10.1071/CH14029_AC

Australian Journal of Chemistry 2014, 67(6), 933-943

SUPPLEMENTARY MATERIAL

Reaction of 2-pyridylmethylthiourea Derivatives with $[(en)_2Co(OSO_2CF_3)_2]^+$ Induces Hypodentate Coordination of an Ethylenediamine Ligand

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Table S1. Bond lengths (Å) for $[C_{18}H_{31}CoN_7S](ClO_4)_2 \cdot H_2O$ {**[Co-4a](ClO$_4$)$_2$·H$_2$O (*endo* isomer)**}. Standard deviations are in parentheses. The unit cell contained two cations unrelated by symmetry. Refer to Figure 5 for the numbering scheme.

Co(1)-N(9)	1.9431(16)	Co(1)-N(4)	1.9545(18)
Co(1)-N(8)	1.9558(19)	Co(1)-N(1)	1.9732(18)
Co(1)-N(5)	1.9916(18)	Co(1)-S(1)	2.2895(6)
S(1)-C(17)	1.7394(19)	N(1)-C(2)	1.497(3)
C(2)-C(3)	1.508(4)	C(3)-N(4)	1.485(3)
N(5)-C(6)	1.493(3)	C(6)-C(7)	1.507(3)
C(7)-N(8)	1.487(3)	N(9)-C(17)	1.315(2)
N(9)-C(10)	1.423(2)	C(10)-C(11)	1.391(3)
C(10)-C(15)	1.392(3)	C(11)-C(12)	1.391(3)
C(12)-C(13)	1.395(3)	C(13)-C(14)	1.388(3)
C(13)-C(16)	1.509(3)	C(14)-C(15)	1.392(3)
C(17)-N(18)	1.336(3)	N(18)-C(19)	1.452(3)
C(19)-C(20)	1.508(3)	C(20)-N(25)	1.340(3)
C(20)-C(21)	1.392(3)	C(21)-C(22)	1.381(4)
C(22)-C(23)	1.384(4)	C(23)-C(24)	1.387(3)
C(24)-N(25)	1.343(3)	Co(2)-N(34)	1.9261(17)
Co(2)-N(30)	1.950(2)	Co(2)-N(29)	1.963(2)
Co(2)-N(26)	1.9704(19)	Co(2)-N(33)	1.9922(19)
Co(2)-S(2)	2.2996(6)	S(2)-C(42)	1.743(2)
N(26)-C(27B)	1.414(7)	N(26)-C(27A)	1.556(5)
C(27A)-C(28A)	1.507(6)	C(28A)-N(29)	1.431(4)
C(27B)-C(28B)	1.503(11)	C(28B)-N(29)	1.640(8)
N(30)-C(31B)	1.469(8)	N(30)-C(31A)	1.517(6)
C(31A)-C(32A)	1.504(8)	C(32A)-N(33)	1.495(5)
C(31B)-C(32B)	1.496(11)	C(32B)-N(33)	1.533(7)
N(34)-C(42)	1.312(3)	N(34)-C(35)	1.425(3)

C(35)-C(36)	1.389(3)	C(35)-C(40)	1.398(3)
C(36)-C(37)	1.391(3)	C(37)-C(38)	1.393(4)
C(38)-C(39)	1.378(4)	C(38)-C(41)	1.506(3)
C(39)-C(40)	1.388(3)	C(42)-N(43)	1.335(3)
N(43)-C(44)	1.452(3)	C(44)-C(45)	1.505(3)
C(45)-N(50)	1.340(3)	C(45)-C(46)	1.388(3)
C(46)-C(47)	1.395(4)	C(47)-C(48)	1.370(5)
C(48)-C(49)	1.374(4)	C(49)-N(50)	1.341(3)
Cl(1)-O(3A)	1.345(11)	Cl(1)-O(1)	1.421(2)
Cl(1)-O(2)	1.426(2)	Cl(1)-O(3B)	1.431(16)
Cl(1)-O(4)	1.448(3)	Cl(2)-O(7)	1.424(3)
Cl(2)-O(6)	1.439(2)	Cl(2)-O(12)	1.4410(19)
Cl(2)-O(8)	1.4426(19)	O(5)-Cl(3)	1.452(2)
Cl(3)-O(10)	1.4262(19)	Cl(3)-O(11)	1.428(2)
Cl(3)-O(9)	1.434(2)	Cl(4)-O(15A)	1.308(9)
Cl(4)-O(16A)	1.351(7)	Cl(4)-O(13)	1.411(4)
Cl(4)-O(16B)	1.428(6)	Cl(4)-O(15B)	1.429(9)
Cl(4)-O(14B)	1.441(6)	Cl(4)-O(14A)	1.465(4)

Table S2. Bond angles (°) for $[C_{18}H_{31}CoN_7S](ClO_4)_2 \cdot H_2O$ {**[Co-4a](ClO$_4$)$_2$·H$_2$O (*endo* isomer)**}. Standard deviations are in parentheses. The unit cell contained two cations unrelated by symmetry. Refer to Figure 5 for the numbering scheme.

