Supporting Information

For

First-Row Transition Metal Complexes of ENENES Ligands: The Ability of the Thioether Donor to Impact the Coordination Chemistry

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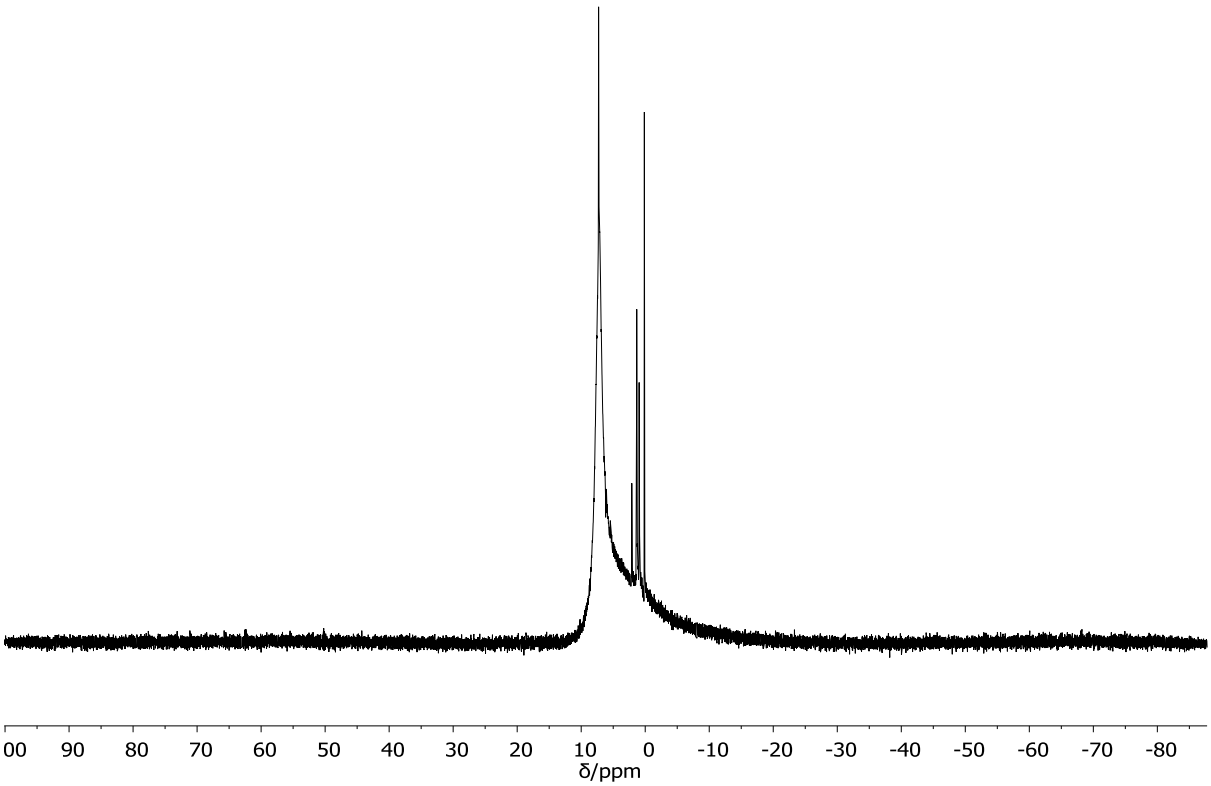

Figure S1. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Mn complex **1** after filtration.

