

Supporting Information

Synthesis, structure and magnetism of homodinuclear complexes of Co, Ni and Cu supported by a novel bitriazine scaffold.

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2. ¹³C NMR spectrum of compound 1.
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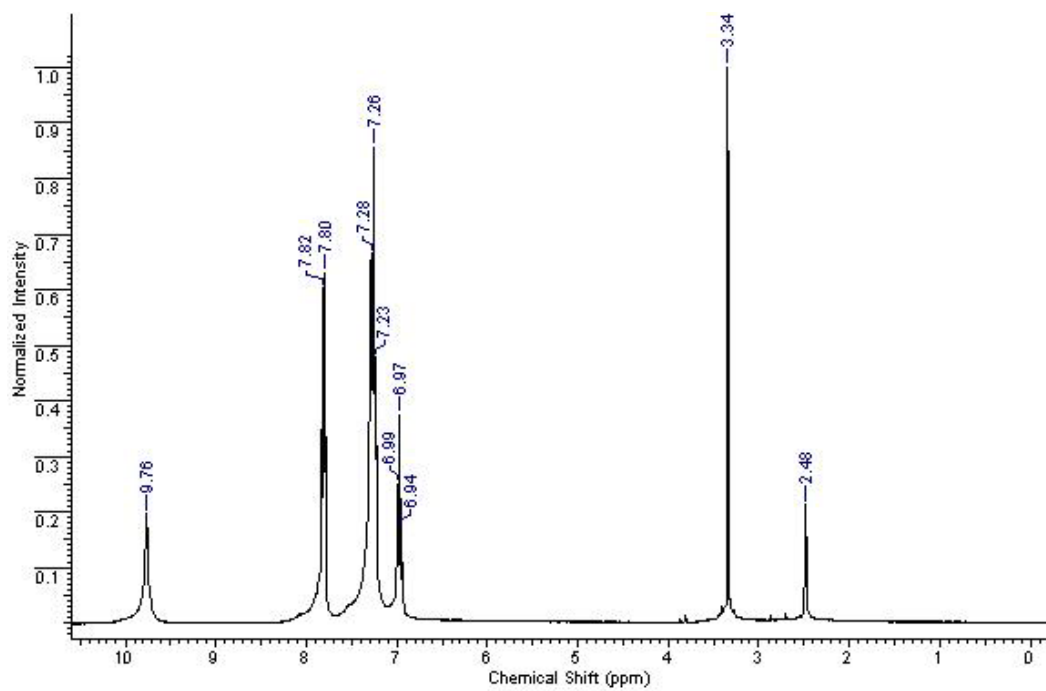


Figure S1. ¹H NMR Spectrum of compound 1.

