38(1)
C(7X)	6462(2)	7248(1)	-140(1)	35(1)
C(7Y)	6079(2)	6373(1)	267(1)	29(1)
N(8)	4156(1)	371(1)	3397(1)	26(1)

Structure of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(benzene) SUPPLEMENTARY

C(81)	4016(2)	40(1)	4233(1)	30(1)
C(82)	3809(2)	-911(1)	4582(1)	31(1)
C(83)	3729(2)	-1591(1)	4056(1)	27(1)
C(84)	3879(2)	-1242(1)	3189(1)	32(1)
C(85)	4076(2)	-277(1)	2892(1)	32(1)
C(86)	3497(2)	-2616(1)	4404(1)	30(1)
C(87)	3869(2)	-3123(2)	5125(1)	36(1)
C(88)	3652(2)	-4081(2)	5440(1)	44(1)
C(89)	3051(2)	-4555(2)	5060(1)	43(1)
C(8X)	2675(2)	-4069(2)	4348(1)	41(1)
C(8Y)	2896(2)	-3106(2)	4017(1)	35(1)
C(1A)	7579(3)	3698(2)	-1434(2)	63(1)
C(2A)	8181(3)	2856(2)	-1020(2)	65(1)
C(3A)	9056(3)	2940(2)	-633(2)	63(1)
C(4A)	9330(3)	3867(2)	-658(2)	58(1)
C(5A)	8721(3)	4715(2)	-1071(2)	57(1)
C(6A)	7851(3)	4627(2)	-1459(2)	60(1)

Table 12S. Bond lengths [A] and angles [deg] for [Ni(4-PhPy)2(DBM)2]*(benzene).

Ni-O(3)	2.0140(11)
Ni-O(6)	2.0145(11)
Ni-O(4)	2.0227(12)
Ni-O(1)	2.0323(12)
Ni-N(8)	2.1198(15)
Ni-N(7)	2.1296(14)
O(1)-C(1)	1.261(2)
C(1)-C(2)	1.413(2)
C(1)-C(11)	1.508(2)
C(11)-C(16)	1.384(3)
C(11)-C(12)	1.388(3)
C(12)-C(13)	1.389(3)
C(13)-C(14)	1.375(4)
C(14)-C(15)	1.373(4)
C(15)-C(16)	1.387(3)
C(2)-C(3)	1.397(2)
O(3)-C(3)	1.270(2)
C(3)-C(31)	1.509(2)
C(31)-C(36)	1.387(2)
C(31)-C(32)	1.394(2)
C(32)-C(33)	1.390(2)
C(33)-C(34)	1.380(3)
C(34)-C(35)	1.374(3)
C(35)-C(36)	1.388(2)
O(4)-C(4)	1.261(2)
C(4)-C(5)	1.409(2)
C(4)-C(41)	1.504(2)
C(41)-C(42)	1.388(2)
C(41)-C(46)	1.392(3)
C(42)-C(43)	1.386(3)
C(43)-C(44)	1.378(3)
C(44)-C(45)	1.367(3)
C(45)-C(46)	1.387(3)
C(5)-C(6)	1.398(2)
O(6)-C(6)	1.270(2)
C(6)-C(61)	1.509(2)
C(61)-C(66)	1.387(2)
C(61)-C(62)	1.391(3)
C(62)-C(63)	1.387(3)
C(63)-C(64)	1.376(3)
C(64)-C(65)	1.379(3)
C(65)-C(66)	1.390(2)
N(7)-C(71)	1.342(2)
N(7)-C(75)	1.343(2)
C(71)-C(72)	1.378(2)
C(72)-C(73)	1.396(2)
C(73)-C(74)	1.392(2)
C(73)-C(76)	1.478(2)
C(74)-C(75)	1.377(2)
C(76)-C(7Y)	1.395(2)
C(76)-C(77)	1.398(2)
C(77)-C(78)	1.382(3)
C(78)-C(79)	1.381(3)
C(79)-C(7X)	1.387(3)

C(7X)-C(7Y)	1.374(3)
N(8)-C(85)	1.340(2)
N(8)-C(81)	1.343(2)
C(81)-C(82)	1.379(2)
C(82)-C(83)	1.399(2)
C(83)-C(84)	1.394(2)
C(83)-C(86)	1.481(2)
C(84)-C(85)	1.377(3)
C(86)-C(87)	1.398(2)
C(86)-C(8Y)	1.402(3)
C(87)-C(88)	1.380(3)
C(88)-C(89)	1.380(3)
C(89)-C(8X)	1.379(3)
C(8X)-C(8Y)	1.393(3)
C(1A)-C(2A)	1.369(4)
C(1A)-C(6A)	1.372(4)
C(2A)-C(3A)	1.371(4)
C(3A)-C(4A)	1.371(4)
C(4A)-C(5A)	1.375(3)
C(5A)-C(6A)	1.369(4)

O(3)-Ni-O(6)	179.29(5)
O(3)-Ni-O(4)	88.37(5)
O(6)-Ni-O(4)	91.22(5)
O(3)-Ni-O(1)	90.64(5)
O(6)-Ni-O(1)	89.78(5)
O(4)-Ni-O(1)	178.86(5)
O(3)-Ni-N(8)	89.53(5)
O(6)-Ni-N(8)	89.91(5)
O(4)-Ni-N(8)	91.32(5)
O(1)-Ni-N(8)	89.23(5)
O(3)-Ni-N(7)	89.26(5)
O(6)-Ni-N(7)	91.31(5)
O(4)-Ni-N(7)	88.75(5)
O(1)-Ni-N(7)	90.67(5)
N(8)-Ni-N(7)	178.78(5)
C(1)-O(1)-Ni	124.58(10)
O(1)-C(1)-C(2)	126.52(15)
O(1)-C(1)-C(11)	116.36(14)
C(2)-C(1)-C(11)	117.06(15)
C(16)-C(11)-C(12)	119.64(17)
C(16)-C(11)-C(1)	121.44(17)
C(12)-C(11)-C(1)	118.90(17)
C(11)-C(12)-C(13)	119.7(2)
C(14)-C(13)-C(12)	120.4(2)
C(15)-C(14)-C(13)	119.8(2)
C(14)-C(15)-C(16)	120.6(2)
C(11)-C(16)-C(15)	119.8(2)
C(3)-C(2)-C(1)	125.27(16)
C(3)-O(3)-Ni	126.53(10)
O(3)-C(3)-C(2)	124.98(15)
O(3)-C(3)-C(31)	114.77(14)
C(2)-C(3)-C(31)	120.16(15)
C(36)-C(31)-C(32)	118.12(15)
C(36)-C(31)-C(3)	117.92(15)
C(32)-C(31)-C(3)	123.86(15)
C(33)-C(32)-C(31)	120.48(17)
C(34)-C(33)-C(32)	120.57(18)
C(35)-C(34)-C(33)	119.36(17)