N(9)-Co(1)-N(4)	91.73(7)	N(9)-Co(1)-N(8)	89.96(8)
N(4)-Co(1)-N(8)	177.74(8)	N(9)-Co(1)-N(1)	169.08(8)
N(4)-Co(1)-N(1)	85.21(8)	N(8)-Co(1)-N(1)	93.40(8)
N(9)-Co(1)-N(5)	98.05(7)	N(4)-Co(1)-N(5)	92.88(8)
N(8)-Co(1)-N(5)	85.39(8)	N(1)-Co(1)-N(5)	92.58(8)
N(9)-Co(1)-S(1)	72.11(5)	N(4)-Co(1)-S(1)	88.92(6)
N(8)-Co(1)-S(1)	93.02(6)	N(1)-Co(1)-S(1)	97.32(6)
N(5)-Co(1)-S(1)	170.05(6)	C(17)-S(1)-Co(1)	77.14(7)
C(2)-N(1)-Co(1)	110.01(14)	N(1)-C(2)-C(3)	106.71(19)
N(4)-C(3)-C(2)	106.97(19)	C(3)-N(4)-Co(1)	109.67(14)
C(6)-N(5)-Co(1)	109.49(14)	N(5)-C(6)-C(7)	107.07(18)
N(8)-C(7)-C(6)	107.0(2)	C(7)-N(8)-Co(1)	108.65(14)
C(17)-N(9)-C(10)	123.16(16)	C(17)-N(9)-Co(1)	101.18(12)
C(10)-N(9)-Co(1)	135.38(13)	C(11)-C(10)-C(15)	119.43(18)
C(11)-C(10)-N(9)	120.57(17)	C(15)-C(10)-N(9)	119.97(18)
C(12)-C(11)-C(10)	120.32(19)	C(11)-C(12)-C(13)	120.7(2)
C(14)-C(13)-C(12)	118.48(19)	C(14)-C(13)-C(16)	120.7(2)
C(12)-C(13)-C(16)	120.8(2)	C(13)-C(14)-C(15)	121.3(2)
C(10)-C(15)-C(14)	119.8(2)	N(9)-C(17)-N(18)	126.03(18)
N(9)-C(17)-S(1)	109.55(14)	N(18)-C(17)-S(1)	124.41(15)
C(17)-N(18)-C(19)	123.55(18)	N(18)-C(19)-C(20)	114.52(18)
N(25)-C(20)-C(21)	122.4(2)	N(25)-C(20)-C(19)	117.93(18)
C(21)-C(20)-C(19)	119.5(2)	C(22)-C(21)-C(20)	119.2(2)
C(21)-C(22)-C(23)	119.0(2)	C(22)-C(23)-C(24)	118.2(2)
N(25)-C(24)-C(23)	123.6(3)	C(20)-N(25)-C(24)	117.6(2)
N(34)-Co(2)-N(30)	91.73(8)	N(34)-Co(2)-N(29)	91.34(8)

N(30)-Co(2)-N(29)	176.91(9)	N(34)-Co(2)-N(26)	169.50(8)
N(30)-Co(2)-N(26)	91.82(9)	N(29)-Co(2)-N(26)	85.23(9)
N(34)-Co(2)-N(33)	95.18(8)	N(30)-Co(2)-N(33)	85.34(9)
N(29)-Co(2)-N(33)	93.99(8)	N(26)-Co(2)-N(33)	94.95(8)
N(34)-Co(2)-S(2)	71.97(5)	N(30)-Co(2)-S(2)	91.83(6)
N(29)-Co(2)-S(2)	89.49(6)	N(26)-Co(2)-S(2)	98.04(6)
N(33)-Co(2)-S(2)	166.79(6)	C(42)-S(2)-Co(2)	76.75(7)
C(27B)-N(26)-Co(2)	114.3(3)	C(27A)-N(26)-Co(2)	106.57(18)
C(28A)-C(27A)-N(26)	107.8(3)	N(29)-C(28A)-C(27A)	104.3(3)
N(26)-C(27B)-C(28B)	101.2(6)	C(27B)-C(28B)-N(29)	108.9(5)
C(28A)-N(29)-Co(2)	111.7(2)	C(28B)-N(29)-Co(2)	104.4(3)
C(31B)-N(30)-Co(2)	109.5(3)	C(31A)-N(30)-Co(2)	109.9(2)
C(32A)-C(31A)-N(30)	106.8(4)	N(33)-C(32A)-C(31A)	105.4(4)
N(30)-C(31B)-C(32B)	106.1(7)	C(31B)-C(32B)-N(33)	105.9(5)
C(32A)-N(33)-Co(2)	108.0(2)	C(32B)-N(33)-Co(2)	107.6(3)
C(42)-N(34)-C(35)	122.06(17)	C(42)-N(34)-Co(2)	102.07(13)
C(35)-N(34)-Co(2)	135.67(14)	C(36)-C(35)-C(40)	119.6(2)
C(36)-C(35)-N(34)	120.51(19)	C(40)-C(35)-N(34)	119.87(19)
C(35)-C(36)-C(37)	119.8(2)	C(36)-C(37)-C(38)	121.1(2)
C(39)-C(38)-C(37)	118.3(2)	C(39)-C(38)-C(41)	120.1(3)
C(37)-C(38)-C(41)	121.6(3)	C(38)-C(39)-C(40)	121.8(2)
C(39)-C(40)-C(35)	119.3(2)	N(34)-C(42)-N(43)	125.43(19)
N(34)-C(42)-S(2)	109.10(15)	N(43)-C(42)-S(2)	125.46(16)
C(42)-N(43)-C(44)	124.33(18)	N(43)-C(44)-C(45)	114.26(18)
N(50)-C(45)-C(46)	122.5(2)	N(50)-C(45)-C(44)	117.69(18)
C(46)-C(45)-C(44)	119.8(2)	C(45)-C(46)-C(47)	118.5(3)
C(48)-C(47)-C(46)	119.1(3)	C(47)-C(48)-C(49)	118.6(3)
N(50)-C(49)-C(48)	123.6(3)	C(45)-N(50)-C(49)	117.6(2)
O(3A)-Cl(1)-O(1)	116.2(4)	O(3A)-Cl(1)-O(2)	101.9(5)

