

Table 20S. Bond lengths [Å] and angles [deg] for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{chlorobenzene})$.

Ni-O(3)	2.0115(15)
Ni-O(6)	2.0146(15)
Ni-O(4)	2.0243(16)
Ni-O(1)	2.0311(16)
Ni-N(8)	2.1206(19)
Ni-N(7)	2.1303(19)
O(1)-C(1)	1.267(3)
C(1)-C(2)	1.405(3)
C(1)-C(11)	1.499(3)
C(11)-C(12)	1.380(3)
C(11)-C(16)	1.399(3)
C(12)-C(13)	1.382(3)
C(13)-C(14)	1.374(4)
C(14)-C(15)	1.372(4)
C(15)-C(16)	1.376(4)
C(2)-C(3)	1.389(3)
O(3)-C(3)	1.272(3)
C(3)-C(31)	1.505(3)
C(31)-C(36)	1.379(3)
C(31)-C(32)	1.391(3)
C(32)-C(33)	1.379(3)
C(33)-C(34)	1.371(4)
C(34)-C(35)	1.378(4)
C(35)-C(36)	1.384(3)
O(4)-C(4)	1.266(3)
C(4)-C(5)	1.403(3)
C(4)-C(41)	1.502(3)
C(41)-C(42)	1.376(3)
C(41)-C(46)	1.395(3)
C(42)-C(43)	1.378(3)
C(43)-C(44)	1.378(4)
C(44)-C(45)	1.371(4)
C(45)-C(46)	1.382(4)
C(5)-C(6)	1.391(3)
O(6)-C(6)	1.276(3)
C(6)-C(61)	1.503(3)
C(61)-C(66)	1.380(3)
C(61)-C(62)	1.399(3)
C(62)-C(63)	1.376(4)
C(63)-C(64)	1.370(4)
C(64)-C(65)	1.376(4)
C(65)-C(66)	1.379(3)
N(7)-C(71)	1.338(3)
N(7)-C(75)	1.344(3)
C(71)-C(72)	1.378(3)
C(72)-C(73)	1.390(3)
C(73)-C(74)	1.381(3)
C(73)-C(76)	1.481(3)
C(74)-C(75)	1.373(3)
C(76)-C(77)	1.389(3)
C(76)-C(7Y)	1.396(3)
C(77)-C(78)	1.379(3)
C(78)-C(79)	1.377(3)
C(79)-C(7X)	1.369(4)

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

SUPPLEMENTARY

C(7X)-C(7Y)	1.381(3)
N(8)-C(85)	1.329(3)
N(8)-C(81)	1.340(3)
C(81)-C(82)	1.381(3)
C(82)-C(83)	1.383(3)
C(83)-C(84)	1.390(3)
C(83)-C(86)	1.488(3)
C(84)-C(85)	1.383(3)
C(86)-C(8Y)	1.392(3)
C(86)-C(87)	1.395(3)
C(87)-C(88)	1.379(3)
C(88)-C(89)	1.367(4)
C(89)-C(8X)	1.378(4)
C(8X)-C(8Y)	1.387(3)
ClA-C(1A)	1.714(3)
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
ClB-C(1B)	1.713(3)
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
ClC-C(1C)	1.716(3)
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
ClD-C(1D)	1.719(4)
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)	179.22(7)
O(3)-Ni-O(4)	88.84(6)
O(6)-Ni-O(4)	90.95(6)
O(3)-Ni-O(1)	90.73(6)
O(6)-Ni-O(1)	89.48(6)
O(4)-Ni-O(1)	179.35(6)
O(3)-Ni-N(8)	89.31(7)
O(6)-Ni-N(8)	89.94(7)
O(4)-Ni-N(8)	91.30(7)
O(1)-Ni-N(8)	89.18(7)
O(3)-Ni-N(7)	89.27(7)
O(6)-Ni-N(7)	91.48(7)
O(4)-Ni-N(7)	88.78(7)
O(1)-Ni-N(7)	90.73(7)
N(8)-Ni-N(7)	178.57(8)
C(1)-O(1)-Ni	124.54(15)

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

SUPPLEMENTARY

O(1)-C(1)-C(2)	126.3(2)
O(1)-C(1)-C(11)	115.4(2)
C(2)-C(1)-C(11)	118.3(2)
C(12)-C(11)-C(16)	118.7(2)
C(12)-C(11)-C(1)	120.2(2)
C(16)-C(11)-C(1)	121.1(2)
C(11)-C(12)-C(13)	120.8(3)
C(14)-C(13)-C(12)	119.8(3)
C(15)-C(14)-C(13)	120.0(3)
C(14)-C(15)-C(16)	120.6(3)
C(15)-C(16)-C(11)	119.9(3)
C(3)-C(2)-C(1)	125.9(2)
C(3)-O(3)-Ni	126.46(14)
O(3)-C(3)-C(2)	124.9(2)
O(3)-C(3)-C(31)	114.3(2)
C(2)-C(3)-C(31)	120.7(2)
C(36)-C(31)-C(32)	117.3(2)
C(36)-C(31)-C(3)	118.7(2)
C(32)-C(31)-C(3)	123.9(2)
C(33)-C(32)-C(31)	121.3(2)
C(34)-C(33)-C(32)	120.4(3)
C(33)-C(34)-C(35)	119.5(2)
C(34)-C(35)-C(36)	119.7(3)
C(31)-C(36)-C(35)	121.8(2)
C(4)-O(4)-Ni	125.45(15)
O(4)-C(4)-C(5)	125.3(2)
O(4)-C(4)-C(41)	115.7(2)
C(5)-C(4)-C(41)	119.0(2)
C(42)-C(41)-C(46)	118.2(2)
C(42)-C(41)-C(4)	119.1(2)
C(46)-C(41)-C(4)	122.7(2)
C(41)-C(42)-C(43)	121.1(3)
C(44)-C(43)-C(42)	120.5(3)
C(45)-C(44)-C(43)	119.1(3)
C(44)-C(45)-C(46)	120.8(3)
C(45)-C(46)-C(41)	120.4(3)
C(6)-C(5)-C(4)	126.5(2)
C(6)-O(6)-Ni	124.98(15)
O(6)-C(6)-C(5)	125.5(2)
O(6)-C(6)-C(61)	114.4(2)
C(5)-C(6)-C(61)	120.1(2)
C(66)-C(61)-C(62)	118.3(2)
C(66)-C(61)-C(6)	118.8(2)
C(62)-C(61)-C(6)	122.9(2)
C(63)-C(62)-C(61)	119.6(3)
C(64)-C(63)-C(62)	121.7(3)
C(63)-C(64)-C(65)	119.0(3)
C(64)-C(65)-C(66)	120.2(3)
C(65)-C(66)-C(61)	121.2(3)
C(71)-N(7)-C(75)	116.4(2)
C(71)-N(7)-Ni	122.16(14)
C(75)-N(7)-Ni	121.37(16)
N(7)-C(71)-C(72)	123.1(2)
C(71)-C(72)-C(73)	120.4(2)
C(74)-C(73)-C(72)	116.2(2)
C(74)-C(73)-C(76)	121.7(2)
C(72)-C(73)-C(76)	122.2(2)
C(75)-C(74)-C(73)	120.4(2)
N(7)-C(75)-C(74)	123.5(2)

Structure of [Ni(4-PhPy)₂(DBM)₂]*(chlorobenzene)

SUPPLEMENTARY

C(77)-C(76)-C(7Y)	117.6(2)
C(77)-C(76)-C(73)	122.1(2)
C(7Y)-C(76)-C(73)	120.4(2)
C(78)-C(77)-C(76)	121.1(2)
C(79)-C(78)-C(77)	120.2(3)
C(7X)-C(79)-C(78)	119.9(2)
C(79)-C(7X)-C(7Y)	120.1(2)
C(7X)-C(7Y)-C(76)	121.1(2)
C(85)-N(8)-C(81)	116.5(2)
C(85)-N(8)-Ni	120.50(15)
C(81)-N(8)-Ni	122.73(16)
N(8)-C(81)-C(82)	123.3(2)
C(81)-C(82)-C(83)	120.2(2)
C(82)-C(83)-C(84)	116.3(2)
C(82)-C(83)-C(86)	122.4(2)
C(84)-C(83)-C(86)	121.3(2)
C(85)-C(84)-C(83)	119.9(2)
N(8)-C(85)-C(84)	123.7(2)
C(8Y)-C(86)-C(87)	118.2(2)
C(8Y)-C(86)-C(83)	121.1(2)
C(87)-C(86)-C(83)	120.7(2)
C(88)-C(87)-C(86)	120.3(3)
C(89)-C(88)-C(87)	121.1(3)
C(88)-C(89)-C(8X)	119.7(3)
C(89)-C(8X)-C(8Y)	119.9(3)
C(8X)-C(8Y)-C(86)	120.8(3)
C(2A)-C(1A)-C(6A)	120.0
C(2A)-C(1A)-ClA	119.54(15)
C(6A)-C(1A)-ClA	120.07(15)
C(1A)-C(2A)-C(3A)	120.0
C(4A)-C(3A)-C(2A)	120.0
C(3A)-C(4A)-C(5A)	120.0
C(4A)-C(5A)-C(6A)	120.0
C(5A)-C(6A)-C(1A)	120.0
C(2B)-C(1B)-C(6B)	120.0
C(2B)-C(1B)-ClB	119.69(14)
C(6B)-C(1B)-ClB	120.31(14)
C(3B)-C(2B)-C(1B)	120.0
C(4B)-C(3B)-C(2B)	120.0
C(3B)-C(4B)-C(5B)	120.0
C(6B)-C(5B)-C(4B)	120.0
C(5B)-C(6B)-C(1B)	120.0
C(2C)-C(1C)-C(6C)	120.0
C(2C)-C(1C)-ClC	120.37(15)
C(6C)-C(1C)-ClC	119.63(15)
C(1C)-C(2C)-C(3C)	120.0
C(2C)-C(3C)-C(4C)	120.0
C(5C)-C(4C)-C(3C)	120.0
C(4C)-C(5C)-C(6C)	120.0
C(5C)-C(6C)-C(1C)	120.0
C(2D)-C(1D)-C(6D)	120.0
C(2D)-C(1D)-ClD	119.55(19)
C(6D)-C(1D)-ClD	119.6(2)
C(1D)-C(2D)-C(3D)	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 21S. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{chlorobenzene})$.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ni	25(1)	29(1)	20(1)	-3(1)	-5(1)	-3(1)
O(1)	30(1)	32(1)	24(1)	-5(1)	-10(1)	-2(1)
C(1)	25(1)	31(1)	25(1)	1(1)	-7(1)	-8(1)
C(11)	25(1)	45(2)	23(1)	5(1)	-8(1)	-7(1)
C(12)	44(2)	50(2)	31(1)	8(1)	-17(1)	-19(1)
C(13)	50(2)	83(2)	36(2)	7(2)	-22(1)	-32(2)
C(14)	32(2)	115(3)	36(2)	17(2)	-16(1)	-13(2)
C(15)	44(2)	69(2)	57(2)	7(2)	-20(2)	10(2)
C(16)	33(2)	49(2)	46(2)	-4(1)	-16(1)	-2(1)
C(2)	25(1)	40(2)	28(1)	-8(1)	-6(1)	-1(1)
O(3)	25(1)	33(1)	21(1)	-5(1)	-6(1)	-2(1)
C(3)	24(1)	26(1)	25(1)	-4(1)	-2(1)	-6(1)
C(31)	31(1)	29(1)	24(1)	-5(1)	-4(1)	-9(1)
C(32)	29(2)	61(2)	35(2)	-20(1)	-2(1)	-11(1)
C(33)	32(2)	70(2)	37(2)	-23(1)	6(1)	-17(1)
C(34)	64(2)	48(2)	25(1)	-8(1)	-4(1)	-24(2)
C(35)	57(2)	50(2)	33(2)	-9(1)	-19(1)	-3(2)
C(36)	42(2)	40(2)	27(1)	-10(1)	-10(1)	0(1)
O(4)	25(1)	34(1)	23(1)	-3(1)	-5(1)	-1(1)
C(4)	30(2)	27(1)	30(1)	-1(1)	-8(1)	-7(1)
C(41)	28(1)	38(2)	28(1)	0(1)	-5(1)	-5(1)
C(42)	33(2)	44(2)	34(1)	-2(1)	-11(1)	-3(1)
C(43)	51(2)	62(2)	48(2)	-5(2)	-26(2)	-6(2)
C(44)	35(2)	76(2)	53(2)	3(2)	-22(2)	1(2)
C(45)	33(2)	70(2)	53(2)	-4(2)	-11(1)	6(2)
C(46)	33(2)	48(2)	40(2)	-9(1)	-9(1)	2(1)
C(5)	24(1)	44(2)	28(1)	-10(1)	-2(1)	-3(1)
O(6)	27(1)	32(1)	22(1)	-5(1)	-5(1)	-4(1)
C(6)	28(1)	26(1)	24(1)	-2(1)	-1(1)	-9(1)
C(61)	32(2)	35(1)	28(1)	-9(1)	0(1)	-16(1)
C(62)	32(2)	62(2)	41(2)	-24(1)	0(1)	-9(1)
C(63)	42(2)	89(2)	50(2)	-43(2)	10(2)	-18(2)
C(64)	61(2)	105(3)	32(2)	-33(2)	3(2)	-35(2)
C(65)	58(2)	80(2)	29(2)	-15(2)	-7(1)	-25(2)
C(66)	41(2)	52(2)	28(1)	-9(1)	-6(1)	-17(1)
N(7)	26(1)	32(1)	22(1)	-1(1)	-7(1)	-4(1)
C(71)	36(2)	35(1)	21(1)	-5(1)	-7(1)	-5(1)
C(72)	42(2)	29(1)	27(1)	-5(1)	-12(1)	-8(1)
C(73)	22(1)	36(1)	25(1)	2(1)	-11(1)	-6(1)
C(74)	36(2)	35(1)	20(1)	-2(1)	-7(1)	-8(1)
C(75)	38(2)	32(1)	23(1)	-4(1)	-8(1)	-7(1)
C(76)	26(1)	31(1)	29(1)	-3(1)	-7(1)	-4(1)
C(77)	62(2)	42(2)	32(1)	5(1)	-22(1)	-23(1)
C(78)	75(2)	41(2)	44(2)	2(1)	-26(2)	-31(2)
C(79)	55(2)	35(2)	38(2)	4(1)	-13(1)	-16(1)
C(7X)	53(2)	37(2)	34(1)	4(1)	-15(1)	-12(1)
C(7Y)	37(2)	35(1)	29(1)	-4(1)	-14(1)	-8(1)
N(8)	31(1)	33(1)	25(1)	-3(1)	-11(1)	-5(1)