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C(34)-C(35)-C(36)	120.38(18)
C(31)-C(36)-C(35)	121.06(18)
C(4)-O(4)-Ni	125.42(10)
O(4)-C(4)-C(5)	125.79(15)
O(4)-C(4)-C(41)	115.81(14)
C(5)-C(4)-C(41)	118.40(15)
C(42)-C(41)-C(46)	118.63(16)
C(42)-C(41)-C(4)	118.31(16)
C(46)-C(41)-C(4)	123.03(15)
C(43)-C(42)-C(41)	120.51(18)
C(44)-C(43)-C(42)	120.24(19)
C(45)-C(44)-C(43)	119.73(18)
C(44)-C(45)-C(46)	120.7(2)
C(45)-C(46)-C(41)	120.15(18)
C(6)-C(5)-C(4)	125.73(16)
C(6)-O(6)-Ni	125.13(10)
O(6)-C(6)-C(5)	125.92(14)
O(6)-C(6)-C(61)	115.14(14)
C(5)-C(6)-C(61)	118.94(15)
C(66)-C(61)-C(62)	118.68(16)
C(66)-C(61)-C(6)	118.05(16)
C(62)-C(61)-C(6)	123.27(16)
C(63)-C(62)-C(61)	120.47(19)
C(64)-C(63)-C(62)	120.3(2)
C(63)-C(64)-C(65)	119.85(18)
C(64)-C(65)-C(66)	120.1(2)
C(61)-C(66)-C(65)	120.58(18)
C(71)-N(7)-C(75)	116.55(15)
C(71)-N(7)-Ni	122.21(11)
C(75)-N(7)-Ni	121.24(11)
N(7)-C(71)-C(72)	123.52(15)
C(71)-C(72)-C(73)	120.13(16)
C(74)-C(73)-C(72)	115.98(16)
C(74)-C(73)-C(76)	121.36(15)
C(72)-C(73)-C(76)	122.67(16)
C(75)-C(74)-C(73)	120.55(15)
N(7)-C(75)-C(74)	123.26(16)
C(7Y)-C(76)-C(77)	118.10(17)
C(7Y)-C(76)-C(73)	120.29(15)
C(77)-C(76)-C(73)	121.60(15)
C(78)-C(77)-C(76)	120.52(17)
C(79)-C(78)-C(77)	120.48(18)
C(78)-C(79)-C(7X)	119.57(18)
C(7Y)-C(7X)-C(79)	120.11(17)
C(7X)-C(7Y)-C(76)	121.21(17)
C(85)-N(8)-C(81)	116.47(15)
C(85)-N(8)-Ni	120.45(11)
C(81)-N(8)-Ni	122.94(12)
N(8)-C(81)-C(82)	123.77(16)
C(81)-C(82)-C(83)	119.90(15)
C(84)-C(83)-C(82)	115.91(16)
C(84)-C(83)-C(86)	122.28(16)
C(82)-C(83)-C(86)	121.81(15)
C(85)-C(84)-C(83)	120.59(16)
N(8)-C(85)-C(84)	123.35(16)
C(87)-C(86)-C(8Y)	118.15(17)
C(87)-C(86)-C(83)	121.11(16)
C(8Y)-C(86)-C(83)	120.74(16)
C(88)-C(87)-C(86)	120.49(18)

C(89)-C(88)-C(87)	121.05(19)
C(8X)-C(89)-C(88)	119.45(19)
C(89)-C(8X)-C(8Y)	120.28(19)
C(8X)-C(8Y)-C(86)	120.59(18)
C(2A)-C(1A)-C(6A)	119.8(3)
C(1A)-C(2A)-C(3A)	120.0(3)
C(2A)-C(3A)-C(4A)	120.3(2)
C(3A)-C(4A)-C(5A)	119.7(3)
C(6A)-C(5A)-C(4A)	119.9(2)
C(5A)-C(6A)-C(1A)	120.4(2)