O(1)-Cl(1)-O(2)	110.47(14)	O(1)-Cl(1)-O(3B)	107.8(6)
O(2)-Cl(1)-O(3B)	115.9(6)	O(3A)-Cl(1)-O(4)	110.6(3)
O(1)-Cl(1)-O(4)	107.83(18)	O(2)-Cl(1)-O(4)	109.6(2)
O(3B)-Cl(1)-O(4)	104.8(7)	O(7)-Cl(2)-O(6)	110.55(15)
O(7)-Cl(2)-O(12)	109.42(16)	O(6)-Cl(2)-O(12)	108.94(13)
O(7)-Cl(2)-O(8)	109.97(16)	O(6)-Cl(2)-O(8)	109.76(13)
O(12)-Cl(2)-O(8)	108.15(13)	O(10)-Cl(3)-O(11)	110.91(14)
O(10)-Cl(3)-O(9)	111.10(14)	O(11)-Cl(3)-O(9)	109.49(14)
O(10)-Cl(3)-O(5)	108.94(14)	O(11)-Cl(3)-O(5)	108.40(16)
O(9)-Cl(3)-O(5)	107.91(15)	O(15A)-Cl(4)-O(16A)	125.1(7)
O(15A)-Cl(4)-O(13)	111.0(8)	O(16A)-Cl(4)-O(13)	97.8(5)
O(15A)-Cl(4)-O(16B)	78.5(6)	O(13)-Cl(4)-O(16B)	110.1(4)
O(16A)-Cl(4)-O(15B)	148.8(7)	O(13)-Cl(4)-O(15B)	106.8(6)
O(16B)-Cl(4)-O(15B)	104.7(6)	O(15A)-Cl(4)-O(14B)	122.3(8)
O(16A)-Cl(4)-O(14B)	74.2(5)	O(13)-Cl(4)-O(14B)	119.7(3)
O(16B)-Cl(4)-O(14B)	106.4(6)	O(15B)-Cl(4)-O(14B)	108.2(6)
O(15A)-Cl(4)-O(14A)	112.5(5)	O(16A)-Cl(4)-O(14A)	111.2(4)
O(13)-Cl(4)-O(14A)	93.2(3)	O(16B)-Cl(4)-O(14A)	149.1(5)
O(15B)-Cl(4)-O(14A)	86.7(5)		

Table S3. Bond lengths (Å) for $[C_{17}H_{30}CoN_7S](ClO_4)_3 \cdot 0.5H_2O$ {**[Co-1a](ClO$_4$)$_3$·0.5H$_2$O (*hypodentate*)**}. Standard deviations are in parentheses. The unit cell contained two cations unrelated by symmetry. Refer to Figure 6 for the numbering scheme.

Co(1A)-N(2A)	1.850(5)	Co(1A)-N(3A)	1.952(5)
Co(1A)-N(5A)	1.976(5)	Co(1A)-N(4A)	1.983(5)
Co(1A)-N(1A)	1.982(5)	Co(1A)-S(1A)	2.3224(19)
S(1A)-C(7A)	1.737(7)	N(1A)-C(1A)	1.355(9)
N(1A)-C(5A)	1.359(8)	C(1A)-C(2A)	1.381(10)
C(2A)-C(3A)	1.375(11)	C(3A)-C(4A)	1.370(11)
C(4A)-C(5A)	1.365(9)	C(5A)-C(6A)	1.509(9)
C(6A)-N(2A)	1.448(8)	N(2A)-C(7A)	1.291(8)
C(7A)-N(7A)	1.369(8)	N(7A)-C(12A)	1.417(8)
N(3A)-C(8A)	1.494(8)	C(8A)-C(9A)	1.499(9)
C(9A)-N(4A)	1.489(8)	N(5A)-C(10A)	1.403(14)
C(10A)-C(11A)	1.554(15)	C(11A)-N(6A)	1.458(17)
C(10C)-C(11C)	1.566(17)	C(11C)-N(6C)	1.459(18)
C(12A)-C(17A)	1.374(9)	C(12A)-C(13A)	1.392(9)
C(13A)-C(14A)	1.369(10)	C(14A)-C(15A)	1.369(13)
C(15A)-C(16A)	1.392(13)	C(16A)-C(17A)	1.377(11)
Co(1B)-N(2B)	1.865(5)	Co(1B)-N(3D)	1.91(6)
Co(1B)-N(1B)	1.958(5)	Co(1B)-N(3B)	1.959(18)
Co(1B)-N(5B)	1.974(5)	Co(1B)-N(4D)	1.96(5)
Co(1B)-N(4B)	2.003(16)	Co(1B)-S(1B)	2.3002(17)
S(1B)-C(7B)	1.758(6)	N(1B)-C(5B)	1.344(7)
N(1B)-C(1B)	1.346(7)	C(1B)-C(2B)	1.370(8)
C(2B)-C(3B)	1.375(9)	C(3B)-C(4B)	1.384(8)
C(4B)-C(5B)	1.392(8)	C(5B)-C(6B)	1.517(8)
C(6B)-N(2B)	1.446(7)	N(2B)-C(7B)	1.292(7)
C(7B)-N(7B)	1.346(7)	N(7B)-C(12B)	1.411(7)