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

SUPPLEMENTARY

C(81)	42(2)	32(1)	24(1)	-3(1)	-10(1)	-8(1)
C(82)	44(2)	35(2)	26(1)	0(1)	-10(1)	-7(1)
C(83)	29(1)	32(1)	32(1)	-1(1)	-8(1)	-5(1)
C(84)	45(2)	41(2)	31(1)	-7(1)	-14(1)	-13(1)
C(85)	41(2)	41(2)	27(1)	2(1)	-14(1)	-13(1)
C(86)	27(1)	31(1)	39(1)	-5(1)	-5(1)	-5(1)
C(87)	45(2)	38(2)	41(2)	2(1)	-10(1)	-14(1)
C(88)	51(2)	38(2)	51(2)	6(1)	-13(2)	-13(1)
C(89)	46(2)	33(2)	58(2)	4(1)	-5(2)	-11(1)
C(8X)	33(2)	42(2)	73(2)	-16(2)	-10(2)	-10(1)
C(8Y)	37(2)	37(2)	55(2)	-4(1)	-15(1)	-6(1)
ClA	53(2)	124(3)	70(2)	-30(2)	-28(1)	-3(2)
ClB	80(2)	115(3)	71(2)	4(2)	-35(2)	-26(2)
ClC	160(5)	57(3)	112(4)	11(2)	-90(4)	-19(3)
ClD	34(3)	79(4)	52(4)	2(3)	-17(2)	7(3)

Table 22S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{chlorobenzene})$.

	x	y	z	U(eq)
H(12)	8230	1746	3520	48
H(13)	9875	1262	4137	62
H(14)	10996	-408	4133	75
H(15)	10482	-1589	3508	73
H(16)	8900	-1106	2839	52
H(2)	8263	-136	1705	39
H(32)	8982	-239	347	50
H(33)	9589	-461	-1121	57
H(34)	8100	53	-1865	55
H(35)	5967	753	-1116	56
H(36)	5367	992	352	45
H(42)	1720	1936	1728	45
H(43)	118	2346	1081	62
H(44)	-1727	3571	1632	67
H(45)	-1925	4405	2819	67
H(46)	-348	3973	3494	51
H(5)	805	3035	4253	40
H(62)	377	3805	5378	55
H(63)	-177	4129	6820	74
H(64)	1215	3466	7615	78
H(65)	3188	2420	6965	65
H(66)	3761	2070	5526	48
H(71)	4725	3824	3385	38
H(72)	5219	5359	2776	39
H(74)	6376	4285	416	37
H(75)	5828	2789	1079	38
H(77)	6541	6441	2090	51
H(78)	7039	7967	1412	58
H(79)	6961	8453	10	52
H(7X)	6361	7418	-708	49
H(7Y)	5840	5897	-32	39
H(81)	4086	472	4611	39
H(82)	3724	-1113	5169	43
H(84)	3766	-1646	2811	44
H(85)	4093	-34	2327	42
H(87)	4264	-2790	5358	50
H(88)	3959	-4417	5840	58
H(89)	2922	-5204	5221	59
H(8X)	2230	-4380	4065	59
H(8Y)	2547	-2751	3555	51
H(2A)	8496	2037	-879	60
H(3A)	9828	2356	-173	60
H(4A)	10136	3997	-231	60
H(5A)	9112	5318	-996	60
H(6A)	7780	4999	-1702	60
H(2B)	9323	2500	-477	60
H(3B)	7811	2175	-1023	60
H(4B)	6691	3480	-1744	60
H(5B)	7084	5110	-1918	60

Structure of [Ni(4-PhPy)₂(DBM)₂]*(chlorobenzene)**SUPPLEMENTARY**

H(6B)	8596	5436	-1371	60
H(2C)	7864	2412	-1388	60
H(3C)	6763	3870	-1971	60
H(4C)	7133	5452	-1882	60
H(5C)	8606	5576	-1209	60
H(6C)	9707	4117	-626	60
H(2D)	7554	3136	-1696	60
H(3D)	8819	1816	-1088	60
H(4D)	10157	2172	-405	60
H(5D)	10230	3848	-330	60
H(6D)	8965	5168	-938	60

Table 23S. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{bromobenzene})$.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	4705(1)	1769(1)	2885(1)	23(1)
O(1)	6341(1)	1285(1)	3191(1)	29(1)
C(1)	7319(2)	700(2)	2754(1)	28(1)
C(11)	8396(2)	382(2)	3127(1)	31(1)
C(12)	8692(2)	1080(2)	3526(1)	39(1)
C(13)	9672(2)	794(2)	3892(2)	51(1)
C(14)	10328(2)	-185(3)	3876(2)	59(1)
C(15)	10030(2)	-881(2)	3484(2)	58(1)
C(16)	9080(2)	-597(2)	3103(2)	44(1)
C(2)	7512(2)	356(2)	1935(1)	34(1)
O(3)	5555(1)	1179(1)	1719(1)	27(1)
C(3)	6682(2)	655(1)	1450(1)	27(1)
C(31)	7107(2)	407(2)	513(1)	30(1)
C(32)	8358(2)	-45(2)	58(2)	54(1)
C(33)	8706(2)	-181(2)	-826(2)	57(1)
C(34)	7838(2)	105(2)	-1262(1)	45(1)
C(35)	6599(2)	536(2)	-814(1)	43(1)
C(36)	6239(2)	685(2)	66(1)	35(1)
O(4)	3076(1)	2267(1)	2573(1)	28(1)
C(4)	1993(2)	2627(1)	3096(1)	26(1)
C(41)	911(2)	2901(2)	2727(1)	29(1)
C(42)	1017(2)	2447(2)	1993(1)	36(1)
C(43)	63(2)	2701(2)	1614(2)	49(1)
C(44)	-1019(2)	3424(2)	1962(2)	53(1)
C(45)	-1133(2)	3881(2)	2685(2)	53(1)
C(46)	-186(2)	3626(2)	3073(1)	41(1)
C(5)	1734(2)	2774(2)	3978(1)	31(1)
O(6)	3845(1)	2339(1)	4060(1)	27(1)
C(6)	2641(2)	2635(1)	4402(1)	25(1)
C(61)	2215(2)	2843(2)	5346(1)	28(1)
C(62)	1038(2)	3449(2)	5767(1)	41(1)
C(63)	722(2)	3622(2)	6638(2)	55(1)
C(64)	1543(2)	3203(2)	7096(2)	57(1)
C(65)	2704(2)	2599(2)	6689(1)	50(1)
C(66)	3028(2)	2423(2)	5818(1)	36(1)
N(7)	5291(1)	3141(1)	2310(1)	27(1)
C(71)	5130(2)	3912(2)	2785(1)	31(1)
C(72)	5411(2)	4835(2)	2427(1)	32(1)
C(73)	5887(2)	5009(2)	1525(1)	27(1)
C(74)	6076(2)	4198(2)	1040(1)	31(1)
C(75)	5768(2)	3301(2)	1443(1)	31(1)
C(76)	6145(2)	5993(2)	1107(1)	29(1)
C(77)	6463(2)	6664(2)	1523(1)	43(1)
C(78)	6709(3)	7579(2)	1123(2)	52(1)
C(79)	6656(2)	7847(2)	288(1)	42(1)
C(7X)	6337(2)	7195(2)	-133(1)	38(1)
C(7Y)	6074(2)	6284(2)	274(1)	32(1)

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

SUPPLEMENTARY

N(8)	4141(2)	385(1)	3412(1)	28(1)
C(81)	4022(2)	39(2)	4238(1)	31(1)
C(82)	3779(2)	-902(2)	4568(1)	32(1)
C(83)	3656(2)	-1550(2)	4033(1)	30(1)
C(84)	3779(2)	-1187(2)	3176(1)	34(1)
C(85)	4008(2)	-234(2)	2902(1)	33(1)
C(86)	3426(2)	-2576(2)	4348(1)	33(1)
C(87)	3841(2)	-3093(2)	5025(1)	38(1)
C(88)	3650(2)	-4061(2)	5298(2)	45(1)
C(89)	3035(2)	-4529(2)	4916(2)	49(1)
C(8X)	2604(2)	-4028(2)	4253(2)	48(1)
C(8Y)	2795(2)	-3058(2)	3969(2)	41(1)
BrA	7203(5)	3422(8)	-1937(4)	144(4)
C(1A)	8322(7)	3519(7)	-1327(5)	44(1)
C(2A)	8961(14)	2655(9)	-993(11)	44(1)
C(3A)	9779(16)	2725(13)	-547(12)	44(1)
C(4A)	9958(15)	3659(15)	-434(11)	44(1)
C(5A)	9318(18)	4523(13)	-767(13)	44(1)
C(6A)	8500(15)	4453(9)	-1213(11)	44(1)
BrB	10205(1)	4276(1)	-438(1)	77(1)
C(1B)	9009(5)	4032(2)	-924(4)	44(1)
C(2B)	8773(4)	3069(2)	-847(3)	44(1)
C(3B)	7887(4)	2880(2)	-1187(3)	44(1)
C(4B)	7236(4)	3655(3)	-1604(3)	44(1)
C(5B)	7471(4)	4618(3)	-1681(3)	44(1)
C(6B)	8358(5)	4807(2)	-1341(4)	44(1)
BrC	9619(1)	2042(1)	-498(1)	73(1)
C(1C)	8762(5)	3197(2)	-1000(4)	44(1)
C(2C)	7886(4)	3129(2)	-1400(3)	44(1)
C(3C)	7281(5)	3987(3)	-1763(4)	44(1)
C(4C)	7554(5)	4913(3)	-1726(4)	44(1)
C(5C)	8430(6)	4982(2)	-1327(5)	44(1)
C(6C)	9034(6)	4123(2)	-964(5)	44(1)
BrD	7378(2)	5094(2)	-1978(2)	71(1)
C(1D)	8232(4)	4118(4)	-1324(3)	44(1)
C(2D)	8041(10)	3138(4)	-1206(7)	44(1)
C(3D)	8667(11)	2425(5)	-728(8)	44(1)
C(4D)	9483(10)	2692(7)	-367(7)	44(1)
C(5D)	9674(11)	3672(8)	-485(8)	44(1)
C(6D)	9048(9)	4386(6)	-963(7)	44(1)

Table 24S. Bond lengths [Å] and angles [deg] for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{bromobenzene})$.