Table 13S. Anisotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(benzene).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni	21(1)	26(1)	17(1)	-3(1)	-6(1)	-3(1)
O(1)	26(1)	32(1)	22(1)	-6(1)	-9(1)	-4(1)
C(1)	24(1)	28(1)	23(1)	2(1)	-8(1)	-8(1)
C(11)	23(1)	40(1)	20(1)	2(1)	-5(1)	-8(1)
C(12)	38(1)	48(1)	31(1)	3(1)	-15(1)	-16(1)
C(13)	44(1)	86(2)	34(1)	6(1)	-19(1)	-32(1)
C(14)	29(1)	105(2)	33(1)	8(1)	-16(1)	-8(1)
C(15)	41(1)	68(2)	49(1)	3(1)	-19(1)	11(1)
C(16)	35(1)	44(1)	41(1)	-4(1)	-14(1)	2(1)
C(2)	23(1)	37(1)	25(1)	-7(1)	-6(1)	-2(1)
O(3)	23(1)	29(1)	21(1)	-5(1)	-6(1)	-4(1)
C(3)	23(1)	25(1)	21(1)	-4(1)	-3(1)	-7(1)
C(31)	28(1)	26(1)	21(1)	-5(1)	-3(1)	-10(1)
C(32)	27(1)	49(1)	29(1)	-13(1)	-3(1)	-13(1)
C(33)	33(1)	53(1)	32(1)	-19(1)	6(1)	-17(1)
C(34)	54(1)	45(1)	21(1)	-10(1)	-2(1)	-22(1)
C(35)	50(1)	48(1)	28(1)	-10(1)	-16(1)	-6(1)
C(36)	33(1)	40(1)	26(1)	-10(1)	-8(1)	-3(1)
O(4)	23(1)	33(1)	21(1)	-4(1)	-6(1)	-3(1)
C(4)	23(1)	26(1)	24(1)	-2(1)	-7(1)	-6(1)
C(41)	23(1)	32(1)	26(1)	-1(1)	-8(1)	-5(1)
C(42)	30(1)	42(1)	30(1)	-6(1)	-12(1)	-2(1)
C(43)	44(1)	61(1)	42(1)	-11(1)	-24(1)	-4(1)
C(44)	35(1)	76(2)	46(1)	-6(1)	-25(1)	1(1)
C(45)	29(1)	62(2)	48(1)	-11(1)	-13(1)	10(1)
C(46)	29(1)	47(1)	35(1)	-10(1)	-11(1)	2(1)
C(5)	21(1)	41(1)	24(1)	-9(1)	-4(1)	-4(1)
O(6)	23(1)	29(1)	19(1)	-4(1)	-5(1)	-6(1)
C(6)	27(1)	22(1)	21(1)	-4(1)	-4(1)	-7(1)
C(61)	29(1)	31(1)	21(1)	-6(1)	-3(1)	-12(1)
C(62)	32(1)	54(1)	34(1)	-19(1)	-3(1)	-6(1)
C(63)	38(1)	76(2)	43(1)	-32(1)	4(1)	-9(1)
C(64)	58(2)	77(2)	25(1)	-22(1)	0(1)	-22(1)
C(65)	54(1)	61(1)	26(1)	-9(1)	-13(1)	-18(1)
C(66)	37(1)	38(1)	24(1)	-8(1)	-7(1)	-9(1)
N(7)	24(1)	28(1)	21(1)	-2(1)	-7(1)	-5(1)
C(71)	34(1)	32(1)	20(1)	-3(1)	-6(1)	-8(1)
C(72)	36(1)	29(1)	24(1)	-6(1)	-8(1)	-7(1)
C(73)	25(1)	30(1)	25(1)	1(1)	-11(1)	-6(1)
C(74)	30(1)	32(1)	19(1)	-2(1)	-6(1)	-8(1)
C(75)	33(1)	30(1)	21(1)	-4(1)	-9(1)	-7(1)
C(76)	26(1)	27(1)	27(1)	-2(1)	-8(1)	-4(1)
C(77)	52(1)	37(1)	28(1)	2(1)	-18(1)	-17(1)
C(78)	60(1)	38(1)	39(1)	0(1)	-21(1)	-23(1)
C(79)	45(1)	31(1)	35(1)	1(1)	-10(1)	-13(1)
C(7X)	41(1)	33(1)	27(1)	2(1)	-11(1)	-7(1)
C(7Y)	34(1)	29(1)	26(1)	-3(1)	-12(1)	-6(1)
N(8)	27(1)	30(1)	22(1)	-3(1)	-8(1)	-6(1)

Structure of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(benzene) SUPPLEMENTARY

C(81)	38(1)	30(1)	23(1)	-5(1)	-9(1)	-8(1)
C(82)	38(1)	33(1)	22(1)	0(1)	-10(1)	-9(1)
C(83)	26(1)	27(1)	28(1)	-2(1)	-9(1)	-6(1)
C(84)	39(1)	36(1)	26(1)	-6(1)	-10(1)	-13(1)
C(85)	40(1)	37(1)	22(1)	-1(1)	-13(1)	-14(1)
C(86)	26(1)	28(1)	33(1)	-6(1)	-4(1)	-4(1)
C(87)	40(1)	35(1)	35(1)	0(1)	-11(1)	-12(1)
C(88)	48(1)	37(1)	45(1)	7(1)	-14(1)	-12(1)
C(89)	40(1)	30(1)	54(1)	0(1)	-6(1)	-12(1)
C(8X)	33(1)	37(1)	55(1)	-12(1)	-9(1)	-10(1)
C(8Y)	31(1)	35(1)	41(1)	-6(1)	-11(1)	-7(1)
C(1A)	46(2)	89(2)	50(1)	-19(1)	-10(1)	-8(1)
C(2A)	87(2)	50(2)	60(2)	-10(1)	-16(2)	-24(2)
C(3A)	83(2)	49(2)	49(1)	2(1)	-23(1)	1(1)
C(4A)	55(2)	71(2)	45(1)	-17(1)	-11(1)	-10(1)
C(5A)	59(2)	47(1)	47(1)	-9(1)	10(1)	-14(1)
C(6A)	53(2)	60(2)	41(1)	0(1)	-1(1)	10(1)

Table 14S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(benzene).

	x	y	z	U(eq)
H(12)	8194	1790	3512	45
H(13)	9906	1306	4110	60
H(14)	11044	-388	4156	69
H(15)	10543	-1592	3551	68
H(16)	8910	-1110	2884	50
H(2)	8259	-137	1723	35
H(32)	8993	-201	359	41
H(33)	9591	-405	-1119	48
H(34)	8061	99	-1869	47
H(35)	5915	766	-1126	49
H(36)	5305	981	348	40
H(42)	1663	1923	1695	41
H(43)	41	2335	1023	56
H(44)	-1792	3625	1514	62
H(45)	-2019	4482	2687	59
H(46)	-444	4046	3399	46
H(5)	722	3128	4184	35
H(62)	269	3864	5304	48
H(63)	-334	4210	6751	65
H(64)	1056	3504	7583	63
H(65)	3074	2467	6963	54
H(66)	3695	2123	5512	39
H(71)	4555	3884	3377	35
H(72)	5061	5423	2786	36
H(74)	6268	4345	421	32
H(75)	5714	2842	1074	33
H(77)	6532	6425	2123	44
H(78)	7166	7911	1435	51
H(79)	7141	8428	12	45
H(7X)	6445	7459	-718	42
H(7Y)	5790	5988	-34	35
H(81)	4062	487	4605	36
H(82)	3721	-1105	5178	37
H(84)	3846	-1673	2799	39
H(85)	4159	-60	2300	38
H(87)	4275	-2806	5400	43
H(88)	3920	-4419	5926	53
H(89)	2897	-5211	5287	52
H(8X)	2264	-4393	4082	49
H(8Y)	2637	-2778	3525	42
H(1A)	6974	3640	-1704	76
H(2A)	7992	2212	-999	78
H(3A)	9475	2353	-347	76
H(4A)	9937	3924	-390	69
H(5A)	8903	5360	-1087	68
H(6A)	7434	5212	-1747	72