N(3B)-C(8B)	1.487(15)	C(8B)-C(9B)	1.468(10)
C(9B)-N(4B)	1.491(11)	N(3D)-C(8D)	1.49(2)
C(8D)-C(9D)	1.466(18)	C(9D)-N(4D)	1.494(19)
N(5B)-C(10B)	1.478(7)	C(10B)-C(11B)	1.519(9)
C(11B)-N(6B)	1.481(8)	C(12B)-C(17B)	1.396(8)
C(12B)-C(13B)	1.409(9)	C(13B)-C(14B)	1.374(9)
C(14B)-C(15B)	1.383(9)	C(15B)-C(16B)	1.382(9)
C(16B)-C(17B)	1.373(9)	Cl(1)-O(3)	1.433(5)
Cl(1)-O(2)	1.435(4)	Cl(1)-O(4)	1.444(5)
Cl(1)-O(1)	1.449(4)	Cl(2)-O(6)	1.430(4)
Cl(2)-O(5)	1.433(5)	Cl(2)-O(7)	1.440(5)
Cl(2)-O(8)	1.447(5)	Cl(3)-O(11)	1.407(5)
Cl(3)-O(9)	1.428(5)	Cl(3)-O(12)	1.433(5)
Cl(3)-O(10)	1.441(5)	Cl(4)-O(16)	1.419(5)
Cl(4)-O(14)	1.438(5)	Cl(4)-O(13)	1.450(5)
Cl(4)-O(15)	1.450(5)	Cl(5)-O(19)	1.282(15)
Cl(5)-O(17)	1.429(10)	Cl(5)-O(18)	1.509(12)
Cl(5)-O(20)	1.485(17)	Cl(5')-O(19')	1.287(18)
Cl(5')-O(17')	1.425(12)	Cl(5')-O(20')	1.479(19)
Cl(5')-O(18')	1.521(15)	Cl(6)-O(23)	1.422(10)
Cl(6)-O(21)	1.422(10)	Cl(6)-O(24)	1.433(9)
Cl(6)-O(22)	1.479(9)	Cl(6')-O(23')	1.420(13)
Cl(6')-O(21')	1.423(13)	Cl(6')-O(22')	1.455(12)
Cl(6')-O(24')	1.477(12)		
O(1W)-H(1W1)	0.838(10)	O(1W)-H(2W1)	0.838(10)

Table S4. Bond angles (°) for $[C_{17}H_{30}CoN_7S](ClO_4)_3 \cdot 0.5H_2O$ {**[Co-1a](ClO$_4$)$_3$·0.5H$_2$O (*hypodentate*)**}. Standard deviations are in parentheses. The unit cell contained two cations unrelated by symmetry. Refer to Figure 6 for the numbering scheme.