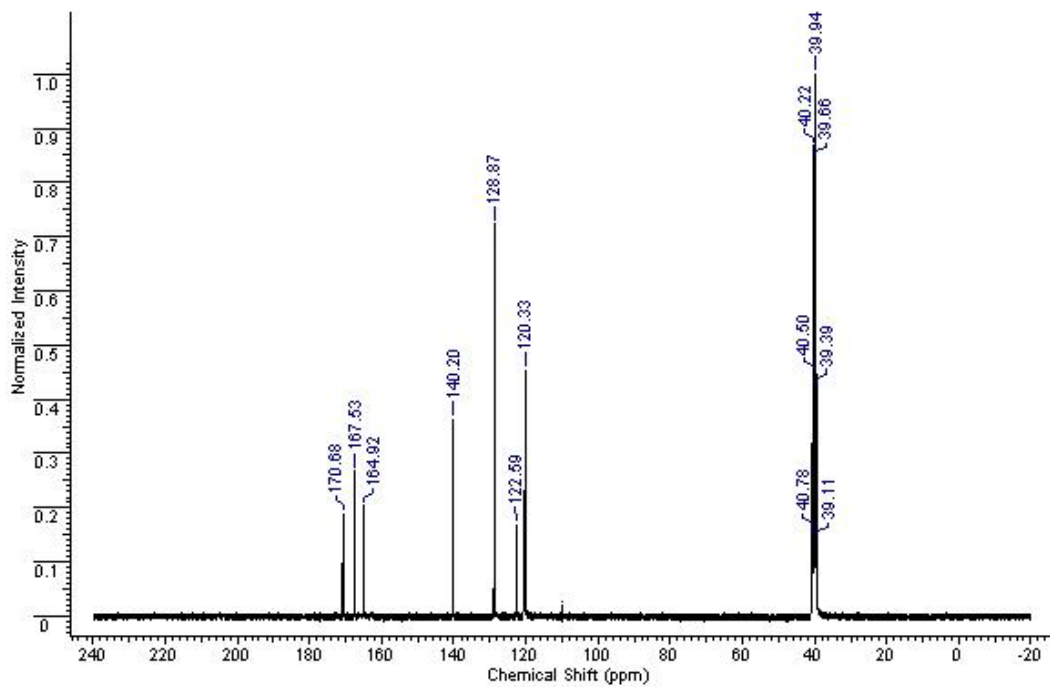


Figure S2. ^{13}C NMR spectrum of compound 1.

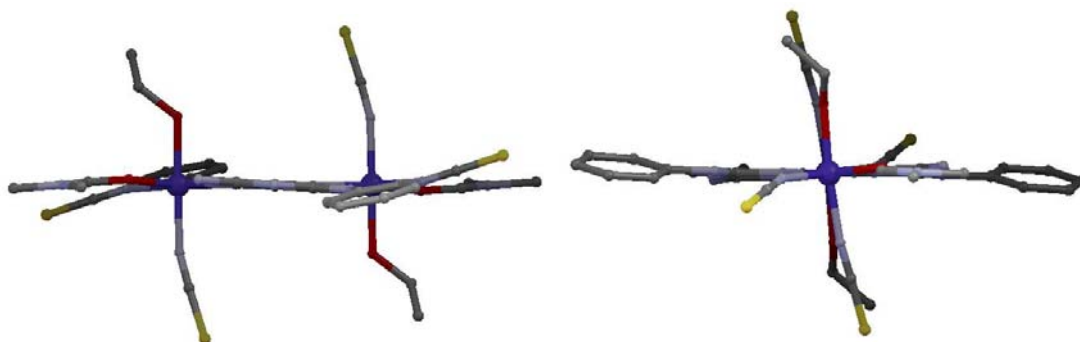


Figure S3. Ball and stick model of complex 2 along the C-C bond in the ligand (left) and along the cobalt centers (right).

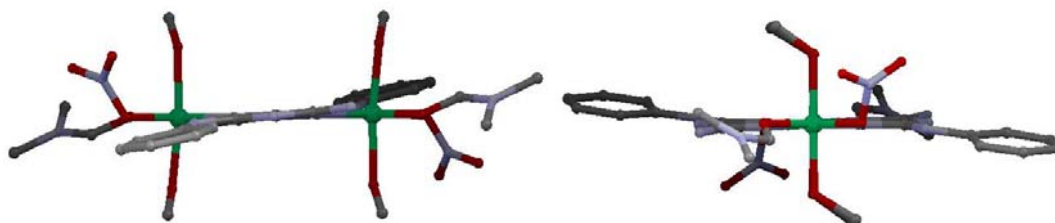


Figure S4. Ball and stick model of complex 3 along the C-C bond in the ligand (left) and along the nickel centers (right).



Figure S5. Ball and stick model of complex 4 along the C-C bond in the ligand (left) and along the copper centers (right).