Table 15S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(fluorobenzene). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni	4619(1)	1780(1)	2855(1)	23(1)
O(1)	6289(1)	1302(1)	3168(1)	27(1)
C(1)	7287(2)	706(2)	2743(2)	26(1)
C(11)	8389(2)	379(2)	3128(2)	29(1)
C(12)	8687(2)	1082(2)	3501(2)	39(1)
C(13)	9687(3)	784(3)	3871(2)	49(1)
C(14)	10362(3)	-207(3)	3880(2)	60(1)
C(15)	10062(3)	-916(3)	3514(2)	57(1)
C(16)	9091(2)	-627(2)	3124(2)	41(1)
C(2)	7485(2)	361(2)	1935(2)	30(1)
O(3)	5492(1)	1197(1)	1697(1)	25(1)
C(3)	6648(2)	671(2)	1436(1)	22(1)
C(31)	7082(2)	432(2)	504(2)	25(1)
C(32)	8357(2)	2(2)	49(2)	34(1)
C(33)	8709(2)	-120(2)	-825(2)	40(1)
C(34)	7805(3)	173(2)	-1270(2)	39(1)
C(35)	6539(3)	586(2)	-826(2)	42(1)
C(36)	6188(2)	712(2)	51(2)	34(1)
O(4)	2974(1)	2263(1)	2517(1)	26(1)
C(4)	1882(2)	2664(2)	3011(2)	24(1)
C(41)	795(2)	2938(2)	2614(2)	27(1)
C(42)	921(2)	2447(2)	1909(2)	33(1)
C(43)	-31(3)	2690(2)	1503(2)	47(1)
C(44)	-1122(3)	3445(2)	1799(2)	52(1)
C(45)	-1255(2)	3940(2)	2502(2)	51(1)
C(46)	-320(2)	3694(2)	2916(2)	39(1)
C(5)	1615(2)	2851(2)	3873(2)	31(1)
O(6)	3724(1)	2360(1)	4013(1)	24(1)
C(6)	2509(2)	2703(2)	4325(2)	24(1)
C(61)	2064(2)	2948(2)	5253(2)	27(1)
C(62)	862(2)	3582(2)	5629(2)	40(1)
C(63)	511(3)	3793(2)	6487(2)	54(1)
C(64)	1329(3)	3388(3)	6972(2)	56(1)
C(65)	2519(3)	2763(2)	6610(2)	47(1)
C(66)	2877(2)	2546(2)	5753(2)	33(1)
N(7)	5112(2)	3195(1)	2288(1)	26(1)
C(71)	4949(2)	3954(2)	2763(2)	30(1)
C(72)	5249(2)	4880(2)	2410(2)	30(1)
C(73)	5763(2)	5050(2)	1520(2)	24(1)
C(74)	5929(2)	4261(2)	1027(2)	28(1)
C(75)	5593(2)	3359(2)	1426(2)	29(1)
C(76)	6119(2)	6027(2)	1108(2)	28(1)
C(77)	6534(2)	6618(2)	1534(2)	37(1)
C(78)	6905(3)	7502(2)	1127(2)	43(1)
C(79)	6873(2)	7814(2)	292(2)	39(1)
C(7X)	6450(2)	7243(2)	-133(2)	35(1)
C(7Y)	6076(2)	6367(2)	272(2)	30(1)

Structure of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(fluorobenzene) SUPPLEMENTARY

N(8)	4153(2)	364(2)	3394(1)	28(1)
C(81)	4013(2)	34(2)	4234(2)	31(1)
C(82)	3809(2)	-910(2)	4579(2)	33(1)
C(83)	3725(2)	-1595(2)	4059(2)	29(1)
C(84)	3872(2)	-1251(2)	3195(2)	32(1)
C(85)	4071(2)	-285(2)	2898(2)	33(1)
C(86)	3495(2)	-2627(2)	4407(2)	30(1)
C(87)	3863(2)	-3127(2)	5125(2)	38(1)
C(88)	3650(3)	-4080(2)	5442(2)	44(1)
C(89)	3060(2)	-4563(2)	5056(2)	43(1)
C(8X)	2685(2)	-4085(2)	4350(2)	42(1)
C(8Y)	2902(2)	-3119(2)	4021(2)	37(1)
FA	7127(4)	3365(3)	-1984(3)	88(2)
C(1A)	7698(7)	3557(3)	-1514(5)	50(1)
C(2A)	8422(6)	2765(3)	-1111(5)	50(1)
C(3A)	9245(5)	2971(4)	-723(4)	50(1)
C(4A)	9344(7)	3968(4)	-738(5)	50(1)
C(5A)	8621(8)	4760(3)	-1140(6)	50(1)
C(6A)	7797(8)	4555(3)	-1529(6)	50(1)
FB	9930(2)	3959(19)	-502(18)	83(6)
C(1B)	9110(3)	3852(16)	-820(3)	50(1)
C(2B)	8830(4)	2901(17)	-730(3)	50(1)
C(3B)	7860(3)	2780(2)	-1040(3)	50(1)
C(4B)	7190(3)	3610(3)	-1440(2)	50(1)
C(5B)	7480(3)	4560(2)	-1530(2)	50(1)
C(6B)	8440(3)	4683(17)	-1230(3)	50(1)
FC	9651(5)	2128(3)	-372(3)	81(2)
C(1C)	8974(6)	2940(3)	-606(5)	50(1)
C(2C)	8155(7)	2904(3)	-1069(5)	50(1)
C(3C)	7645(7)	3784(4)	-1512(5)	50(1)
C(4C)	7953(8)	4700(4)	-1492(5)	50(1)
C(5C)	8772(8)	4736(3)	-1028(6)	50(1)
C(6C)	9282(7)	3856(3)	-585(5)	50(1)
FD	7650(4)	5810(2)	-1400(3)	74(7)
C(1D)	8160(4)	4880(2)	-1360(2)	50(1)
C(2D)	7690(5)	4210(3)	-1660(4)	50(1)
C(3D)	8040(6)	3160(3)	-1450(4)	50(1)
C(4D)	8860(6)	2790(2)	-950(4)	50(1)
C(5D)	9330(6)	3460(3)	-650(4)	50(1)
C(6D)	8980(5)	4500(3)	-850(4)	50(1)

Table 16S. Bond lengths [A] and angles [deg] for [Ni(4-PhPy)2(DBM)2]*(fluorobenzene).