N(2A)-Co(1A)-N(3A)	91.2(2)	N(2A)-Co(1A)-N(5A)	93.2(3)
N(3A)-Co(1A)-N(5A)	175.3(3)	N(2A)-Co(1A)-N(4A)	174.5(2)
N(3A)-Co(1A)-N(4A)	84.8(2)	N(5A)-Co(1A)-N(4A)	90.7(2)
N(2A)-Co(1A)-N(1A)	81.6(2)	N(3A)-Co(1A)-N(1A)	93.6(2)
N(5A)-Co(1A)-N(1A)	88.8(2)	N(4A)-Co(1A)-N(1A)	102.4(2)
N(2A)-Co(1A)-S(1A)	71.17(17)	N(3A)-Co(1A)-S(1A)	88.20(17)
N(5A)-Co(1A)-S(1A)	91.53(16)	N(4A)-Co(1A)-S(1A)	104.85(16)
N(1A)-Co(1A)-S(1A)	152.77(18)	C(7A)-S(1A)-Co(1A)	75.4(2)
C(1A)-N(1A)-C(5A)	118.2(6)	C(1A)-N(1A)-Co(1A)	126.5(5)
C(5A)-N(1A)-Co(1A)	114.9(4)	N(1A)-C(1A)-C(2A)	120.9(8)
C(3A)-C(2A)-C(1A)	120.0(8)	C(4A)-C(3A)-C(2A)	119.0(7)
C(5A)-C(4A)-C(3A)	119.2(8)	N(1A)-C(5A)-C(4A)	122.4(7)
N(1A)-C(5A)-C(6A)	115.6(6)	C(4A)-C(5A)-C(6A)	122.0(7)
N(2A)-C(6A)-C(5A)	106.1(5)	C(7A)-N(2A)-C(6A)	132.7(6)
C(7A)-N(2A)-Co(1A)	105.7(4)	C(6A)-N(2A)-Co(1A)	121.5(4)
N(2A)-C(7A)-N(7A)	124.7(6)	N(2A)-C(7A)-S(1A)	107.6(5)
N(7A)-C(7A)-S(1A)	127.6(5)	C(7A)-N(7A)-C(12A)	125.2(6)
C(8A)-N(3A)-Co(1A)	109.2(4)	N(3A)-C(8A)-C(9A)	106.6(5)
N(4A)-C(9A)-C(8A)	106.0(5)	C(9A)-N(4A)-Co(1A)	109.8(4)
C(10A)-N(5A)-Co(1A)	124.3(7)	N(5A)-C(10A)-C(11A)	115.9(12)
N(6A)-C(11A)-C(10A)	111.9(12)	N(6C)-C(11C)-C(10C)	110.4(15)
C(17A)-C(12A)-C(13A)	120.8(7)	C(17A)-C(12A)-N(7A)	119.8(6)
C(13A)-C(12A)-N(7A)	119.3(6)	C(14A)-C(13A)-C(12A)	118.7(7)
C(15A)-C(14A)-C(13A)	122.0(8)	C(14A)-C(15A)-C(16A)	118.2(8)
C(17A)-C(16A)-C(15A)	121.4(8)	C(12A)-C(17A)-C(16A)	118.9(8)
N(2B)-Co(1B)-N(3D)	93.2(8)	N(2B)-Co(1B)-N(1B)	83.3(2)

N(3D)-Co(1B)-N(1B)	91(3)	N(2B)-Co(1B)-N(3B)	90.1(3)
N(1B)-Co(1B)-N(3B)	90.6(9)	N(2B)-Co(1B)-N(5B)	94.4(2)
N(3D)-Co(1B)-N(5B)	172.3(9)	N(1B)-Co(1B)-N(5B)	90.8(2)
N(3B)-Co(1B)-N(5B)	175.5(3)	N(2B)-Co(1B)-N(4D)	174(2)
N(3D)-Co(1B)-N(4D)	86.8(10)	N(1B)-Co(1B)-N(4D)	102(2)
N(5B)-Co(1B)-N(4D)	85.6(8)	N(2B)-Co(1B)-N(4B)	172.7(5)
N(1B)-Co(1B)-N(4B)	101.7(7)	N(3B)-Co(1B)-N(4B)	84.6(3)
N(5B)-Co(1B)-N(4B)	90.9(3)	N(2B)-Co(1B)-S(1B)	71.54(15)
N(3D)-Co(1B)-S(1B)	90(3)	N(1B)-Co(1B)-S(1B)	154.89(15)
N(3B)-Co(1B)-S(1B)	89.1(9)	N(5B)-Co(1B)-S(1B)	91.47(16)
N(4D)-Co(1B)-S(1B)	103(2)	N(4B)-Co(1B)-S(1B)	103.3(7)
C(7B)-S(1B)-Co(1B)	76.2(2)	C(5B)-N(1B)-C(1B)	118.5(5)
C(5B)-N(1B)-Co(1B)	113.8(4)	C(1B)-N(1B)-Co(1B)	127.6(4)
N(1B)-C(1B)-C(2B)	122.7(6)	C(1B)-C(2B)-C(3B)	119.1(6)
C(2B)-C(3B)-C(4B)	119.0(6)	C(3B)-C(4B)-C(5B)	119.1(6)
N(1B)-C(5B)-C(4B)	121.5(5)	N(1B)-C(5B)-C(6B)	117.4(5)
C(4B)-C(5B)-C(6B)	121.2(5)	N(2B)-C(6B)-C(5B)	106.1(5)
C(7B)-N(2B)-C(6B)	134.9(5)	C(7B)-N(2B)-Co(1B)	105.7(4)
C(6B)-N(2B)-Co(1B)	119.4(4)	N(2B)-C(7B)-N(7B)	126.6(6)
N(2B)-C(7B)-S(1B)	106.5(4)	N(7B)-C(7B)-S(1B)	126.8(5)
C(7B)-N(7B)-C(12B)	127.5(5)	C(8B)-N(3B)-Co(1B)	109.2(8)
C(9B)-C(8B)-N(3B)	107.1(11)	C(8B)-C(9B)-N(4B)	107.1(9)
C(9B)-N(4B)-Co(1B)	108.3(8)	C(8D)-N(3D)-Co(1B)	109(3)
C(9D)-C(8D)-N(3D)	108(2)	C(8D)-C(9D)-N(4D)	108(2)
C(9D)-N(4D)-Co(1B)	108(2)	C(10B)-N(5B)-Co(1B)	118.5(4)
N(5B)-C(10B)-C(11B)	113.0(5)	N(6B)-C(11B)-C(10B)	109.3(5)
C(17B)-C(12B)-C(13B)	119.5(6)	C(17B)-C(12B)-N(7B)	118.5(6)
C(13B)-C(12B)-N(7B)	122.0(6)	C(14B)-C(13B)-C(12B)	119.3(6)
C(13B)-C(14B)-C(15B)	121.1(7)	C(16B)-C(15B)-C(14B)	119.3(7)