Ni-O(3)	2.0113(12)
Ni-O(6)	2.0123(12)
Ni-O(4)	2.0280(13)
Ni-O(1)	2.0287(13)
Ni-N(8)	2.1220(17)
Ni-N(7)	2.1308(16)
O(1)-C(1)	1.262(2)
C(1)-C(2)	1.416(3)
C(1)-C(11)	1.499(3)
C(11)-C(16)	1.388(3)
C(11)-C(12)	1.390(3)
C(12)-C(13)	1.393(3)
C(13)-C(14)	1.379(4)
C(14)-C(15)	1.380(4)
C(15)-C(16)	1.380(3)
C(2)-C(3)	1.392(3)
O(3)-C(3)	1.273(2)
C(3)-C(31)	1.507(2)
C(31)-C(36)	1.378(3)
C(31)-C(32)	1.397(3)
C(32)-C(33)	1.394(3)
C(33)-C(34)	1.363(4)
C(34)-C(35)	1.375(3)
C(35)-C(36)	1.389(3)
O(4)-C(4)	1.265(2)
C(4)-C(5)	1.407(3)
C(4)-C(41)	1.501(3)
C(41)-C(42)	1.387(3)
C(41)-C(46)	1.401(3)
C(42)-C(43)	1.380(3)
C(43)-C(44)	1.390(3)
C(44)-C(45)	1.371(4)
C(45)-C(46)	1.383(3)
C(5)-C(6)	1.393(3)
O(6)-C(6)	1.275(2)
C(6)-C(61)	1.504(2)
C(61)-C(66)	1.381(3)
C(61)-C(62)	1.402(3)
C(62)-C(63)	1.389(3)
C(63)-C(64)	1.371(4)
C(64)-C(65)	1.384(3)
C(65)-C(66)	1.388(3)
N(7)-C(71)	1.342(2)
N(7)-C(75)	1.344(2)
C(71)-C(72)	1.381(3)
C(72)-C(73)	1.396(3)
C(73)-C(74)	1.393(3)
C(73)-C(76)	1.475(3)
C(74)-C(75)	1.376(3)
C(76)-C(77)	1.391(3)
C(76)-C(7Y)	1.395(3)
C(77)-C(78)	1.379(3)
C(78)-C(79)	1.387(3)
C(79)-C(7X)	1.378(3)
C(7X)-C(7Y)	1.380(3)

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

SUPPLEMENTARY

N(8)-C(85)	1.338(2)
N(8)-C(81)	1.345(2)
C(81)-C(82)	1.381(3)
C(82)-C(83)	1.392(3)
C(83)-C(84)	1.397(3)
C(83)-C(86)	1.483(3)
C(84)-C(85)	1.378(3)
C(86)-C(87)	1.396(3)
C(86)-C(8Y)	1.403(3)
C(87)-C(88)	1.385(3)
C(88)-C(89)	1.381(4)
C(89)-C(8X)	1.378(4)
C(8X)-C(8Y)	1.391(3)
BrA-C(1A)	1.901(3)
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
BrB-C(1B)	1.900(2)
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
BrC-C(1C)	1.903(2)
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
BrD-C(1D)	1.900(3)
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)	179.06(5)
O(3)-Ni-O(4)	89.17(5)
O(6)-Ni-O(4)	90.84(5)
O(3)-Ni-O(1)	90.82(5)
O(6)-Ni-O(1)	89.18(5)
O(4)-Ni-O(1)	179.39(5)
O(3)-Ni-N(8)	88.97(6)
O(6)-Ni-N(8)	90.09(6)
O(4)-Ni-N(8)	91.06(6)
O(1)-Ni-N(8)	89.55(6)
O(3)-Ni-N(7)	89.04(6)
O(6)-Ni-N(7)	91.90(6)
O(4)-Ni-N(7)	88.51(6)
O(1)-Ni-N(7)	90.88(6)
N(8)-Ni-N(7)	177.96(6)
C(1)-O(1)-Ni	124.92(12)
O(1)-C(1)-C(2)	126.14(17)

Structure of [Ni(4-PhPy)₂(DBM)₂]*(bromobenzene)

SUPPLEMENTARY

O(1)-C(1)-C(11)	116.31(16)
C(2)-C(1)-C(11)	117.49(16)
C(16)-C(11)-C(12)	119.3(2)
C(16)-C(11)-C(1)	121.64(19)
C(12)-C(11)-C(1)	119.05(19)
C(11)-C(12)-C(13)	119.9(2)
C(14)-C(13)-C(12)	120.1(2)
C(13)-C(14)-C(15)	120.1(2)
C(14)-C(15)-C(16)	120.1(3)
C(15)-C(16)-C(11)	120.5(2)
C(3)-C(2)-C(1)	125.53(17)
C(3)-O(3)-Ni	126.34(12)
O(3)-C(3)-C(2)	125.18(16)
O(3)-C(3)-C(31)	114.22(16)
C(2)-C(3)-C(31)	120.53(16)
C(36)-C(31)-C(32)	117.91(18)
C(36)-C(31)-C(3)	118.62(17)
C(32)-C(31)-C(3)	123.37(19)
C(33)-C(32)-C(31)	120.1(2)
C(34)-C(33)-C(32)	121.3(2)
C(33)-C(34)-C(35)	118.9(2)
C(34)-C(35)-C(36)	120.6(2)
C(31)-C(36)-C(35)	121.2(2)
C(4)-O(4)-Ni	125.22(12)
O(4)-C(4)-C(5)	125.65(17)
O(4)-C(4)-C(41)	115.69(16)
C(5)-C(4)-C(41)	118.65(16)
C(42)-C(41)-C(46)	118.43(19)
C(42)-C(41)-C(4)	118.91(17)
C(46)-C(41)-C(4)	122.61(18)
C(43)-C(42)-C(41)	120.9(2)
C(42)-C(43)-C(44)	120.2(2)
C(45)-C(44)-C(43)	119.5(2)
C(44)-C(45)-C(46)	120.7(2)
C(45)-C(46)-C(41)	120.3(2)
C(6)-C(5)-C(4)	125.80(17)
C(6)-O(6)-Ni	124.99(12)
O(6)-C(6)-C(5)	125.77(16)
O(6)-C(6)-C(61)	114.67(16)
C(5)-C(6)-C(61)	119.56(16)
C(66)-C(61)-C(62)	118.52(18)
C(66)-C(61)-C(6)	118.31(16)
C(62)-C(61)-C(6)	123.17(18)
C(63)-C(62)-C(61)	119.8(2)
C(64)-C(63)-C(62)	120.9(2)
C(63)-C(64)-C(65)	119.8(2)
C(64)-C(65)-C(66)	119.7(2)
C(61)-C(66)-C(65)	121.3(2)
C(71)-N(7)-C(75)	116.36(17)
C(71)-N(7)-Ni	122.22(12)
C(75)-N(7)-Ni	121.30(13)
N(7)-C(71)-C(72)	123.55(17)
C(71)-C(72)-C(73)	120.21(18)
C(74)-C(73)-C(72)	115.80(18)
C(74)-C(73)-C(76)	121.66(17)
C(72)-C(73)-C(76)	122.52(18)
C(75)-C(74)-C(73)	120.63(17)
N(7)-C(75)-C(74)	123.42(18)
C(77)-C(76)-C(7Y)	117.64(19)

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

SUPPLEMENTARY

C(77)-C(76)-C(73)	121.70(18)
C(7Y)-C(76)-C(73)	120.66(18)
C(78)-C(77)-C(76)	121.2(2)
C(77)-C(78)-C(79)	120.3(2)
C(7X)-C(79)-C(78)	119.4(2)
C(79)-C(7X)-C(7Y)	120.2(2)
C(7X)-C(7Y)-C(76)	121.32(19)
C(85)-N(8)-C(81)	116.49(17)
C(85)-N(8)-Ni	120.39(13)
C(81)-N(8)-Ni	122.81(13)
N(8)-C(81)-C(82)	123.61(18)
C(81)-C(82)-C(83)	119.85(18)
C(82)-C(83)-C(84)	116.39(19)
C(82)-C(83)-C(86)	122.10(18)
C(84)-C(83)-C(86)	121.51(18)
C(85)-C(84)-C(83)	120.06(18)
N(8)-C(85)-C(84)	123.60(18)
C(87)-C(86)-C(8Y)	118.2(2)
C(87)-C(86)-C(83)	120.86(19)
C(8Y)-C(86)-C(83)	120.96(19)
C(88)-C(87)-C(86)	120.3(2)
C(89)-C(88)-C(87)	120.9(2)
C(8X)-C(89)-C(88)	119.8(2)
C(89)-C(8X)-C(8Y)	120.0(2)
C(8X)-C(8Y)-C(86)	120.9(2)
C(2A)-C(1A)-C(6A)	120.0
C(2A)-C(1A)-BrA	119.96(15)
C(6A)-C(1A)-BrA	120.04(15)
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(6A)-C(5A)-C(4A)	120.0
C(5A)-C(6A)-C(1A)	120.0
C(2B)-C(1B)-C(6B)	120.0
C(2B)-C(1B)-BrB	119.21(13)
C(6B)-C(1B)-BrB	120.78(13)
C(1B)-C(2B)-C(3B)	120.0
C(4B)-C(3B)-C(2B)	120.0
C(5B)-C(4B)-C(3B)	120.0
C(4B)-C(5B)-C(6B)	120.0
C(5B)-C(6B)-C(1B)	120.0
C(2C)-C(1C)-C(6C)	120.0
C(2C)-C(1C)-BrC	121.54(13)
C(6C)-C(1C)-BrC	118.46(13)
C(3C)-C(2C)-C(1C)	120.0
C(2C)-C(3C)-C(4C)	120.0
C(5C)-C(4C)-C(3C)	120.0
C(4C)-C(5C)-C(6C)	120.0
C(5C)-C(6C)-C(1C)	120.0
C(2D)-C(1D)-C(6D)	120.0
C(2D)-C(1D)-BrD	120.07(15)
C(6D)-C(1D)-BrD	119.93(15)
C(1D)-C(2D)-C(3D)	120.0
C(4D)-C(3D)-C(2D)	120.0
C(3D)-C(4D)-C(5D)	120.0
C(4D)-C(5D)-C(6D)	120.0
C(5D)-C(6D)-C(1D)	120.0