Ni-O(3)	2.0107(15)
Ni-O(6)	2.0118(15)
Ni-O(4)	2.0243(15)
Ni-O(1)	2.0303(15)
Ni-N(8)	2.116(2)
Ni-N(7)	2.1339(19)
O(1)-C(1)	1.261(3)
C(1)-C(2)	1.406(3)
C(1)-C(11)	1.509(3)
C(11)-C(12)	1.378(3)
C(11)-C(16)	1.391(3)
C(12)-C(13)	1.392(3)
C(13)-C(14)	1.364(4)
C(14)-C(15)	1.380(4)
C(15)-C(16)	1.384(4)
C(2)-C(3)	1.389(3)
O(3)-C(3)	1.278(2)
C(3)-C(31)	1.505(3)
C(31)-C(36)	1.385(3)
C(31)-C(32)	1.398(3)
C(32)-C(33)	1.380(3)
C(33)-C(34)	1.384(4)
C(34)-C(35)	1.381(4)
C(35)-C(36)	1.386(3)
O(4)-C(4)	1.265(3)
C(4)-C(5)	1.396(3)
C(4)-C(41)	1.509(3)
C(41)-C(42)	1.375(3)
C(41)-C(46)	1.398(3)
C(42)-C(43)	1.386(3)
C(43)-C(44)	1.379(4)
C(44)-C(45)	1.373(4)
C(45)-C(46)	1.378(3)
C(5)-C(6)	1.394(3)
O(6)-C(6)	1.278(2)
C(6)-C(61)	1.500(3)
C(61)-C(66)	1.379(3)
C(61)-C(62)	1.401(3)
C(62)-C(63)	1.387(4)
C(63)-C(64)	1.364(4)
C(64)-C(65)	1.382(4)
C(65)-C(66)	1.386(3)
N(7)-C(71)	1.333(3)
N(7)-C(75)	1.342(3)
C(71)-C(72)	1.381(3)
C(72)-C(73)	1.389(3)
C(73)-C(74)	1.383(3)
C(73)-C(76)	1.488(3)
C(74)-C(75)	1.383(3)
C(76)-C(7Y)	1.389(3)
C(76)-C(77)	1.397(3)
C(77)-C(78)	1.379(4)
C(78)-C(79)	1.378(4)
C(79)-C(7X)	1.381(3)

C(7X)-C(7Y)	1.370(3)
N(8)-C(85)	1.331(3)
N(8)-C(81)	1.351(3)
C(81)-C(82)	1.368(3)
C(82)-C(83)	1.399(3)
C(83)-C(84)	1.390(3)
C(83)-C(86)	1.487(3)
C(84)-C(85)	1.380(3)
C(86)-C(87)	1.394(3)
C(86)-C(8Y)	1.396(3)
C(87)-C(88)	1.373(4)
C(88)-C(89)	1.386(4)
C(89)-C(8X)	1.372(4)
C(8X)-C(8Y)	1.394(4)
FA-C(1A)	1.249(5)
C(1A)-C(2A)	1.3900
C(1A)-C(6A)	1.3900
C(2A)-C(3A)	1.3900
C(3A)-C(4A)	1.3900
C(4A)-C(5A)	1.3900
C(5A)-C(6A)	1.3900
FB-C(1B)	1.251(5)
C(1B)-C(2B)	1.3900
C(1B)-C(6B)	1.3900
C(2B)-C(3B)	1.3900
C(3B)-C(4B)	1.3900
C(4B)-C(5B)	1.3900
C(5B)-C(6B)	1.3900
FC-C(1C)	1.251(5)
C(1C)-C(2C)	1.3900
C(1C)-C(6C)	1.3900
C(2C)-C(3C)	1.3900
C(3C)-C(4C)	1.3900
C(4C)-C(5C)	1.3900
C(5C)-C(6C)	1.3900
FD-C(1D)	1.255(5)
C(1D)-C(2D)	1.3900
C(1D)-C(6D)	1.3900
C(2D)-C(3D)	1.3900
C(3D)-C(4D)	1.3900
C(4D)-C(5D)	1.3900
C(5D)-C(6D)	1.3900
O(3)-Ni-O(6)	179.29(6)
O(3)-Ni-O(4)	88.33(6)
O(6)-Ni-O(4)	91.07(6)
O(3)-Ni-O(1)	90.72(6)
O(6)-Ni-O(1)	89.88(6)
O(4)-Ni-O(1)	178.83(7)
O(3)-Ni-N(8)	89.59(7)
O(6)-Ni-N(8)	90.05(7)
O(4)-Ni-N(8)	91.50(7)
O(1)-Ni-N(8)	89.19(7)
O(3)-Ni-N(7)	89.26(7)
O(6)-Ni-N(7)	91.10(7)
O(4)-Ni-N(7)	88.64(7)
O(1)-Ni-N(7)	90.65(7)
N(8)-Ni-N(7)	178.84(8)
C(1)-O(1)-Ni	124.60(15)

O(1)-C(1)-C(2)	126.4(2)
O(1)-C(1)-C(11)	116.1(2)
C(2)-C(1)-C(11)	117.5(2)
C(12)-C(11)-C(16)	119.7(2)
C(12)-C(11)-C(1)	119.6(2)
C(16)-C(11)-C(1)	120.7(2)
C(11)-C(12)-C(13)	120.0(3)
C(14)-C(13)-C(12)	120.4(3)
C(13)-C(14)-C(15)	119.9(3)
C(14)-C(15)-C(16)	120.4(3)
C(15)-C(16)-C(11)	119.6(3)
C(3)-C(2)-C(1)	125.8(2)
C(3)-O(3)-Ni	126.27(14)
O(3)-C(3)-C(2)	124.8(2)
O(3)-C(3)-C(31)	114.27(19)
C(2)-C(3)-C(31)	120.84(19)
C(36)-C(31)-C(32)	117.6(2)
C(36)-C(31)-C(3)	118.4(2)
C(32)-C(31)-C(3)	123.9(2)
C(33)-C(32)-C(31)	120.9(2)
C(32)-C(33)-C(34)	120.8(2)
C(35)-C(34)-C(33)	118.9(2)
C(34)-C(35)-C(36)	120.2(2)
C(31)-C(36)-C(35)	121.6(2)
C(4)-O(4)-Ni	125.19(15)
O(4)-C(4)-C(5)	125.8(2)
O(4)-C(4)-C(41)	115.2(2)
C(5)-C(4)-C(41)	119.0(2)
C(42)-C(41)-C(46)	118.6(2)
C(42)-C(41)-C(4)	118.8(2)
C(46)-C(41)-C(4)	122.6(2)
C(41)-C(42)-C(43)	121.2(2)
C(44)-C(43)-C(42)	119.8(3)
C(45)-C(44)-C(43)	119.4(2)
C(44)-C(45)-C(46)	121.2(3)
C(45)-C(46)-C(41)	119.9(3)
C(6)-C(5)-C(4)	126.5(2)
C(6)-O(6)-Ni	125.41(14)
O(6)-C(6)-C(5)	125.1(2)
O(6)-C(6)-C(61)	114.9(2)
C(5)-C(6)-C(61)	120.0(2)
C(66)-C(61)-C(62)	118.6(2)
C(66)-C(61)-C(6)	118.8(2)
C(62)-C(61)-C(6)	122.6(2)
C(63)-C(62)-C(61)	120.0(3)
C(64)-C(63)-C(62)	120.5(3)
C(63)-C(64)-C(65)	120.2(3)
C(64)-C(65)-C(66)	119.7(3)
C(61)-C(66)-C(65)	121.0(2)
C(71)-N(7)-C(75)	117.0(2)
C(71)-N(7)-Ni	122.15(16)
C(75)-N(7)-Ni	120.86(16)
N(7)-C(71)-C(72)	123.2(2)
C(71)-C(72)-C(73)	120.1(2)
C(74)-C(73)-C(72)	116.7(2)
C(74)-C(73)-C(76)	121.1(2)
C(72)-C(73)-C(76)	122.2(2)
C(73)-C(74)-C(75)	120.0(2)
N(7)-C(75)-C(74)	123.1(2)