C(17B)-C(16B)-C(15B)	121.2(6)	C(16B)-C(17B)-C(12B)	119.6(6)
O(3)-Cl(1)-O(2)	109.5(3)	O(3)-Cl(1)-O(4)	110.5(3)
O(2)-Cl(1)-O(4)	109.7(3)	O(3)-Cl(1)-O(1)	109.5(3)
O(2)-Cl(1)-O(1)	109.6(3)	O(4)-Cl(1)-O(1)	107.9(3)
O(6)-Cl(2)-O(5)	110.0(3)	O(6)-Cl(2)-O(7)	110.2(3)
O(5)-Cl(2)-O(7)	109.5(3)	O(6)-Cl(2)-O(8)	109.9(3)
O(5)-Cl(2)-O(8)	110.4(3)	O(7)-Cl(2)-O(8)	106.8(3)
O(11)-Cl(3)-O(9)	112.9(3)	O(11)-Cl(3)-O(12)	108.8(4)
O(9)-Cl(3)-O(12)	107.9(3)	O(11)-Cl(3)-O(10)	108.4(3)
O(9)-Cl(3)-O(10)	109.2(3)	O(12)-Cl(3)-O(10)	109.6(4)
O(16)-Cl(4)-O(14)	109.1(3)	O(16)-Cl(4)-O(13)	109.0(4)
O(14)-Cl(4)-O(13)	108.1(3)	O(16)-Cl(4)-O(15)	111.9(3)
O(14)-Cl(4)-O(15)	109.2(3)	O(13)-Cl(4)-O(15)	109.4(3)
O(19)-Cl(5)-O(17)	110.2(12)	O(19)-Cl(5)-O(18)	108.5(10)
O(17)-Cl(5)-O(18)	102.2(11)	O(19)-Cl(5)-O(20)	118.5(10)
O(17)-Cl(5)-O(20)	113.7(12)	O(18)-Cl(5)-O(20)	102.0(8)
O(19')-Cl(5')-O(17')	109.7(19)	O(19')-Cl(5')-O(20')	120.1(15)
O(17')-Cl(5')-O(20')	112.2(18)	O(19')-Cl(5')-O(18')	107.6(13)
O(17')-Cl(5')-O(18')	102.7(18)	O(20')-Cl(5')-O(18')	102.7(13)
O(23)-Cl(6)-O(21)	111.5(9)	O(23)-Cl(6)-O(24)	111.8(7)
O(21)-Cl(6)-O(24)	107.7(9)	O(23)-Cl(6)-O(22)	109.3(8)
O(21)-Cl(6)-O(22)	107.9(8)	O(24)-Cl(6)-O(22)	108.5(6)
O(23')-Cl(6')-O(21')	110.4(14)	O(23')-Cl(6')-O(22')	110.1(12)
O(21')-Cl(6')-O(22')	112.1(14)	O(23')-Cl(6')-O(24')	110.9(11)
O(21')-Cl(6')-O(24')	106.0(15)	O(22')-Cl(6')-O(24')	107.2(10)
H(1W1)-O(1W)-H(2W1)	105(3)		