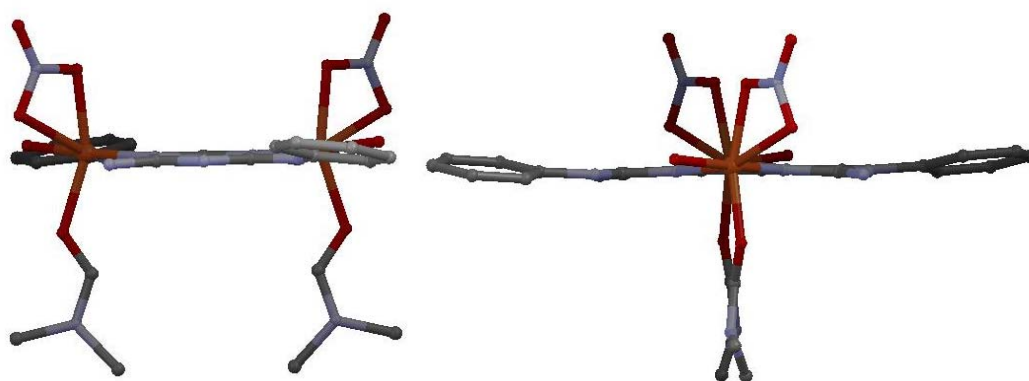


Figure S6. Ball and stick model of complex 5 along the C-C bond in the ligand (left) and along the copper centers (right).

Table S1. Selected Bond Distances (Å) and Angles (deg) for complex 2

Co(1)-N(7)	2.056(5)	N(7)-C(15)	1.142(6)
Co(1)-O(2)	2.058(4)	N(8)-C(16)	1.159(6)
Co(1)-N(8)	2.071(4)	S(1)-C(15)	1.630(6)
Co(1)-O(1)	2.158(3)	S(2)-C(16)	1.592(6)
Co(1)-N(3a)	2.180(4)	C(3)-C(3a)	1.521(9)
Co(1)-N(1)	2.188(4)	Co(1)...Co(1a)	5.828
N(7)-Co(1)-O(2)	174.90(17)	N(7)-Co(1)-N(1)	94.57(16)
N(7)-Co(1)-N(8)	93.57(17)	O(2)-Co(1)-N(1)	87.75(14)
O(2)-Co(1)-N(8)	90.50(16)	N(8)-Co(1)-N(1)	99.91(15)
N(7)-Co(1)-O(1)	89.22(16)	O(1)-Co(1)-N(1)	169.51(13)
O(2)-Co(1)-O(1)	87.74(14)	N(3a)-Co(1)-N(1)	175.29(16)
N(8)-Co(1)-O(1)	89.59(15)	C(15)-N(7)-Co(1)	164.9(4)
N(7)-Co(1)-N(3a)	85.93(16)	C(16)-N(8)-Co(1)	157.9(4)
O(2)-Co(1)-N(3a)	90.26(14)	N(7)-C(15)-S(1)	177.3(5)
N(8)-Co(1)-N(3a)	175.29(16)	N(8)-C(16)-S(2)	179.0(5)
O(1)-Co(1)-N(3a)	95.09(13)		

Table S2. Selected Bond Distances (Å) and Angles (deg) for complex 3

Ni(1)-O(3)	2.0462(12)	O(4)-N(7)	1.315(2)
Ni(1)-O(1)	2.0561(15)	O(5)-N(7)	1.216(2)
Ni(1)-O(2)	2.0603(14)	O(6)-N(7)	1.211(2)
Ni(1)-O(4)	2.0943(13)	O(7)-N(8)	1.238(2)
Ni(1)-N(2a)	2.0992(14)	O(8)-N(8)	1.243(2)
Ni(1)-N(1)	2.1231(13)	O(9)-N(8)	1.259(2)
C(1)-C(1a)	1.500(3)	H(1H)...O(7)	2.19(2)
Ni(1)...Ni(1a)	5.645		
O(3)-Ni(1)-O(1)	89.90(6)	O(1)-Ni(1)-N(1)	89.36(6)
O(3)-Ni(1)-O(2)	87.52(5)	O(2)-Ni(1)-N(1)	93.84(5)
O(1)-Ni(1)-O(2)	173.50(6)	O(4)-Ni(1)-N(1)	96.71(5)
O(3)-Ni(1)-O(4)	89.26(5)	N(2a)-Ni(1)-N(1)	78.39(5)
O(1)-Ni(1)-O(4)	88.26(6)	N(7)-O(4)-Ni(1)	119.24(11)
O(2)-Ni(1)-O(4)	85.75(6)	O(5)-N(7)-O(4)	118.06(17)
O(3)-Ni(1)-N(2a)	95.65(5)	O(6)-N(7)-O(5)	123.3(2)
O(1)-Ni(1)-N(2a)	92.35(6)	O(6)-N(7)-O(4)	118.64(18)
O(2)-Ni(1)-N(2a)	93.84(6)	O(7)-N(8)-O(8)	120.40(18)
O(4)-Ni(1)-N(2a)	175.06(5)	O(7)-N(8)-O(9)	119.94(18)
O(3)-Ni(1)-N(1)	173.96(5)	O(8)-N(8)-O(9)	119.63(18)