C(7Y)-C(76)-C(77)	117.9(2)
C(7Y)-C(76)-C(73)	120.5(2)
C(77)-C(76)-C(73)	121.6(2)
C(78)-C(77)-C(76)	120.6(2)
C(79)-C(78)-C(77)	120.4(3)
C(78)-C(79)-C(7X)	119.7(3)
C(7Y)-C(7X)-C(79)	120.1(2)
C(7X)-C(7Y)-C(76)	121.4(2)
C(85)-N(8)-C(81)	116.3(2)
C(85)-N(8)-Ni	120.90(17)
C(81)-N(8)-Ni	122.63(16)
N(8)-C(81)-C(82)	123.5(2)
C(81)-C(82)-C(83)	120.4(2)
C(84)-C(83)-C(82)	115.8(2)
C(84)-C(83)-C(86)	121.9(2)
C(82)-C(83)-C(86)	122.3(2)
C(85)-C(84)-C(83)	120.3(2)
N(8)-C(85)-C(84)	123.8(2)
C(87)-C(86)-C(8Y)	118.3(2)
C(87)-C(86)-C(83)	121.0(2)
C(8Y)-C(86)-C(83)	120.8(2)
C(88)-C(87)-C(86)	120.7(3)
C(87)-C(88)-C(89)	120.7(3)
C(8X)-C(89)-C(88)	119.6(3)
C(89)-C(8X)-C(8Y)	120.2(3)
C(8X)-C(8Y)-C(86)	120.5(3)
FA-C(1A)-C(2A)	120.01(18)
FA-C(1A)-C(6A)	118.92(18)
C(2A)-C(1A)-C(6A)	120.0
C(3A)-C(2A)-C(1A)	120.0
C(2A)-C(3A)-C(4A)	120.0
C(5A)-C(4A)-C(3A)	120.0
C(4A)-C(5A)-C(6A)	120.0
C(5A)-C(6A)-C(1A)	120.0
FB-C(1B)-C(2B)	119.1(2)
FB-C(1B)-C(6B)	120.7(2)
C(2B)-C(1B)-C(6B)	120.0
C(1B)-C(2B)-C(3B)	120.0
C(4B)-C(3B)-C(2B)	120.0
C(3B)-C(4B)-C(5B)	120.0
C(4B)-C(5B)-C(6B)	120.0
C(5B)-C(6B)-C(1B)	120.0
FC-C(1C)-C(2C)	119.55(19)
FC-C(1C)-C(6C)	118.59(19)
C(2C)-C(1C)-C(6C)	120.0
C(3C)-C(2C)-C(1C)	120.0
C(2C)-C(3C)-C(4C)	120.0
C(3C)-C(4C)-C(5C)	120.0
C(6C)-C(5C)-C(4C)	120.0
C(5C)-C(6C)-C(1C)	120.0
FD-C(1D)-C(2D)	119.1(3)
FD-C(1D)-C(6D)	119.4(3)
C(2D)-C(1D)-C(6D)	120.0
C(3D)-C(2D)-C(1D)	120.0
C(2D)-C(3D)-C(4D)	120.0
C(5D)-C(4D)-C(3D)	120.0
C(6D)-C(5D)-C(4D)	120.0
C(5D)-C(6D)-C(1D)	120.0