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

SUPPLEMENTARY

Table 25S. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{bromobenzene})$.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ni	22(1)	28(1)	18(1)	-4(1)	-5(1)	-1(1)
O(1)	28(1)	34(1)	25(1)	-8(1)	-10(1)	1(1)
C(1)	24(1)	33(1)	27(1)	-2(1)	-8(1)	-4(1)
C(11)	23(1)	44(1)	25(1)	1(1)	-8(1)	-6(1)
C(12)	39(1)	51(1)	30(1)	4(1)	-15(1)	-14(1)
C(13)	46(1)	83(2)	34(1)	7(1)	-20(1)	-29(1)
C(14)	30(1)	106(2)	35(1)	13(1)	-15(1)	-6(1)
C(15)	40(1)	68(2)	53(2)	5(1)	-18(1)	13(1)
C(16)	34(1)	49(1)	45(1)	-6(1)	-15(1)	4(1)
C(2)	24(1)	43(1)	33(1)	-15(1)	-9(1)	4(1)
O(3)	24(1)	33(1)	23(1)	-8(1)	-7(1)	0(1)
C(3)	25(1)	32(1)	24(1)	-8(1)	-4(1)	-6(1)
C(31)	28(1)	36(1)	26(1)	-11(1)	-4(1)	-8(1)
C(32)	26(1)	94(2)	43(1)	-37(1)	-5(1)	-3(1)
C(33)	34(1)	92(2)	43(1)	-38(1)	7(1)	-16(1)
C(34)	58(1)	51(1)	24(1)	-12(1)	0(1)	-22(1)
C(35)	59(1)	43(1)	26(1)	-6(1)	-16(1)	-6(1)
C(36)	39(1)	37(1)	26(1)	-8(1)	-9(1)	-1(1)
O(4)	24(1)	33(1)	22(1)	-4(1)	-7(1)	-1(1)
C(4)	25(1)	25(1)	26(1)	-2(1)	-6(1)	-3(1)
C(41)	25(1)	33(1)	27(1)	0(1)	-8(1)	-3(1)
C(42)	34(1)	41(1)	32(1)	-3(1)	-13(1)	-1(1)
C(43)	47(1)	64(2)	43(1)	-6(1)	-26(1)	-5(1)
C(44)	33(1)	80(2)	47(1)	2(1)	-22(1)	-1(1)
C(45)	30(1)	68(2)	49(1)	-2(1)	-12(1)	10(1)
C(46)	31(1)	51(1)	36(1)	-7(1)	-10(1)	5(1)
C(5)	23(1)	40(1)	26(1)	-8(1)	-4(1)	-1(1)
O(6)	24(1)	34(1)	21(1)	-6(1)	-5(1)	-3(1)
C(6)	27(1)	24(1)	22(1)	-5(1)	-3(1)	-5(1)
C(61)	26(1)	34(1)	23(1)	-10(1)	-1(1)	-10(1)
C(62)	29(1)	55(1)	36(1)	-20(1)	-4(1)	-4(1)
C(63)	36(1)	80(2)	43(1)	-37(1)	5(1)	-6(1)
C(64)	47(1)	98(2)	28(1)	-29(1)	1(1)	-21(1)
C(65)	45(1)	80(2)	26(1)	-16(1)	-9(1)	-14(1)
C(66)	34(1)	51(1)	23(1)	-9(1)	-5(1)	-9(1)
N(7)	25(1)	33(1)	21(1)	-3(1)	-6(1)	-4(1)
C(71)	36(1)	35(1)	22(1)	-2(1)	-10(1)	-7(1)
C(72)	39(1)	33(1)	25(1)	-5(1)	-11(1)	-7(1)
C(73)	22(1)	34(1)	25(1)	-1(1)	-9(1)	-4(1)
C(74)	32(1)	35(1)	21(1)	-4(1)	-4(1)	-6(1)
C(75)	34(1)	33(1)	23(1)	-6(1)	-5(1)	-6(1)
C(76)	27(1)	33(1)	26(1)	-3(1)	-8(1)	-3(1)
C(77)	68(2)	41(1)	33(1)	4(1)	-26(1)	-21(1)
C(78)	84(2)	41(1)	43(1)	3(1)	-30(1)	-26(1)
C(79)	57(1)	31(1)	37(1)	4(1)	-16(1)	-10(1)
C(7X)	47(1)	36(1)	30(1)	2(1)	-14(1)	-5(1)
C(7Y)	37(1)	34(1)	27(1)	-5(1)	-12(1)	-5(1)
N(8)	29(1)	31(1)	22(1)	-4(1)	-10(1)	-2(1)

SUPPLEMENTARY

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

C(81)	38(1)	31(1)	24(1)	-4(1)	-11(1)	-6(1)
C(82)	37(1)	34(1)	23(1)	0(1)	-9(1)	-4(1)
C(83)	27(1)	30(1)	30(1)	-5(1)	-8(1)	-2(1)
C(84)	42(1)	36(1)	29(1)	-5(1)	-15(1)	-10(1)
C(85)	40(1)	38(1)	24(1)	-1(1)	-14(1)	-9(1)
C(86)	28(1)	31(1)	34(1)	-3(1)	-6(1)	-3(1)
C(87)	39(1)	35(1)	37(1)	2(1)	-9(1)	-10(1)
C(88)	47(1)	37(1)	47(1)	6(1)	-12(1)	-9(1)
C(89)	44(1)	33(1)	57(2)	-2(1)	-2(1)	-10(1)
C(8X)	40(1)	41(1)	62(2)	-13(1)	-9(1)	-13(1)
C(8Y)	37(1)	38(1)	47(1)	-6(1)	-14(1)	-6(1)
BrA	49(3)	288(11)	74(4)	-11(5)	-18(2)	5(4)
BrB	80(1)	103(1)	51(1)	-3(1)	-30(1)	-12(1)
BrC	112(1)	50(1)	72(1)	8(1)	-56(1)	-8(1)
BrD	36(1)	120(3)	45(1)	-17(1)	-16(1)	15(1)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{bromobenzene})$

SUPPLEMENTARY

Table 26S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{bromobenzene})$.

	x	y	z	U(eq)
H(12)	8227	1751	3550	46
H(13)	9889	1275	4152	61
H(14)	10985	-382	4135	70
H(15)	10480	-1556	3476	69
H(16)	8893	-1075	2822	53
H(2)	8273	-118	1696	41
H(32)	8974	-261	351	65
H(33)	9563	-478	-1132	69
H(34)	8085	9	-1864	54
H(35)	5984	734	-1109	51
H(36)	5379	984	364	42
H(42)	1755	1956	1747	43
H(43)	146	2381	1114	59
H(44)	-1675	3601	1701	64
H(45)	-1869	4377	2923	63
H(46)	-280	3945	3577	50
H(5)	863	2986	4314	37
H(62)	459	3741	5458	49
H(63)	-75	4036	6920	66
H(64)	1316	3328	7692	69
H(65)	3276	2305	7003	60
H(66)	3826	2007	5542	43
H(71)	4806	3818	3400	37
H(72)	5281	5354	2795	38
H(74)	6421	4264	424	37
H(75)	5900	2767	1090	37
H(77)	6512	6487	2092	52
H(78)	6914	8030	1420	62
H(79)	6838	8473	9	50
H(7X)	6298	7373	-705	46
H(7Y)	5840	5847	-20	39
H(81)	4109	464	4615	37
H(82)	3697	-1106	5159	38
H(84)	3705	-1598	2782	41
H(85)	4074	-4	2318	40
H(87)	4256	-2780	5300	46
H(88)	3947	-4409	5754	54
H(89)	2910	-5193	5108	58
H(8X)	2177	-4346	3991	57
H(8Y)	2494	-2716	3513	49
H(2A)	8839	2017	-1071	53
H(3A)	10216	2135	-319	53
H(4A)	10517	3707	-128	53
H(5A)	9441	5161	-689	53
H(6A)	8063	5043	-1441	53
H(2B)	9218	2540	-562	53
H(3B)	7725	2222	-1134	53
H(4B)	6629	3526	-1836	53
H(5B)	7027	5148	-1966	53
H(6B)	8520	5465	-1393	53

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

SUPPLEMENTARY

H(2C)	7700	2496	-1425	53
H(3C)	6682	3941	-2036	53
H(4C)	7141	5500	-1975	53
H(5C)	8616	5615	-1302	53
H(6C)	9634	4170	-691	53
H(2D)	7483	2955	-1452	53
H(3D)	8536	1754	-647	53
H(4D)	9911	2205	-40	53
H(5D)	10232	3855	-238	53
H(6D)	9179	5056	-1044	53

Table 27S. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{toluene})$.U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	4663 (1)	1784 (1)	2861 (1)	24 (1)
O(1)	6316 (2)	1297 (1)	3176 (1)	29 (1)
C(1)	7298 (2)	698 (2)	2747 (2)	28 (1)
C(11)	8379 (2)	357 (2)	3136 (2)	31 (1)
C(12)	8700 (3)	1046 (2)	3511 (2)	41 (1)
C(13)	9686 (3)	748 (3)	3872 (2)	55 (1)
C(14)	10319 (3)	-245 (3)	3886 (2)	65 (1)
C(15)	10004 (3)	-932 (3)	3517 (2)	64 (1)
C(16)	9047 (3)	-631 (2)	3131 (2)	46 (1)
C(2)	7501 (2)	348 (2)	1933 (2)	32 (1)
O(3)	5541 (2)	1199 (1)	1696 (1)	26 (1)
C(3)	6671 (2)	661 (2)	1437 (1)	26 (1)
C(31)	7106 (2)	406 (2)	505 (1)	29 (1)
C(32)	8375 (3)	-36 (2)	45 (2)	46 (1)
C(33)	8728 (3)	-170 (2)	-832 (2)	55 (1)
C(34)	7851 (3)	125 (2)	-1277 (2)	50 (1)
C(35)	6590 (3)	550 (2)	-830 (2)	48 (1)
C(36)	6232 (3)	693 (2)	48 (2)	38 (1)
O(4)	3025 (2)	2264 (1)	2540 (1)	28 (1)
C(4)	1927 (2)	2639 (2)	3051 (2)	27 (1)
C(41)	842 (2)	2897 (2)	2674 (2)	33 (1)
C(42)	972 (3)	2419 (2)	1956 (2)	39 (1)
C(43)	8 (3)	2653 (2)	1571 (2)	56 (1)
C(44)	-1100 (3)	3374 (3)	1906 (2)	58 (1)
C(45)	-1227 (3)	3849 (3)	2606 (2)	59 (1)
C(46)	-275 (3)	3619 (2)	3004 (2)	45 (1)
C(5)	1664 (2)	2816 (2)	3925 (2)	35 (1)
O(6)	3776 (2)	2357 (1)	4031 (1)	27 (1)
C(6)	2566 (2)	2681 (2)	4354 (1)	27 (1)
C(61)	2124 (2)	2925 (2)	5292 (2)	33 (1)
C(62)	946 (3)	3551 (2)	5685 (2)	51 (1)
C(63)	610 (3)	3753 (3)	6551 (2)	67 (1)
C(64)	1438 (4)	3353 (3)	7020 (2)	73 (1)
C(65)	2590 (3)	2750 (3)	6645 (2)	60 (1)
C(66)	2944 (3)	2524 (2)	5782 (2)	41 (1)
N(7)	5211 (2)	3163 (1)	2289 (1)	27 (1)
C(71)	5063 (2)	3917 (2)	2772 (1)	30 (1)
C(72)	5360 (2)	4836 (2)	2419 (2)	31 (1)
C(73)	5848 (2)	5010 (2)	1519 (1)	27 (1)
C(74)	6012 (2)	4234 (2)	1018 (1)	29 (1)
C(75)	5682 (2)	3339 (2)	1421 (2)	31 (1)
C(76)	6153 (2)	5994 (2)	1106 (2)	29 (1)
C(77)	6532 (3)	6610 (2)	1531 (2)	41 (1)
C(78)	6829 (3)	7516 (2)	1133 (2)	48 (1)
C(79)	6755 (3)	7830 (2)	305 (2)	43 (1)
C(7X)	6382 (3)	7229 (2)	-125 (2)	38 (1)
C(7Y)	6082 (2)	6331 (2)	276 (2)	32 (1)
N(8)	4148 (2)	388 (1)	3400 (1)	30 (1)