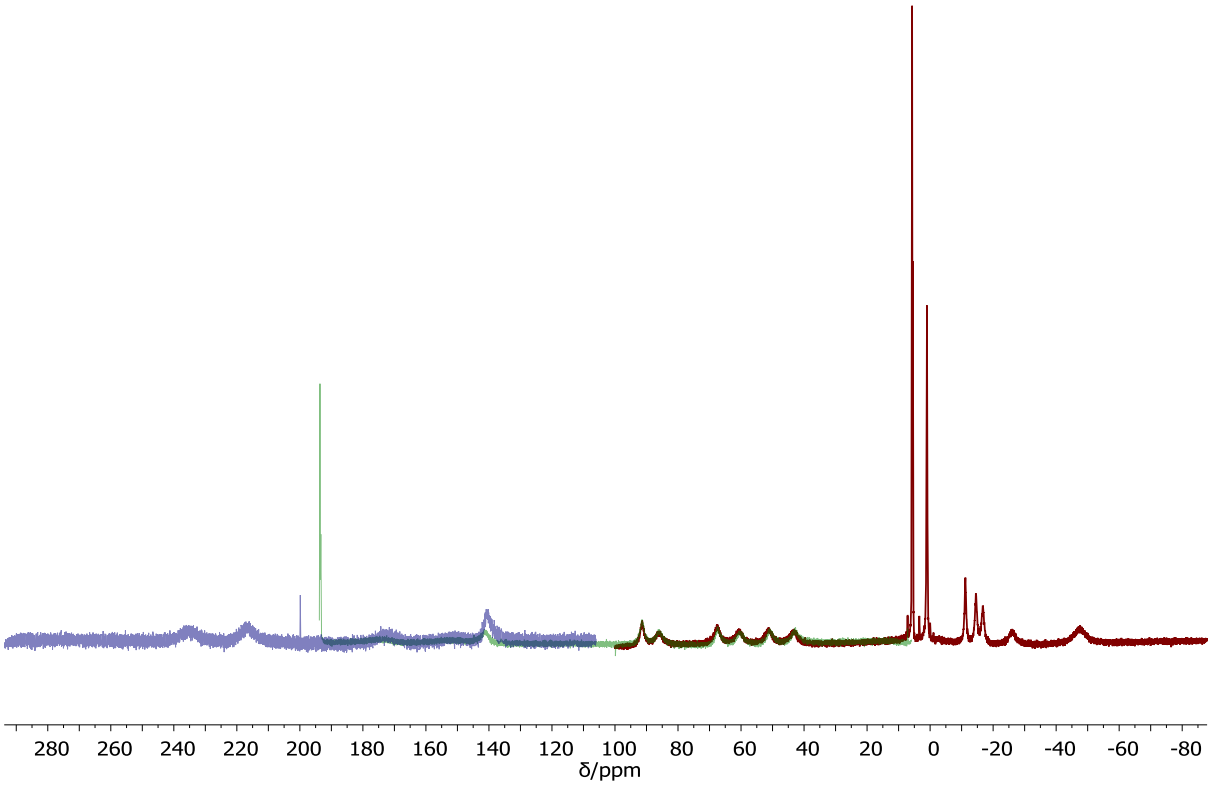

Figure S2. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Fe complex **2**; each spectrum in regions shown were taken separately and superimposed to give spectrum shown.