Table 17S. Anisotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(fluorobenzene).
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ni	19(1)	26(1)	19(1)	-4(1)	-4(1)	1(1)
O(1)	23(1)	31(1)	24(1)	-7(1)	-8(1)	2(1)
C(1)	22(1)	26(1)	27(1)	0(1)	-6(1)	-2(1)
C(11)	23(1)	36(2)	22(1)	3(1)	-5(1)	-3(1)
C(12)	40(2)	48(2)	34(2)	4(1)	-16(1)	-15(1)
C(13)	40(2)	84(3)	34(2)	3(2)	-17(1)	-28(2)
C(14)	25(1)	108(3)	38(2)	9(2)	-14(1)	-5(2)
C(15)	40(2)	67(2)	48(2)	5(2)	-17(2)	15(2)
C(16)	31(1)	45(2)	42(2)	-3(1)	-12(1)	2(1)
C(2)	22(1)	35(2)	28(1)	-10(1)	-8(1)	5(1)
O(3)	20(1)	28(1)	22(1)	-5(1)	-3(1)	-1(1)
C(3)	21(1)	23(1)	21(1)	-2(1)	-4(1)	-5(1)
C(31)	25(1)	22(1)	24(1)	-5(1)	-1(1)	-6(1)
C(32)	24(1)	45(2)	30(2)	-12(1)	-2(1)	-8(1)
C(33)	30(1)	48(2)	37(2)	-17(1)	6(1)	-14(1)
C(34)	51(2)	45(2)	22(1)	-11(1)	-2(1)	-17(1)
C(35)	45(2)	49(2)	31(2)	-12(1)	-16(1)	0(1)
C(36)	29(1)	40(2)	29(1)	-11(1)	-7(1)	1(1)
O(4)	20(1)	32(1)	23(1)	-6(1)	-4(1)	1(1)
C(4)	23(1)	23(1)	25(1)	-2(1)	-6(1)	-4(1)
C(41)	21(1)	31(1)	27(1)	-2(1)	-8(1)	0(1)
C(42)	27(1)	36(2)	32(2)	-5(1)	-10(1)	2(1)
C(43)	44(2)	58(2)	42(2)	-15(2)	-23(1)	1(1)
C(44)	32(2)	77(2)	48(2)	-10(2)	-25(1)	4(1)
C(45)	29(2)	66(2)	49(2)	-13(2)	-14(1)	13(1)
C(46)	30(1)	45(2)	37(2)	-11(1)	-10(1)	7(1)
C(5)	20(1)	40(2)	29(1)	-11(1)	-1(1)	-2(1)
O(6)	20(1)	29(1)	19(1)	-5(1)	-2(1)	-1(1)
C(6)	26(1)	21(1)	23(1)	-3(1)	-2(1)	-5(1)
C(61)	28(1)	31(1)	22(1)	-9(1)	0(1)	-11(1)
C(62)	28(1)	53(2)	36(2)	-22(1)	0(1)	-5(1)
C(63)	35(2)	77(2)	44(2)	-37(2)	7(1)	-8(2)
C(64)	56(2)	86(3)	24(2)	-26(2)	5(1)	-22(2)
C(65)	50(2)	65(2)	25(2)	-10(1)	-9(1)	-14(2)
C(66)	32(1)	40(2)	25(1)	-9(1)	-4(1)	-7(1)
N(7)	23(1)	31(1)	24(1)	-3(1)	-8(1)	-3(1)
C(71)	31(1)	34(2)	21(1)	-6(1)	-6(1)	-5(1)
C(72)	32(1)	31(2)	28(1)	-5(1)	-8(1)	-5(1)
C(73)	19(1)	30(1)	26(1)	0(1)	-11(1)	-4(1)
C(74)	28(1)	35(2)	19(1)	-2(1)	-4(1)	-7(1)
C(75)	30(1)	31(2)	25(1)	-6(1)	-7(1)	-4(1)
C(76)	24(1)	26(1)	32(1)	-3(1)	-9(1)	-1(1)
C(77)	50(2)	38(2)	28(2)	2(1)	-19(1)	-14(1)
C(78)	57(2)	36(2)	44(2)	-1(1)	-21(1)	-18(1)
C(79)	42(2)	33(2)	38(2)	-2(1)	-8(1)	-9(1)
C(7X)	38(1)	33(2)	28(1)	0(1)	-9(1)	-3(1)
C(7Y)	31(1)	27(1)	29(1)	-5(1)	-10(1)	-2(1)
N(8)	27(1)	31(1)	25(1)	-4(1)	-7(1)	-2(1)

C(81)	39(1)	32(2)	22(1)	-6(1)	-8(1)	-8(1)
C(82)	39(1)	34(2)	23(1)	-1(1)	-8(1)	-6(1)
C(83)	24(1)	29(1)	31(1)	-5(1)	-7(1)	0(1)
C(84)	41(2)	34(2)	26(1)	-6(1)	-10(1)	-11(1)
C(85)	38(1)	42(2)	21(1)	-1(1)	-11(1)	-11(1)
C(86)	23(1)	29(1)	31(1)	-7(1)	-3(1)	0(1)
C(87)	40(2)	34(2)	38(2)	-1(1)	-12(1)	-8(1)
C(88)	45(2)	36(2)	46(2)	4(1)	-12(1)	-8(1)
C(89)	37(2)	30(2)	54(2)	1(1)	-6(1)	-7(1)
C(8X)	30(1)	37(2)	58(2)	-14(1)	-7(1)	-6(1)
C(8Y)	30(1)	38(2)	41(2)	-6(1)	-10(1)	-2(1)
FA	63(3)	129(4)	79(3)	-36(3)	-37(2)	2(3)
FB	68(9)	71(9)	74(9)	5(9)	6(8)	3(8)
FC	120(4)	39(3)	106(4)	6(2)	-82(3)	0(2)
FD	66(10)	68(10)	65(10)	5(10)	-4(9)	-3(9)

Table 18S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(fluorobenzene).

	x	y	z	U(eq)
H(12)	8209	1771	3505	47
H(13)	9901	1273	4119	59
H(14)	11038	-408	4139	72
H(15)	10525	-1608	3529	68
H(16)	8906	-1112	2856	49
H(2)	8262	-127	1710	36
H(32)	8990	-209	345	40
H(33)	9582	-409	-1124	47
H(34)	8053	92	-1872	47
H(35)	5906	784	-1122	50
H(36)	5313	997	347	41
H(42)	1674	1932	1698	39
H(43)	67	2338	1021	56
H(44)	-1775	3620	1521	62
H(45)	-2004	4461	2706	62
H(46)	-432	4038	3405	47
H(5)	736	3104	4183	38
H(62)	287	3868	5296	48
H(63)	-305	4223	6740	65
H(64)	1080	3537	7559	67
H(65)	3088	2482	6948	56
H(66)	3694	2115	5507	39
H(71)	4611	3854	3375	35
H(72)	5102	5402	2776	37
H(74)	6274	4340	415	34
H(75)	5708	2831	1074	35
H(77)	6561	6409	2109	44
H(78)	7185	7898	1423	51
H(79)	7139	8419	10	47
H(7X)	6419	7458	-707	42
H(7Y)	5781	5984	-26	36
H(81)	4060	482	4605	37
H(82)	3723	-1103	5174	40
H(84)	3835	-1683	2808	39
H(85)	4154	-70	2306	40
H(87)	4266	-2805	5398	45
H(88)	3909	-4411	5930	53
H(89)	2916	-5223	5279	52
H(8X)	2276	-4412	4086	50
H(8Y)	2645	-2794	3530	44
H(2A)	8354	2083	-1102	59
H(3A)	9740	2430	-448	59
H(4A)	9907	4109	-472	59
H(5A)	8689	5442	-1150	59
H(6A)	7302	5096	-1804	59
H(2B)	9287	2333	-456	59
H(3B)	7668	2133	-971	59
H(4B)	6531	3532	-1645	59
H(5B)	7014	5132	-1804	59

H(6B)	8633	5332	-1290	59
H(2C)	7945	2278	-1083	59
H(3C)	7085	3759	-1829	59
H(4C)	7604	5301	-1794	59
H(5C)	8982	5362	-1014	59
H(6C)	9842	3881	-269	59
H(2D)	7124	4465	-2006	59
H(3D)	7712	2708	-1659	59
H(4D)	9096	2077	-807	59
H(5D)	9892	3203	-302	59
H(6D)	9305	4960	-648	59