SUPPLEMENTARY

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

C(81)	4016(2)	46(2)	4231(2)	33(1)
C(82)	3804(2)	-893(2)	4563(2)	35(1)
C(83)	3697(2)	-1550(2)	4035(2)	31(1)
C(84)	3832(3)	-1190(2)	3174(2)	36(1)
C(85)	4036(2)	-233(2)	2891(2)	35(1)
C(86)	3470(2)	-2573(2)	4364(2)	33(1)
C(87)	3854(3)	-3090(2)	5060(2)	41(1)
C(88)	3661(3)	-4051(2)	5339(2)	48(1)
C(89)	3067(3)	-4511(2)	4959(2)	47(1)
C(8X)	2656(3)	-4012(2)	4277(2)	48(1)
C(8Y)	2863(3)	-3047(2)	3973(2)	41(1)
C(7A)	7240(2)	3205(16)	-1889(17)	69(6)
C(1A)	7992(17)	3471(10)	-1377(11)	45(1)
C(2A)	8693(18)	2713(9)	-956(11)	45(1)
C(3A)	9478(17)	2949(11)	-555(11)	45(1)
C(4A)	9562(17)	3943(13)	-575(12)	45(1)
C(5A)	8861(18)	4701(10)	-997(12)	45(1)
C(6A)	8076(17)	4465(10)	-1398(11)	45(1)
C(7B)	9811(8)	4530(5)	-438(5)	70(2)
C(1B)	9015(6)	4163(3)	-856(4)	45(1)
C(2B)	8916(5)	3161(3)	-699(4)	45(1)
C(3B)	8114(5)	2824(3)	-1023(4)	45(1)
C(4B)	7411(5)	3489(4)	-1504(4)	45(1)
C(5B)	7510(5)	4491(4)	-1661(4)	45(1)
C(6B)	8312(6)	4828(3)	-1337(4)	45(1)
C(7C)	9495(9)	2119(5)	-562(6)	81(3)
C(1C)	8806(5)	3083(2)	-923(4)	45(1)
C(2C)	7939(5)	3062(3)	-1348(4)	45(1)
C(3C)	7351(4)	3950(4)	-1712(3)	45(1)
C(4C)	7629(5)	4859(3)	-1651(3)	45(1)
C(5C)	8497(6)	4879(2)	-1226(4)	45(1)
C(6C)	9085(5)	3992(3)	-862(4)	45(1)
C(7D)	7240(4)	4850(2)	-2050(3)	59(8)
C(1D)	7840(3)	4089(19)	-1450(2)	45(1)
C(2D)	7700(3)	3100(2)	-1360(2)	45(1)
C(3D)	8340(4)	2377(18)	-880(2)	45(1)
C(4D)	9100(3)	2650(2)	-480(2)	45(1)
C(5D)	9240(3)	3640(3)	-570(2)	45(1)
C(6D)	8600(3)	4360(2)	-1060(2)	45(1)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{toluene})$ Table 28S. Bond lengths [Å] and angles [deg] for
 $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{toluene})$.

Ni-O(6)	2.0102(15)
Ni-O(3)	2.0106(15)
Ni-O(4)	2.0210(16)
Ni-O(1)	2.0305(16)
Ni-N(8)	2.123(2)
Ni-N(7)	2.1261(18)
O(1)-C(1)	1.258(3)
C(1)-C(2)	1.412(3)
C(1)-C(11)	1.507(3)
C(11)-C(16)	1.379(4)
C(11)-C(12)	1.382(3)
C(12)-C(13)	1.380(4)
C(13)-C(14)	1.375(5)
C(14)-C(15)	1.371(5)
C(15)-C(16)	1.379(4)
C(2)-C(3)	1.391(3)
O(3)-C(3)	1.268(3)
C(3)-C(31)	1.501(3)
C(31)-C(36)	1.382(3)
C(31)-C(32)	1.397(3)
C(32)-C(33)	1.381(4)
C(33)-C(34)	1.371(4)
C(34)-C(35)	1.378(4)
C(35)-C(36)	1.385(3)
O(4)-C(4)	1.266(3)
C(4)-C(5)	1.404(3)
C(4)-C(41)	1.498(3)
C(41)-C(42)	1.380(3)
C(41)-C(46)	1.392(3)
C(42)-C(43)	1.386(4)
C(43)-C(44)	1.386(4)
C(44)-C(45)	1.353(4)
C(45)-C(46)	1.389(4)
C(5)-C(6)	1.387(3)
O(6)-C(6)	1.272(3)
C(6)-C(61)	1.505(3)
C(61)-C(66)	1.387(4)
C(61)-C(62)	1.390(4)
C(62)-C(63)	1.390(4)
C(63)-C(64)	1.368(5)
C(64)-C(65)	1.350(5)
C(65)-C(66)	1.391(3)
N(7)-C(75)	1.343(3)
N(7)-C(71)	1.344(3)
C(71)-C(72)	1.381(3)
C(72)-C(73)	1.392(3)
C(73)-C(74)	1.382(3)
C(73)-C(76)	1.486(3)
C(74)-C(75)	1.381(3)
C(76)-C(7Y)	1.389(3)
C(76)-C(77)	1.398(3)
C(77)-C(78)	1.382(4)
C(78)-C(79)	1.384(4)
C(79)-C(7X)	1.381(3)
C(7X)-C(7Y)	1.374(3)

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

N(8) - C(85)	1.336(3)
N(8) - C(81)	1.341(3)
C(81) - C(82)	1.372(3)
C(82) - C(83)	1.394(3)
C(83) - C(84)	1.391(3)
C(83) - C(86)	1.483(3)
C(84) - C(85)	1.378(3)
C(86) - C(87)	1.389(4)
C(86) - C(8Y)	1.399(4)
C(87) - C(88)	1.379(4)
C(88) - C(89)	1.363(4)
C(89) - C(8X)	1.377(4)
C(8X) - C(8Y)	1.394(4)
C(7A) - C(1A)	1.511(6)
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
C(7B) - C(1B)	1.513(6)
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
C(7C) - C(1C)	1.508(6)
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
C(7D) - C(1D)	1.511(7)
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(6) - Ni - O(3)	179.43(6)
O(6) - Ni - O(4)	91.05(6)
O(3) - Ni - O(4)	88.79(6)
O(6) - Ni - O(1)	89.39(6)
O(3) - Ni - O(1)	90.77(6)
O(4) - Ni - O(1)	179.56(6)
O(6) - Ni - N(8)	90.19(7)
O(3) - Ni - N(8)	89.26(7)
O(4) - Ni - N(8)	90.93(7)
O(1) - Ni - N(8)	89.07(7)
O(6) - Ni - N(7)	91.43(6)
O(3) - Ni - N(7)	89.12(7)
O(4) - Ni - N(7)	89.20(7)
O(1) - Ni - N(7)	90.78(7)
N(8) - Ni - N(7)	178.38(7)
C(1) - O(1) - Ni	124.30(14)
O(1) - C(1) - C(2)	126.7(2)

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

SUPPLEMENTARY

O(1)-C(1)-C(11)	115.9(2)
C(2)-C(1)-C(11)	117.4(2)
C(16)-C(11)-C(12)	119.4(2)
C(16)-C(11)-C(1)	121.2(2)
C(12)-C(11)-C(1)	119.4(2)
C(13)-C(12)-C(11)	120.3(3)
C(14)-C(13)-C(12)	119.7(3)
C(15)-C(14)-C(13)	120.2(3)
C(14)-C(15)-C(16)	120.1(3)
C(15)-C(16)-C(11)	120.2(3)
C(3)-C(2)-C(1)	125.3(2)
C(3)-O(3)-Ni	126.43(14)
O(3)-C(3)-C(2)	125.1(2)
O(3)-C(3)-C(31)	114.3(2)
C(2)-C(3)-C(31)	120.6(2)
C(36)-C(31)-C(32)	117.3(2)
C(36)-C(31)-C(3)	118.6(2)
C(32)-C(31)-C(3)	123.8(2)
C(33)-C(32)-C(31)	120.6(3)
C(34)-C(33)-C(32)	121.3(3)
C(33)-C(34)-C(35)	118.8(2)
C(34)-C(35)-C(36)	120.1(3)
C(31)-C(36)-C(35)	121.8(3)
C(4)-O(4)-Ni	125.40(14)
O(4)-C(4)-C(5)	125.3(2)
O(4)-C(4)-C(41)	115.7(2)
C(5)-C(4)-C(41)	119.0(2)
C(42)-C(41)-C(46)	118.7(2)
C(42)-C(41)-C(4)	118.7(2)
C(46)-C(41)-C(4)	122.5(2)
C(41)-C(42)-C(43)	120.7(2)
C(42)-C(43)-C(44)	119.9(3)
C(45)-C(44)-C(43)	119.6(3)
C(44)-C(45)-C(46)	121.2(3)
C(45)-C(46)-C(41)	119.8(3)
C(6)-C(5)-C(4)	126.1(2)
C(6)-O(6)-Ni	124.93(14)
O(6)-C(6)-C(5)	126.0(2)
O(6)-C(6)-C(61)	114.4(2)
C(5)-C(6)-C(61)	119.5(2)
C(66)-C(61)-C(62)	118.3(2)
C(66)-C(61)-C(6)	118.5(2)
C(62)-C(61)-C(6)	123.1(2)
C(63)-C(62)-C(61)	119.9(3)
C(64)-C(63)-C(62)	120.6(3)
C(65)-C(64)-C(63)	120.1(3)
C(64)-C(65)-C(66)	120.5(3)
C(61)-C(66)-C(65)	120.5(3)
C(75)-N(7)-C(71)	116.38(19)
C(75)-N(7)-Ni	121.69(15)
C(71)-N(7)-Ni	121.89(15)
N(7)-C(71)-C(72)	123.3(2)
C(71)-C(72)-C(73)	119.8(2)
C(74)-C(73)-C(72)	117.2(2)
C(74)-C(73)-C(76)	121.0(2)
C(72)-C(73)-C(76)	121.9(2)
C(75)-C(74)-C(73)	119.6(2)
N(7)-C(75)-C(74)	123.8(2)
C(75)-C(76)-C(77)	117.5(2)

Structure of [Ni(4-PhPy)₂(DBM)₂]*(toluene)

SUPPLEMENTARY

C(7Y)-C(76)-C(73)	121.0(2)
C(77)-C(76)-C(73)	121.5(2)
C(78)-C(77)-C(76)	120.8(2)
C(77)-C(78)-C(79)	120.4(2)
C(7X)-C(79)-C(78)	119.6(2)
C(7Y)-C(7X)-C(79)	119.8(2)
C(7X)-C(7Y)-C(76)	122.0(2)
C(85)-N(8)-C(81)	116.5(2)
C(85)-N(8)-Ni	120.19(16)
C(81)-N(8)-Ni	123.11(15)
N(8)-C(81)-C(82)	123.5(2)
C(81)-C(82)-C(83)	120.3(2)
C(84)-C(83)-C(82)	115.9(2)
C(84)-C(83)-C(86)	121.8(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)	123.4(2)
C(87)-C(86)-C(8Y)	118.2(2)
C(87)-C(86)-C(83)	121.4(2)
C(8Y)-C(86)-C(83)	120.4(2)
C(88)-C(87)-C(86)	120.3(3)
C(89)-C(88)-C(87)	121.4(3)
C(88)-C(89)-C(8X)	119.6(3)
C(89)-C(8X)-C(8Y)	119.9(3)
C(8X)-C(8Y)-C(86)	120.5(3)
C(2A)-C(1A)-C(6A)	120.0
C(2A)-C(1A)-C(7A)	120.0(3)
C(6A)-C(1A)-C(7A)	119.8(3)
C(1A)-C(2A)-C(3A)	120.0
C(4A)-C(3A)-C(2A)	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
C(2B)-C(1B)-C(6B)	120.0
C(2B)-C(1B)-C(7B)	119.0(2)
C(6B)-C(1B)-C(7B)	120.8(2)
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(6B)-C(5B)-C(4B)	120.0
C(5B)-C(6B)-C(1B)	120.0
C(2C)-C(1C)-C(6C)	120.0
C(2C)-C(1C)-C(7C)	120.4(2)
C(6C)-C(1C)-C(7C)	119.6(2)
C(3C)-C(2C)-C(1C)	120.0
C(2C)-C(3C)-C(4C)	120.0
C(5C)-C(4C)-C(3C)	120.0
C(4C)-C(5C)-C(6C)	120.0
C(5C)-C(6C)-C(1C)	120.0
C(2D)-C(1D)-C(6D)	120.0
C(2D)-C(1D)-C(7D)	119.9(3)
C(6D)-C(1D)-C(7D)	119.9(3)
C(1D)-C(2D)-C(3D)	120.0
C(4D)-C(3D)-C(2D)	120.0
C(5D)-C(4D)-C(3D)	120.0
C(4D)-C(5D)-C(6D)	120.0
C(5D)-C(6D)-C(1D)	120.0