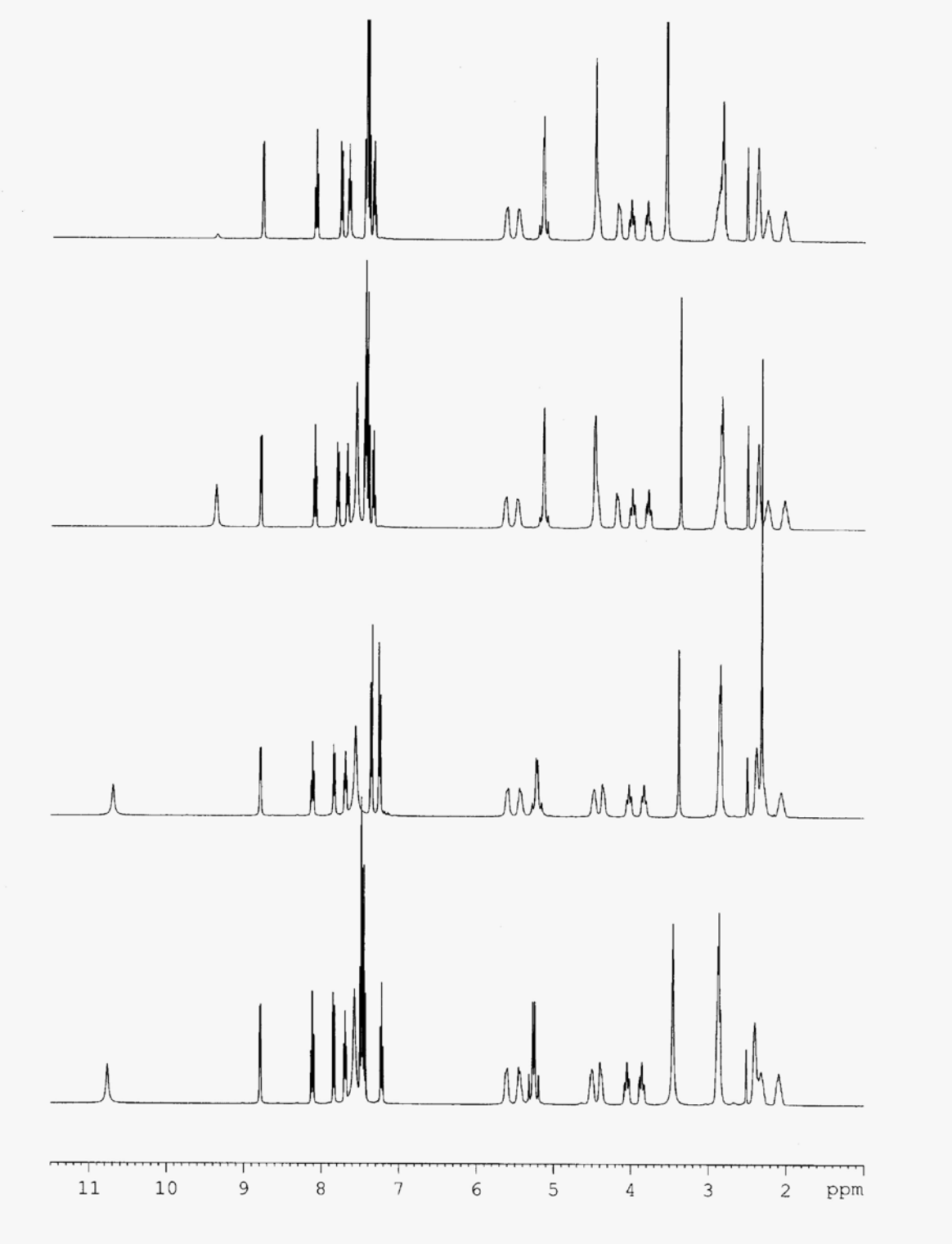

Figure S1. ^{1}H NMR of the hypodentate complexes **Co-1a**$^{3+}$ (lower) followed by **Co-1b**$^{3+}$ and **Co-2**$^{3+}$ in d_6-DMSO. The upper spectrum is that of **Co-2**$^{3+}$ in d_6-DMSO after three drops of D_2O have been added.