Table 19S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [Ni(4-PhPy)2(DBM)2]*(chlorobenzene). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni	4665(1)	1767(1)	2870(1)	25(1)
O(1)	6316(2)	1284(1)	3180(1)	29(1)
C(1)	7307(2)	693(2)	2744(1)	27(1)
C(11)	8379(2)	373(2)	3131(1)	32(1)
C(12)	8691(3)	1064(2)	3512(2)	40(1)
C(13)	9665(3)	778(3)	3881(2)	52(1)
C(14)	10329(3)	-209(3)	3876(2)	62(1)
C(15)	10029(3)	-906(3)	3501(2)	61(1)
C(16)	9080(2)	-624(2)	3115(2)	43(1)
C(2)	7498(2)	349(2)	1936(1)	32(1)
O(3)	5532(1)	1175(1)	1710(1)	27(1)
C(3)	6670(2)	654(2)	1443(1)	26(1)
C(31)	7105(2)	413(2)	509(1)	28(1)
C(32)	8362(2)	-27(2)	52(2)	42(1)
C(33)	8724(3)	-161(2)	-822(2)	48(1)
C(34)	7845(3)	137(2)	-1261(2)	46(1)
C(35)	6588(3)	558(2)	-820(2)	47(1)
C(36)	6234(3)	695(2)	55(2)	37(1)
O(4)	3032(2)	2256(1)	2548(1)	29(1)
C(4)	1941(2)	2634(2)	3056(2)	29(1)
C(41)	859(2)	2905(2)	2676(2)	33(1)
C(42)	973(2)	2436(2)	1960(2)	38(1)
C(43)	22(3)	2681(2)	1573(2)	52(1)
C(44)	-1067(3)	3408(2)	1895(2)	56(1)
C(45)	-1186(3)	3892(2)	2601(2)	56(1)
C(46)	-244(2)	3641(2)	2998(2)	42(1)
C(5)	1680(2)	2802(2)	3928(1)	34(1)
O(6)	3785(2)	2345(1)	4037(1)	27(1)
C(6)	2575(2)	2660(2)	4364(1)	27(1)
C(61)	2143(2)	2899(2)	5298(2)	32(1)
C(62)	956(3)	3519(2)	5696(2)	46(1)
C(63)	633(3)	3712(2)	6552(2)	62(1)
C(64)	1450(3)	3317(3)	7027(2)	65(1)
C(65)	2615(3)	2703(2)	6641(2)	54(1)
C(66)	2954(3)	2497(2)	5785(2)	40(1)
N(7)	5216(2)	3155(1)	2297(1)	27(1)
C(71)	5057(2)	3920(2)	2771(1)	31(1)
C(72)	5353(2)	4839(2)	2411(2)	32(1)
C(73)	5846(2)	5012(2)	1515(1)	28(1)
C(74)	6026(2)	4215(2)	1031(1)	31(1)
C(75)	5702(2)	3320(2)	1432(1)	31(1)
C(76)	6151(2)	5995(2)	1101(2)	30(1)
C(77)	6504(3)	6633(2)	1518(2)	42(1)
C(78)	6800(3)	7541(2)	1116(2)	49(1)
C(79)	6751(3)	7830(2)	287(2)	43(1)
C(7X)	6397(3)	7219(2)	-137(2)	41(1)
C(7Y)	6093(2)	6312(2)	265(1)	32(1)

Structure of $[Ni(4\text{-}PhPy)_2(DBM)_2]$*(chlorobenzene) SUPPLEMENTARY

N(8)	4144(2)	369(1)	3411(1)	29(1)
C(81)	4019(2)	35(2)	4239(1)	33(1)
C(82)	3798(2)	-913(2)	4578(2)	36(1)
C(83)	3684(2)	-1571(2)	4060(2)	32(1)
C(84)	3818(2)	-1223(2)	3201(2)	37(1)
C(85)	4028(2)	-259(2)	2913(2)	35(1)
C(86)	3459(2)	-2603(2)	4391(2)	34(1)
C(87)	3858(3)	-3110(2)	5085(2)	42(1)
C(88)	3665(3)	-4074(2)	5376(2)	48(1)
C(89)	3059(3)	-4543(2)	5008(2)	49(1)
C(8X)	2647(3)	-4055(2)	4326(2)	50(1)
C(8Y)	2840(2)	-3087(2)	4021(2)	43(1)
ClA	7183(3)	3225(2)	-1968(2)	81(1)
C(1A)	8013(8)	3488(3)	-1357(5)	50(1)
C(2A)	8621(8)	2703(3)	-902(5)	50(1)
C(3A)	9412(7)	2893(5)	-483(5)	50(1)
C(4A)	9595(8)	3867(5)	-518(6)	50(1)
C(5A)	8987(10)	4652(4)	-972(6)	50(1)
C(6A)	8196(9)	4462(3)	-1392(6)	50(1)
ClB	10207(3)	4231(2)	-468(2)	86(1)
C(1B)	9102(9)	3999(3)	-873(7)	50(1)
C(2B)	8868(8)	3030(3)	-769(6)	50(1)
C(3B)	7970(7)	2837(4)	-1094(5)	50(1)
C(4B)	7305(6)	3612(5)	-1522(5)	50(1)
C(5B)	7539(7)	4580(5)	-1626(6)	50(1)
C(6B)	8437(9)	4774(4)	-1301(7)	50(1)
ClC	9692(5)	2064(3)	-514(3)	100(2)
C(1C)	8889(10)	3127(3)	-952(7)	50(1)
C(2C)	8015(9)	3054(5)	-1351(7)	50(1)
C(3C)	7360(9)	3920(6)	-1698(7)	50(1)
C(4C)	7581(11)	4860(5)	-1645(8)	50(1)
C(5C)	8455(13)	4933(4)	-1245(10)	50(1)
C(6C)	9110(13)	4067(4)	-899(10)	50(1)
ClD	7416(5)	5225(4)	-1968(3)	58(2)
C(1D)	8140(19)	4276(6)	-1374(13)	50(1)
C(2D)	8097(18)	3281(6)	-1419(12)	50(1)
C(3D)	8849(17)	2497(7)	-1058(11)	50(1)
C(4D)	9644(15)	2708(10)	-652(11)	50(1)
C(5D)	9687(18)	3704(11)	-607(13)	50(1)
C(6D)	8940(2)	4488(9)	-968(14)	50(1)