Table 29S. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{toluene})$.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ni	21(1)	32(1)	16(1)	-5(1)	-3(1)	-1(1)
O(1)	26(1)	35(1)	23(1)	-7(1)	-7(1)	1(1)
C(1)	22(1)	33(1)	25(1)	-2(1)	-6(1)	-5(1)
C(11)	22(1)	46(1)	21(1)	2(1)	-5(1)	-5(1)
C(12)	40(2)	55(2)	31(1)	4(1)	-16(1)	-15(1)
C(13)	45(2)	95(3)	37(2)	8(2)	-19(1)	-34(2)
C(14)	29(2)	122(3)	37(2)	14(2)	-16(1)	-9(2)
C(15)	39(2)	85(2)	51(2)	4(2)	-17(2)	15(2)
C(16)	33(2)	54(2)	43(2)	-5(1)	-12(1)	4(1)
C(2)	23(1)	43(1)	28(1)	-13(1)	-6(1)	3(1)
O(3)	24(1)	33(1)	19(1)	-6(1)	-5(1)	-1(1)
C(3)	23(1)	30(1)	23(1)	-7(1)	-3(1)	-7(1)
C(31)	27(1)	37(1)	22(1)	-10(1)	-1(1)	-10(1)
C(32)	25(1)	77(2)	36(2)	-31(1)	-2(1)	-6(1)
C(33)	34(2)	84(2)	43(2)	-34(2)	9(1)	-19(2)
C(34)	66(2)	61(2)	24(1)	-15(1)	1(1)	-30(2)
C(35)	59(2)	55(2)	29(1)	-13(1)	-15(1)	-6(1)
C(36)	42(2)	44(1)	27(1)	-10(1)	-10(1)	0(1)
O(4)	21(1)	36(1)	21(1)	-4(1)	-4(1)	-1(1)
C(4)	23(1)	29(1)	26(1)	-1(1)	-7(1)	-5(1)
C(41)	26(1)	39(1)	30(1)	-1(1)	-8(1)	-2(1)
C(42)	30(1)	48(2)	34(1)	-5(1)	-9(1)	-1(1)
C(43)	48(2)	75(2)	48(2)	-12(2)	-26(2)	-2(2)
C(44)	34(2)	85(2)	53(2)	-1(2)	-23(2)	1(2)
C(45)	30(2)	78(2)	54(2)	-6(2)	-13(1)	12(1)
C(46)	29(2)	56(2)	43(2)	-8(1)	-9(1)	5(1)
C(5)	22(1)	50(2)	28(1)	-12(1)	0(1)	-5(1)
O(6)	24(1)	33(1)	19(1)	-6(1)	-2(1)	-2(1)
C(6)	27(1)	29(1)	20(1)	-7(1)	2(1)	-7(1)
C(61)	29(1)	44(1)	24(1)	-13(1)	5(1)	-15(1)
C(62)	32(2)	74(2)	45(2)	-33(2)	3(1)	-12(1)
C(63)	40(2)	103(3)	54(2)	-52(2)	14(2)	-19(2)
C(64)	64(2)	124(3)	34(2)	-43(2)	9(2)	-36(2)
C(65)	58(2)	100(3)	27(2)	-20(2)	-3(1)	-31(2)
C(66)	38(2)	61(2)	23(1)	-14(1)	-4(1)	-13(1)
N(7)	24(1)	35(1)	20(1)	-2(1)	-6(1)	-4(1)
C(71)	31(1)	41(1)	17(1)	-5(1)	-6(1)	-7(1)
C(72)	32(1)	37(1)	25(1)	-8(1)	-9(1)	-7(1)
C(73)	20(1)	41(1)	22(1)	-2(1)	-10(1)	-5(1)
C(74)	29(1)	37(1)	16(1)	-3(1)	-4(1)	-5(1)
C(75)	33(1)	38(1)	21(1)	-9(1)	-6(1)	-7(1)
C(76)	24(1)	32(1)	27(1)	-2(1)	-7(1)	-2(1)
C(77)	59(2)	46(2)	27(1)	1(1)	-19(1)	-21(1)
C(78)	64(2)	47(2)	43(2)	-5(1)	-19(2)	-24(2)
C(79)	53(2)	35(1)	38(2)	1(1)	-12(1)	-14(1)
C(7X)	41(2)	42(1)	30(1)	0(1)	-12(1)	-7(1)
C(7Y)	34(1)	37(1)	26(1)	-6(1)	-10(1)	-6(1)
N(8)	29(1)	36(1)	24(1)	-5(1)	-7(1)	-5(1)
C(81)	38(2)	38(1)	22(1)	-4(1)	-9(1)	-7(1)

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

SUPPLEMENTARY

C(82)	42(2)	38(1)	23(1)	-3(1)	-8(1)	-7(1)
C(83)	24(1)	35(1)	28(1)	-3(1)	-5(1)	-3(1)
C(84)	42(2)	41(1)	31(1)	-7(1)	-15(1)	-11(1)
C(85)	39(2)	42(1)	25(1)	-1(1)	-12(1)	-11(1)
C(86)	24(1)	36(1)	35(1)	-5(1)	-3(1)	-4(1)
C(87)	42(2)	42(1)	34(1)	2(1)	-8(1)	-12(1)
C(88)	48(2)	42(2)	48(2)	7(1)	-12(1)	-11(1)
C(89)	39(2)	37(1)	53(2)	0(1)	1(1)	-10(1)
C(8X)	32(2)	45(2)	64(2)	-16(1)	-6(1)	-10(1)
C(8Y)	34(2)	43(2)	44(2)	-7(1)	-11(1)	-4(1)
C(7A)	56(10)	96(11)	54(10)	-16(9)	-16(9)	-9(10)
C(7B)	67(5)	92(6)	59(5)	-11(4)	-11(4)	-38(4)
C(7C)	92(6)	64(5)	79(6)	-7(4)	-29(5)	0(5)
C(7D)	54(11)	63(11)	47(11)	-7(11)	-4(11)	-3(11)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{toluene})$ Table 30S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{toluene})$.

	x	y	z	U(eq)
H(12)	8240	1726	3520	49
H(13)	9927	1228	4109	66
H(14)	10977	-455	4152	77
H(15)	10445	-1617	3527	77
H(16)	8848	-1104	2860	55
H(2)	8266	-142	1706	39
H(32)	9001	-246	339	55
H(33)	9596	-472	-1133	66
H(34)	8107	38	-1882	60
H(35)	5966	745	-1125	57
H(36)	5363	996	344	46
H(42)	1730	1925	1723	46
H(43)	106	2319	1077	67
H(44)	-1766	3532	1647	70
H(45)	-1982	4350	2829	70
H(46)	-385	3954	3499	54
H(5)	785	3050	4252	42
H(62)	370	3841	5362	61
H(63)	-202	4173	6821	81
H(64)	1202	3500	7610	88
H(65)	3163	2477	6972	72
H(66)	3753	2093	5527	49
H(71)	4738	3813	3389	36
H(72)	5231	5348	2789	37
H(74)	6350	4315	401	34
H(75)	5793	2819	1063	37
H(77)	6585	6403	2100	50
H(78)	7086	7927	1430	58
H(79)	6959	8454	33	51
H(7X)	6334	7437	-695	46
H(7Y)	5818	5928	-23	39
H(81)	4072	479	4610	39
H(82)	3730	-1098	5156	42
H(84)	3784	-1607	2779	43
H(85)	4101	-3	2303	42
H(87)	4251	-2779	5344	49
H(88)	3948	-4400	5806	57
H(89)	2938	-5172	5163	57
H(8X)	2232	-4325	4014	57
H(8Y)	2590	-2709	3497	50
H(7A1)	7828	3020	-2468	104
H(7A2)	6562	3787	-1948	104
H(7A3)	6855	2637	-1581	104
H(2A)	8636	2034	-942	54
H(3A)	9957	2431	-267	54
H(4A)	10098	4104	-301	54
H(5A)	8918	5380	-1010	54
H(6A)	7597	4983	-1686	54
H(7B1)	9250	4813	114	105
H(7B2)	10219	5050	-830	105

Structure of [Ni(4-PhPy)₂(DBM)₂]*(toluene)

SUPPLEMENTARY

H(7B3)	10478	3966	-328	105
H(2B)	9397	2706	-371	54
H(3B)	8047	2139	-916	54
H(4B)	6863	3259	-1725	54
H(5B)	7029	4945	-1989	54
H(6B)	8379	5513	-1444	54
H(7C1)	8943	1929	18	121
H(7C2)	10301	2217	-519	121
H(7C3)	9690	1584	-951	121
H(2C)	7749	2442	-1390	54
H(3C)	6758	3936	-2003	54
H(4C)	7227	5465	-1900	54
H(5C)	8687	5500	-1185	54
H(6C)	9678	4006	-572	54
H(7D1)	6326	4837	-1897	89
H(7D2)	7691	4693	-2654	89
H(7D3)	7312	5526	-1972	89
H(2D)	7181	2914	-1636	54
H(3D)	8248	1699	-814	54
H(4D)	9537	2153	-144	54
H(5D)	9759	3821	-297	54
H(6D)	8692	5036	-1119	54