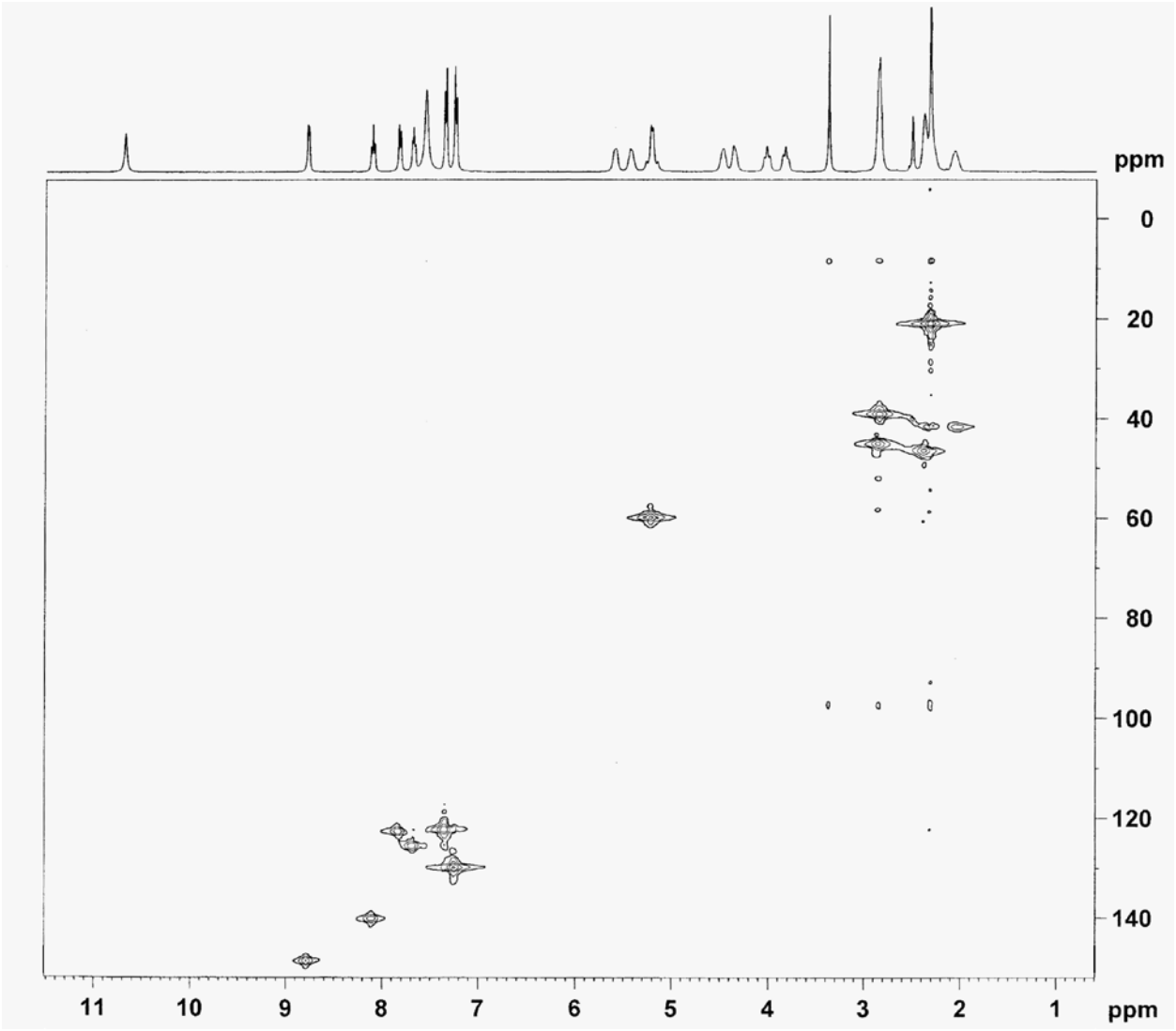

Figure S2. HMQC NMR of the hypodentate complex **Co-1b**$^{3+}$ in d_6-DMSO.

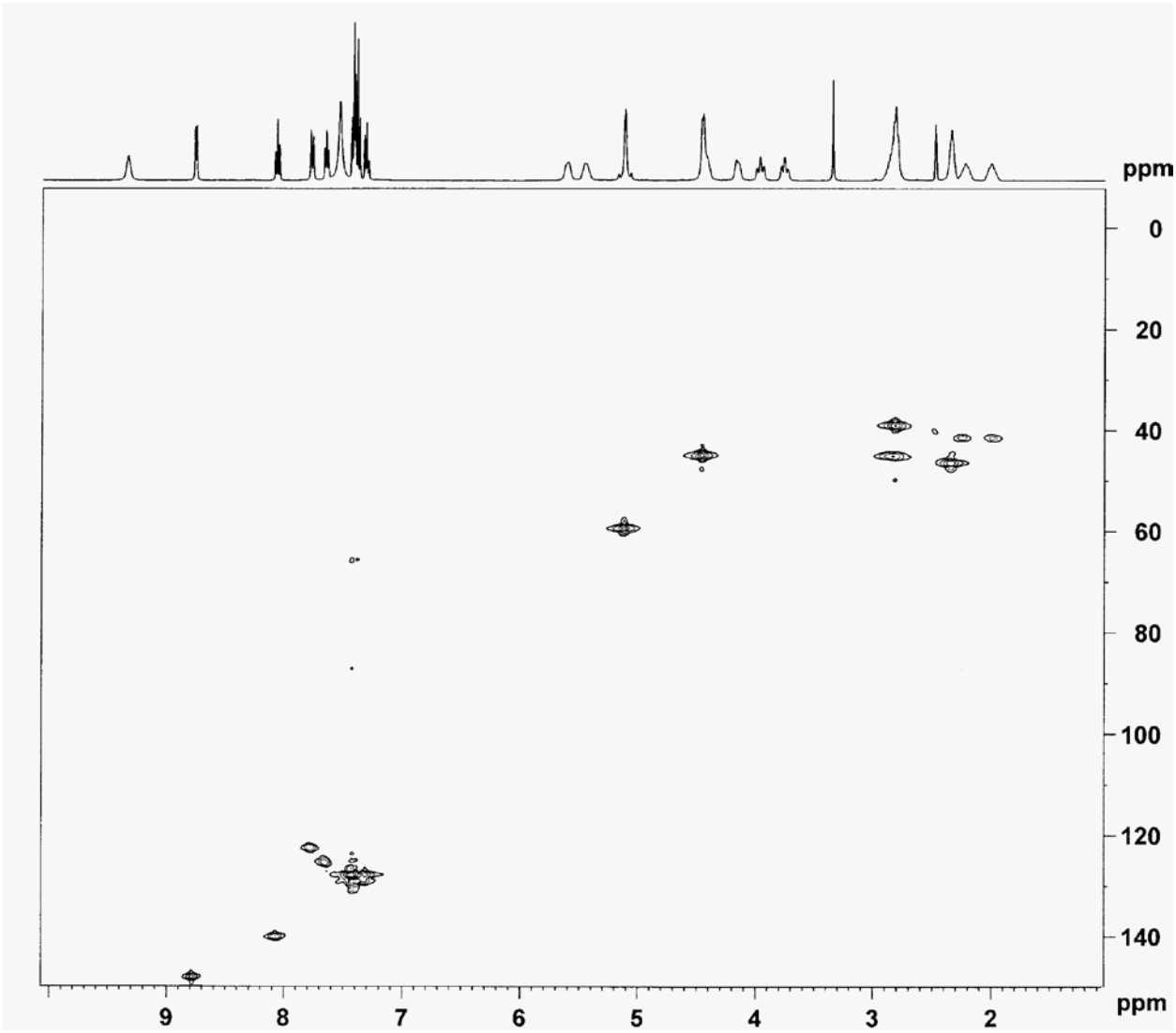

Figure S3. HMQC NMR of the hypodentate complex **Co-2**$^{3+}$ in d_6-DMSO.