Table S3. Selected Bond Distances (Å) and Angles (deg) for complex 4

Cu(1)-O(1)	1.9607(15)	Cu(1)-Cl(2)	2.2907(7)
Cu(1)-N(1)	2.0163(16)	Cu(1)-Cl(1)	2.3214(6)
Cu(1)-N(2a)	2.1805(15)	C(1)-C(1a)	1.500(4)
Cu(1)...Cu(1A)	5.584		
O(1)-Cu(1)-N(1)	172.05(6)	N(2a)-Cu(1)-Cl(2)	113.07(5)
O(1)-Cu(1)-N(2a)	93.68(6)	O(1)-Cu(1)-Cl(1)	90.58(5)
N(1)-Cu(1)-N(2a)	78.38(6)	N(1)-Cu(1)-Cl(1)	93.60(5)
O(1)-Cu(1)-Cl(2)	92.69(6)	N(2a)-Cu(1)-Cl(1)	118.62(5)
N(1)-Cu(1)-Cl(2)	90.08(5)	Cl(2)-Cu(1)-Cl(1)	127.85(2)

Table S4. Selected Bond Distances (Å) and Angles (deg) for complex 5

Cu(1)-O(5)	1.9739(17)	N(6)-O(3)	1.199(3)
Cu(1)-O(4)	2.0117(18)	N(6)-O(2)	1.256(4)
Cu(1)-N(2a)	2.0129(19)	N(6)-O(1)	1.249(4)
Cu(1)-O(2)	2.071(3)	N(8)-O(7)	1.208(4)
Cu(1)-N(1)	2.2086(19)	N(8)-O(6)	1.223(3)
Cu(1)-O(1)	2.429(4)	N(8)-O(8)	1.256(3)
C(1)-C(1a)	1.497(4)	Cu(1)...Cu(1A)	5.634
O(5)-Cu(1)-O(4)	87.47(8)	O(2)-Cu(1)-O(1)	55.43(10)
O(5)-Cu(1)-N(2a)	172.12(7)	N(1)-Cu(1)-O(1)	160.22(8)
O(4)-Cu(1)-N(2a)	96.57(8)	O(4)-Cu(1)-O(1)	96.14(9)
O(5)-Cu(1)-O(2)	87.94(8)	N(2a)-Cu(1)-O(1)	99.81(8)
O(4)-Cu(1)-O(2)	151.45(11)	O(3)-N(6)-O(2)	120.5(3)
N(2a)-Cu(1)-O(2)	91.64(8)	O(3)-N(6)-O(1)	124.2(4)
O(5)-Cu(1)-N(1)	94.27(7)	O(2)-N(6)-O(1)	115.4(3)
O(4)-Cu(1)-N(1)	103.64(8)	O(7)-N(8)-O(6)	120.9(3)
N(2a)-Cu(1)-N(1)	78.22(7)	O(7)-N(8)-O(8)	120.3(3)
O(2)-Cu(1)-N(1)	104.80(9)	O(6)-N(8)-O(8)	118.8(2)
O(5)-Cu(1)-O(1)	86.43(8)		