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{o-xylene})$

Table 31S. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{o-xylene})$.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ni	4704(1)	1763(1)	2865(1)	25(1)
O(1)	6356(1)	1274(1)	3162(1)	30(1)
C(1)	7320(2)	667(1)	2736(1)	28(1)
C(11)	8390(2)	311(1)	3119(1)	33(1)
C(12)	8742(2)	984(2)	3480(1)	42(1)
C(13)	9711(2)	661(2)	3851(1)	54(1)
C(14)	10288(2)	-320(2)	3883(2)	59(1)
C(15)	9942(2)	-990(2)	3529(2)	59(1)
C(16)	9010(2)	-672(2)	3131(1)	45(1)
C(2)	7514(2)	313(1)	1930(1)	31(1)
O(3)	5586(1)	1197(1)	1692(1)	27(1)
C(3)	6695(2)	638(1)	1434(1)	26(1)
C(31)	7128(2)	364(1)	508(1)	26(1)
C(32)	8390(2)	-108(1)	52(1)	34(1)
C(33)	8753(2)	-261(2)	-824(1)	43(1)
C(34)	7887(2)	37(2)	-1264(1)	44(1)
C(35)	6630(2)	488(2)	-819(1)	48(1)
C(36)	6260(2)	648(1)	57(1)	38(1)
O(4)	3068(1)	2240(1)	2559(1)	29(1)
C(4)	1966(2)	2592(1)	3081(1)	28(1)
C(41)	881(2)	2853(1)	2711(1)	32(1)
C(42)	1053(2)	2432(1)	1957(1)	36(1)
C(43)	107(2)	2679(2)	1567(1)	48(1)
C(44)	-1018(2)	3349(2)	1927(2)	56(1)
C(45)	-1196(2)	3775(2)	2669(2)	60(1)
C(46)	-259(2)	3528(2)	3066(1)	47(1)
C(5)	1690(2)	2765(1)	3960(1)	33(1)
O(6)	3804(1)	2318(1)	4044(1)	28(1)
C(6)	2598(2)	2646(1)	4374(1)	28(1)
C(61)	2149(2)	2928(1)	5297(1)	34(1)
C(62)	1000(2)	3583(2)	5676(1)	51(1)
C(63)	666(2)	3825(2)	6533(2)	71(1)
C(64)	1464(2)	3419(2)	7008(2)	76(1)
C(65)	2595(2)	2776(2)	6647(1)	63(1)
C(66)	2944(2)	2526(2)	5797(1)	44(1)
N(7)	5288(1)	3124(1)	2292(1)	28(1)
C(71)	5143(2)	3853(1)	2783(1)	32(1)
C(72)	5436(2)	4764(1)	2432(1)	32(1)
C(73)	5908(2)	4967(1)	1528(1)	29(1)
C(74)	6083(2)	4201(1)	1025(1)	32(1)
C(75)	5759(2)	3310(1)	1423(1)	32(1)
C(76)	6174(2)	5950(1)	1123(1)	31(1)
C(77)	6535(2)	6567(2)	1540(1)	43(1)
C(78)	6771(2)	7484(2)	1152(1)	48(1)
C(79)	6647(2)	7804(1)	344(1)	41(1)
C(7X)	6287(2)	7210(1)	-78(1)	39(1)
C(7Y)	6045(2)	6294(1)	312(1)	36(1)
N(8)	4154(1)	389(1)	3408(1)	30(1)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2](\text{o-xylene})$

SUPPLEMENTARY

C(81)	4039(2)	37(1)	4238(1)	34(1)
C(82)	3812(2)	-890(1)	4573(1)	34(1)
C(83)	3688(2)	-1523(1)	4051(1)	31(1)
C(84)	3807(2)	-1155(1)	3187(1)	37(1)
C(85)	4023(2)	-214(1)	2906(1)	35(1)
C(86)	3457(2)	-2539(1)	4374(1)	35(1)
C(87)	3881(2)	-3061(1)	5041(1)	41(1)
C(88)	3709(2)	-4019(2)	5313(1)	47(1)
C(89)	3089(2)	-4468(2)	4945(2)	48(1)
C(8X)	2637(2)	-3955(2)	4296(2)	49(1)
C(8Y)	2828(2)	-2997(2)	4008(1)	42(1)
C(7A)	7348(5)	3104(4)	-1826(4)	47(2)
C(8A)	7600(5)	5125(3)	-1841(4)	39(2)
C(1A)	8179(3)	3326(2)	-1366(2)	47(1)
C(2A)	8301(3)	4293(2)	-1373(2)	47(1)
C(3A)	9065(3)	4495(2)	-950(2)	47(1)
C(4A)	9708(3)	3730(2)	-520(2)	47(1)
C(5A)	9586(3)	2764(2)	-512(2)	47(1)
C(6A)	8822(3)	2562(2)	-936(2)	47(1)
C(7B)	9639(3)	4359(2)	-531(2)	65(1)
C(8B)	9325(4)	2299(2)	-569(2)	67(3)
C(1B)	8807(2)	4141(2)	-997(1)	47(1)
C(2B)	8659(2)	3188(1)	-1016(1)	47(1)
C(3B)	7886(2)	3028(1)	-1452(2)	47(1)
C(4B)	7261(2)	3820(2)	-1868(2)	47(1)
C(5B)	7409(2)	4774(2)	-1850(2)	47(1)
C(6B)	8182(2)	4934(1)	-1414(2)	47(1)
C(7C)	9363(9)	2279(4)	-589(7)	72(7)
C(8C)	7547(8)	2560(4)	-1537(6)	61(3)
C(1C)	8839(5)	3305(3)	-928(4)	47(1)
C(2C)	7976(5)	3438(3)	-1378(3)	47(1)
C(3C)	7499(5)	4381(3)	-1686(4)	47(1)
C(4C)	7885(6)	5192(3)	-1544(4)	47(1)
C(5C)	8748(6)	5060(3)	-1094(4)	47(1)
C(6C)	9225(6)	4116(3)	-786(4)	47(1)

Table 32S. Bond lengths [Å] and angles [deg] for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{o-xylene})$.

Ni-O(3)	2.0111(12)
Ni-O(6)	2.0143(12)
Ni-O(4)	2.0250(11)
Ni-O(1)	2.0344(11)
Ni-N(8)	2.1269(15)
Ni-N(7)	2.1311(14)
O(1)-C(1)	1.257(2)
C(1)-C(2)	1.414(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)	1.393(3)
C(13)-C(14)	1.370(3)
C(14)-C(15)	1.374(3)
C(15)-C(16)	1.387(3)
C(2)-C(3)	1.399(2)
O(3)-C(3)	1.2679(19)
C(3)-C(31)	1.503(2)
C(31)-C(36)	1.387(2)
C(31)-C(32)	1.399(2)
C(32)-C(33)	1.383(3)
C(33)-C(34)	1.373(3)
C(34)-C(35)	1.381(3)
C(35)-C(36)	1.385(2)
O(4)-C(4)	1.262(2)
C(4)-C(5)	1.411(2)
C(4)-C(41)	1.507(2)
C(41)-C(42)	1.387(2)
C(41)-C(46)	1.389(3)
C(42)-C(43)	1.389(2)
C(43)-C(44)	1.378(3)
C(44)-C(45)	1.371(3)
C(45)-C(46)	1.387(3)
C(5)-C(6)	1.394(2)
O(6)-C(6)	1.266(2)
C(6)-C(61)	1.500(2)
C(61)-C(62)	1.389(3)
C(61)-C(66)	1.395(3)
C(62)-C(63)	1.396(3)
C(63)-C(64)	1.368(4)
C(64)-C(65)	1.362(4)
C(65)-C(66)	1.386(3)
N(7)-C(75)	1.339(2)
N(7)-C(71)	1.343(2)
C(71)-C(72)	1.379(2)
C(72)-C(73)	1.394(2)
C(73)-C(74)	1.389(2)
C(73)-C(76)	1.482(2)
C(74)-C(75)	1.381(2)
C(76)-C(7Y)	1.394(2)
C(76)-C(77)	1.394(2)
C(77)-C(78)	1.381(3)
C(78)-C(79)	1.380(3)
C(79)-C(7X)	1.377(3)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{o-xylene})$

C(7X)-C(7Y)	1.382(3)
N(8)-C(85)	1.336(2)
N(8)-C(81)	1.347(2)
C(81)-C(82)	1.373(2)
C(82)-C(83)	1.388(2)
C(83)-C(84)	1.404(3)
C(83)-C(86)	1.487(2)
C(84)-C(85)	1.374(3)
C(86)-C(87)	1.389(3)
C(86)-C(8Y)	1.392(3)
C(87)-C(88)	1.382(3)
C(88)-C(89)	1.377(3)
C(89)-C(8X)	1.377(3)
C(8X)-C(8Y)	1.390(3)
C(7A)-C(1A)	1.515(3)
C(8A)-C(2A)	1.514(3)
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
C(7B)-C(1B)	1.520(2)
C(8B)-C(2B)	1.522(2)
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
C(7C)-C(1C)	1.516(3)
C(8C)-C(2C)	1.516(3)
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
O(3)-Ni-O(6)	179.22(5)
O(3)-Ni-O(4)	88.69(5)
O(6)-Ni-O(4)	90.92(5)
O(3)-Ni-O(1)	90.72(5)
O(6)-Ni-O(1)	89.66(5)
O(4)-Ni-O(1)	179.37(4)
O(3)-Ni-N(8)	89.19(5)
O(6)-Ni-N(8)	90.14(5)
O(4)-Ni-N(8)	90.69(5)
O(1)-Ni-N(8)	89.07(5)
O(3)-Ni-N(7)	89.44(5)
O(6)-Ni-N(7)	91.23(5)
O(4)-Ni-N(7)	89.58(5)
O(1)-Ni-N(7)	90.64(5)
N(8)-Ni-N(7)	178.59(5)
C(1)-O(1)-Ni	124.24(10)
O(1)-C(1)-C(2)	126.66(15)
O(1)-C(1)-C(11)	116.07(15)
C(2)-C(1)-C(11)	117.24(15)
C(16)-C(11)-C(12)	119.51(17)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{o-xylene})$

SUPPLEMENTARY

C(16)-C(11)-C(1)	121.44(16)
C(12)-C(11)-C(1)	119.05(17)
C(11)-C(12)-C(13)	119.7(2)
C(14)-C(13)-C(12)	120.2(2)
C(13)-C(14)-C(15)	120.44(19)
C(14)-C(15)-C(16)	119.9(2)
C(11)-C(16)-C(15)	120.2(2)
C(3)-C(2)-C(1)	125.21(16)
C(3)-O(3)-Ni	126.41(10)
O(3)-C(3)-C(2)	125.01(15)
O(3)-C(3)-C(31)	114.57(14)
C(2)-C(3)-C(31)	120.36(15)
C(36)-C(31)-C(32)	117.57(16)
C(36)-C(31)-C(3)	118.64(15)
C(32)-C(31)-C(3)	123.66(15)
C(33)-C(32)-C(31)	120.62(17)
C(34)-C(33)-C(32)	121.03(18)
C(33)-C(34)-C(35)	119.12(18)
C(34)-C(35)-C(36)	120.19(18)
C(35)-C(36)-C(31)	121.44(18)
C(4)-O(4)-Ni	125.44(11)
O(4)-C(4)-C(5)	125.48(15)
O(4)-C(4)-C(41)	115.69(15)
C(5)-C(4)-C(41)	118.82(15)
C(42)-C(41)-C(46)	118.43(16)
C(42)-C(41)-C(4)	118.34(16)
C(46)-C(41)-C(4)	123.15(16)
C(41)-C(42)-C(43)	120.75(18)
C(44)-C(43)-C(42)	120.08(19)
C(45)-C(44)-C(43)	119.68(19)
C(44)-C(45)-C(46)	120.6(2)
C(45)-C(46)-C(41)	120.47(19)
C(6)-C(5)-C(4)	125.72(16)
C(6)-O(6)-Ni	125.27(10)
O(6)-C(6)-C(5)	126.08(15)
O(6)-C(6)-C(61)	114.97(14)
C(5)-C(6)-C(61)	118.94(15)
C(62)-C(61)-C(66)	118.18(18)
C(62)-C(61)-C(6)	123.63(17)
C(66)-C(61)-C(6)	118.18(17)
C(61)-C(62)-C(63)	120.1(2)
C(64)-C(63)-C(62)	120.4(2)
C(65)-C(64)-C(63)	120.3(2)
C(64)-C(65)-C(66)	120.2(2)
C(65)-C(66)-C(61)	120.8(2)
C(75)-N(7)-C(71)	116.74(15)
C(75)-N(7)-Ni	121.53(11)
C(71)-N(7)-Ni	121.65(12)
N(7)-C(71)-C(72)	123.14(16)
C(71)-C(72)-C(73)	120.32(16)
C(74)-C(73)-C(72)	116.16(16)
C(74)-C(73)-C(76)	121.72(16)
C(72)-C(73)-C(76)	122.10(16)
C(75)-C(74)-C(73)	120.23(16)
N(7)-C(75)-C(74)	123.38(16)
C(7Y)-C(76)-C(77)	117.80(17)
C(7Y)-C(76)-C(73)	120.36(16)
C(77)-C(76)-C(73)	121.83(16)
C(78)-C(77)-C(76)	120.82(18)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{o-xylene})$

SUPPLEMENTARY

C(79)-C(78)-C(77)	120.25(18)
C(7X)-C(79)-C(78)	120.00(18)
C(79)-C(7X)-C(7Y)	119.72(17)
C(7X)-C(7Y)-C(76)	121.40(17)
C(85)-N(8)-C(81)	116.42(15)
C(85)-N(8)-Ni	120.50(12)
C(81)-N(8)-Ni	122.79(11)
N(8)-C(81)-C(82)	123.59(16)
C(81)-C(82)-C(83)	120.22(16)
C(82)-C(83)-C(84)	116.12(16)
C(82)-C(83)-C(86)	122.73(16)
C(84)-C(83)-C(86)	121.15(16)
C(85)-C(84)-C(83)	119.96(16)
N(8)-C(85)-C(84)	123.68(17)
C(87)-C(86)-C(8Y)	118.22(17)
C(87)-C(86)-C(83)	120.76(16)
C(8Y)-C(86)-C(83)	121.01(17)
C(88)-C(87)-C(86)	120.38(18)
C(89)-C(88)-C(87)	120.96(19)
C(88)-C(89)-C(8X)	119.51(19)
C(89)-C(8X)-C(8Y)	119.85(19)
C(8X)-C(8Y)-C(86)	121.05(19)
C(2A)-C(1A)-C(6A)	120.0
C(2A)-C(1A)-C(7A)	120.1(2)
C(6A)-C(1A)-C(7A)	119.9(2)
C(1A)-C(2A)-C(3A)	120.0
C(1A)-C(2A)-C(8A)	119.9(2)
C(3A)-C(2A)-C(8A)	120.1(2)
C(4A)-C(3A)-C(2A)	120.0
C(5A)-C(4A)-C(3A)	120.0
C(6A)-C(5A)-C(4A)	120.0
C(5A)-C(6A)-C(1A)	120.0
C(2B)-C(1B)-C(6B)	120.0
C(2B)-C(1B)-C(7B)	122.20(14)
C(6B)-C(1B)-C(7B)	117.80(14)
C(3B)-C(2B)-C(1B)	120.0
C(3B)-C(2B)-C(8B)	118.20(14)
C(1B)-C(2B)-C(8B)	121.80(14)
C(2B)-C(3B)-C(4B)	120.0
C(5B)-C(4B)-C(3B)	120.0
C(4B)-C(5B)-C(6B)	120.0
C(5B)-C(6B)-C(1B)	120.0
C(2C)-C(1C)-C(6C)	120.0
C(2C)-C(1C)-C(7C)	120.4(2)
C(6C)-C(1C)-C(7C)	119.6(2)
C(3C)-C(2C)-C(1C)	120.0
C(3C)-C(2C)-C(8C)	119.4(2)
C(1C)-C(2C)-C(8C)	120.6(2)
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

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{o-xylene})$ Table 33S. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2] \cdot (\text{o-xylene})$.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hk a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Ni	24(1)	29(1)	20(1)	-5(1)	-8(1)	0(1)
O(1)	29(1)	35(1)	28(1)	-6(1)	-13(1)	0(1)
C(1)	26(1)	31(1)	28(1)	0(1)	-10(1)	-5(1)
C(11)	26(1)	45(1)	25(1)	3(1)	-9(1)	-7(1)
C(12)	43(1)	55(1)	34(1)	1(1)	-19(1)	-16(1)
C(13)	50(1)	86(2)	37(1)	4(1)	-22(1)	-26(1)
C(14)	32(1)	100(2)	40(1)	11(1)	-18(1)	-5(1)
C(15)	47(1)	67(2)	55(2)	4(1)	-25(1)	10(1)
C(16)	37(1)	49(1)	45(1)	-2(1)	-18(1)	2(1)
C(2)	26(1)	35(1)	31(1)	-8(1)	-10(1)	2(1)
O(3)	25(1)	31(1)	24(1)	-8(1)	-9(1)	2(1)
C(3)	24(1)	25(1)	26(1)	-4(1)	-6(1)	-5(1)
C(31)	28(1)	27(1)	24(1)	-5(1)	-5(1)	-7(1)
C(32)	27(1)	39(1)	34(1)	-11(1)	-5(1)	-7(1)
C(33)	34(1)	47(1)	39(1)	-20(1)	6(1)	-10(1)
C(34)	58(1)	47(1)	26(1)	-11(1)	-6(1)	-14(1)
C(35)	56(1)	57(1)	32(1)	-13(1)	-20(1)	1(1)
C(36)	37(1)	45(1)	30(1)	-11(1)	-11(1)	3(1)
O(4)	25(1)	35(1)	24(1)	-6(1)	-8(1)	1(1)
C(4)	26(1)	28(1)	28(1)	-3(1)	-8(1)	-3(1)
C(41)	25(1)	37(1)	31(1)	-2(1)	-10(1)	-3(1)
C(42)	33(1)	39(1)	35(1)	-5(1)	-14(1)	0(1)
C(43)	47(1)	59(1)	45(1)	-9(1)	-26(1)	-2(1)
C(44)	35(1)	80(2)	52(1)	-8(1)	-24(1)	5(1)
C(45)	35(1)	83(2)	51(1)	-15(1)	-17(1)	17(1)
C(46)	35(1)	63(1)	38(1)	-16(1)	-13(1)	9(1)
C(5)	26(1)	42(1)	28(1)	-11(1)	-5(1)	-1(1)
O(6)	26(1)	34(1)	22(1)	-6(1)	-6(1)	-2(1)
C(6)	30(1)	27(1)	23(1)	-5(1)	-4(1)	-7(1)
C(61)	30(1)	45(1)	27(1)	-13(1)	-1(1)	-16(1)
C(62)	33(1)	73(2)	49(1)	-34(1)	-3(1)	-10(1)
C(63)	39(1)	111(2)	60(2)	-58(2)	10(1)	-17(1)
C(64)	58(2)	142(3)	39(1)	-47(2)	3(1)	-42(2)
C(65)	61(2)	105(2)	30(1)	-19(1)	-8(1)	-32(2)
C(66)	43(1)	64(1)	28(1)	-12(1)	-6(1)	-19(1)
N(7)	25(1)	32(1)	26(1)	-4(1)	-10(1)	-1(1)
C(71)	36(1)	37(1)	22(1)	-3(1)	-12(1)	-6(1)
C(72)	38(1)	35(1)	27(1)	-6(1)	-13(1)	-7(1)
C(73)	22(1)	35(1)	28(1)	0(1)	-10(1)	-3(1)
C(74)	32(1)	38(1)	23(1)	-3(1)	-7(1)	-5(1)
C(75)	34(1)	33(1)	25(1)	-6(1)	-8(1)	-4(1)
C(76)	27(1)	34(1)	32(1)	-2(1)	-10(1)	-6(1)
C(77)	54(1)	48(1)	35(1)	3(1)	-22(1)	-21(1)
C(78)	63(1)	47(1)	46(1)	-1(1)	-24(1)	-26(1)
C(79)	46(1)	36(1)	40(1)	2(1)	-12(1)	-12(1)
C(7X)	46(1)	39(1)	33(1)	3(1)	-15(1)	-9(1)
C(7Y)	40(1)	38(1)	32(1)	-4(1)	-15(1)	-8(1)
N(8)	32(1)	34(1)	26(1)	-3(1)	-12(1)	-4(1)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2](\text{o-xylene})$

SUPPLEMENTARY

C(81)	43(1)	35(1)	27(1)	-6(1)	-15(1)	-5(1)
C(82)	38(1)	38(1)	26(1)	-1(1)	-12(1)	-4(1)
C(83)	28(1)	32(1)	33(1)	-4(1)	-10(1)	-3(1)
C(84)	40(1)	43(1)	33(1)	-8(1)	-15(1)	-11(1)
C(85)	40(1)	43(1)	27(1)	-1(1)	-15(1)	-11(1)
C(86)	31(1)	34(1)	36(1)	-5(1)	-7(1)	-4(1)
C(87)	44(1)	41(1)	40(1)	2(1)	-15(1)	-13(1)
C(88)	52(1)	41(1)	44(1)	5(1)	-15(1)	-12(1)
C(89)	47(1)	36(1)	54(1)	-2(1)	-7(1)	-12(1)
C(8X)	44(1)	45(1)	60(1)	-12(1)	-13(1)	-15(1)
C(8Y)	40(1)	42(1)	46(1)	-6(1)	-16(1)	-7(1)
C(7A)	50(5)	40(5)	53(5)	1(4)	-20(4)	-10(4)
C(8A)	34(3)	42(3)	50(4)	-17(3)	-10(3)	-21(3)
C(7B)	79(3)	71(3)	55(3)	-1(2)	-22(2)	-36(2)
C(8B)	76(4)	47(4)	95(5)	12(3)	-49(4)	-20(3)
C(7C)	77(9)	65(9)	76(9)	1(7)	-36(7)	-8(7)
C(8C)	57(5)	59(5)	71(6)	-28(5)	-19(4)	-10(4)

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{o-xylene})$

SUPPLEMENTARY

Table 34S. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{o-xylene})$.

	x	y	z	U(eq)
H(12)	8324	1660	3473	50
H(13)	9971	1123	4084	65
H(14)	10932	-538	4151	71
H(15)	10341	-1669	3557	71
H(16)	8796	-1131	2866	53
H(2)	8259	-186	1706	37
H(32)	9002	-326	346	41
H(33)	9616	-577	-1125	51
H(34)	8147	-65	-1866	53
H(35)	6018	689	-1114	57
H(36)	5392	958	355	46
H(42)	1827	1969	1704	43
H(43)	236	2384	1050	58
H(44)	-1668	3516	1662	67
H(45)	-1967	4244	2914	72
H(46)	-397	3823	3583	56
H(5)	806	2982	4298	40
H(62)	441	3866	5351	62
H(63)	-121	4273	6789	86
H(64)	1229	3588	7591	91
H(65)	3145	2497	6980	75
H(66)	3734	2076	5551	53
H(71)	4822	3737	3401	38
H(72)	5316	5256	2808	39
H(74)	6426	4290	405	38
H(75)	5876	2803	1062	38
H(77)	6620	6355	2097	51
H(78)	7020	7895	1442	58
H(79)	6810	8435	80	50
H(7X)	6205	7427	-635	47
H(7Y)	5785	5891	21	43
H(81)	4119	452	4611	41
H(82)	3739	-1099	5164	41
H(84)	3738	-1555	2798	44
H(85)	4082	21	2321	42
H(87)	4291	-2757	5313	49
H(88)	4022	-4373	5760	56
H(89)	2974	-5126	5138	58
H(8X)	2195	-4255	4045	59
H(8Y)	2525	-2650	3554	51
H(7A1)	6487	3062	-1402	71
H(7A2)	7752	2472	-2093	71
H(7A3)	7266	3632	-2282	71
H(8A1)	6718	5355	-1447	59
H(8A2)	7566	4887	-2359	59
H(8A3)	8064	5672	-2020	59
H(3A)	9148	5156	-954	57
H(4A)	10230	3868	-230	57
H(5A)	10025	2241	-218	57
H(6A)	8739	1901	-931	57

Structure of $[\text{Ni}(\text{4-PhPy})_2(\text{DBM})_2]^*(\text{o-xylene})$

H(7B1)	9232	4236	102	97
H(7B2)	9723	5052	-668	97
H(7B3)	10499	3930	-726	97
H(8B1)	9206	1690	-726	101
H(8B2)	8947	2334	66	101
H(8B3)	10252	2299	-760	101
H(3B)	7785	2376	-1464	57
H(4B)	6733	3711	-2166	57
H(5B)	6982	5315	-2134	57
H(6B)	8283	5585	-1401	57
H(7C1)	8684	2054	-79	108
H(7C2)	10103	2297	-421	108
H(7C3)	9641	1822	-1049	108
H(8C1)	6890	2793	-1820	91
H(8C2)	7179	2194	-978	91
H(8C3)	8293	2125	-1918	91
H(3C)	6910	4472	-1994	57
H(4C)	7560	5837	-1755	57
H(5C)	9012	5614	-997	57
H(6C)	9814	4025	-478	57