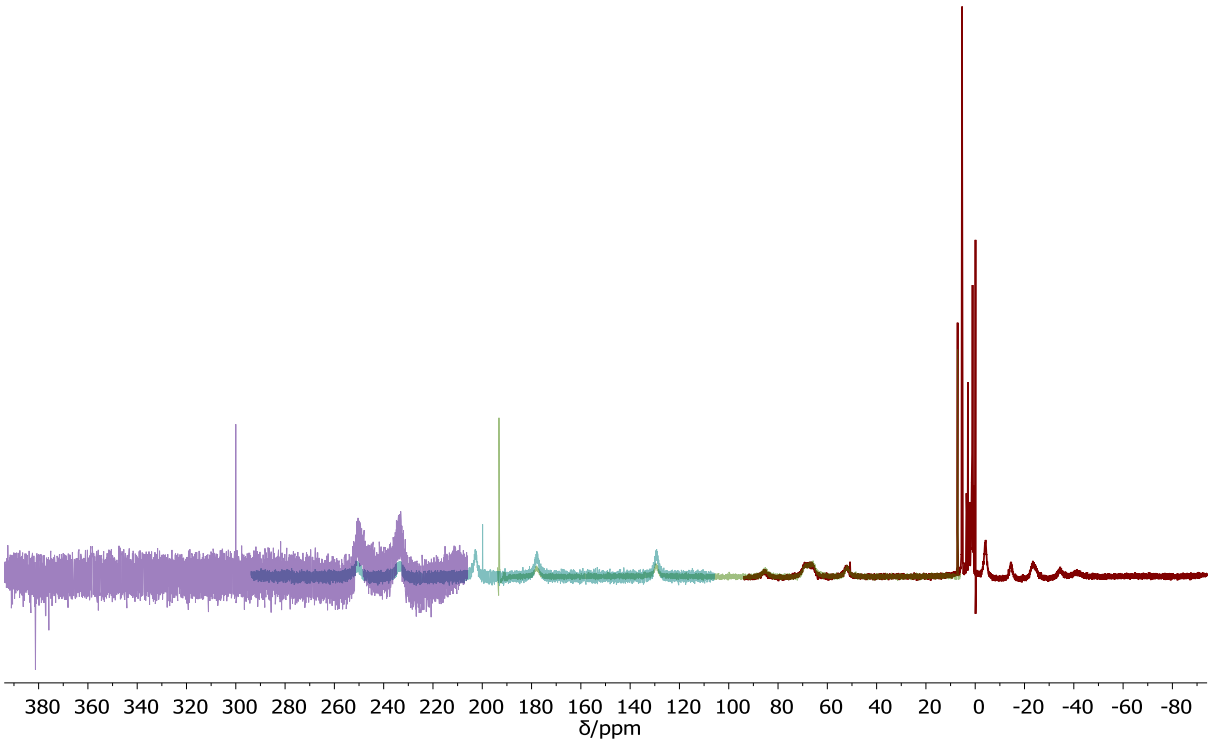

Figure S3. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Co complex **3** after filtration; each spectrum in regions shown were taken separately and superimposed to give spectrum shown.

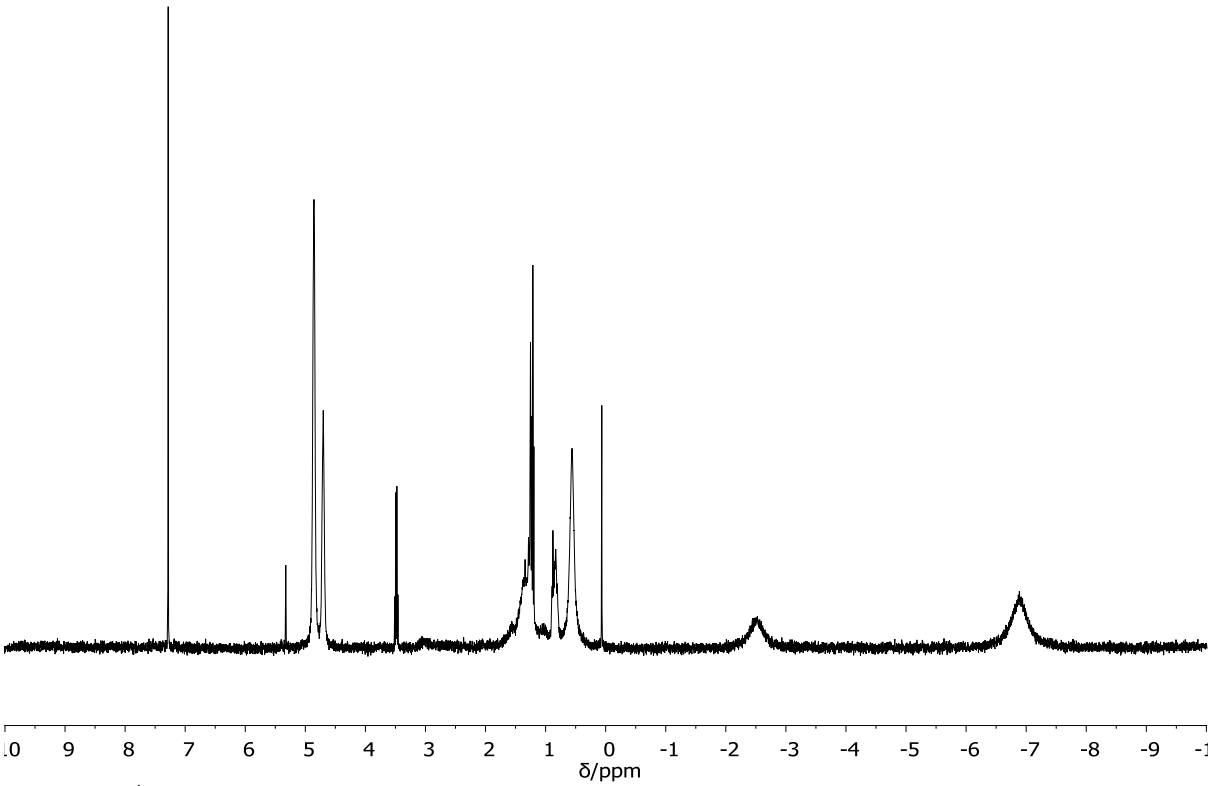

Figure S4. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Co complex **4** after filtration**.**

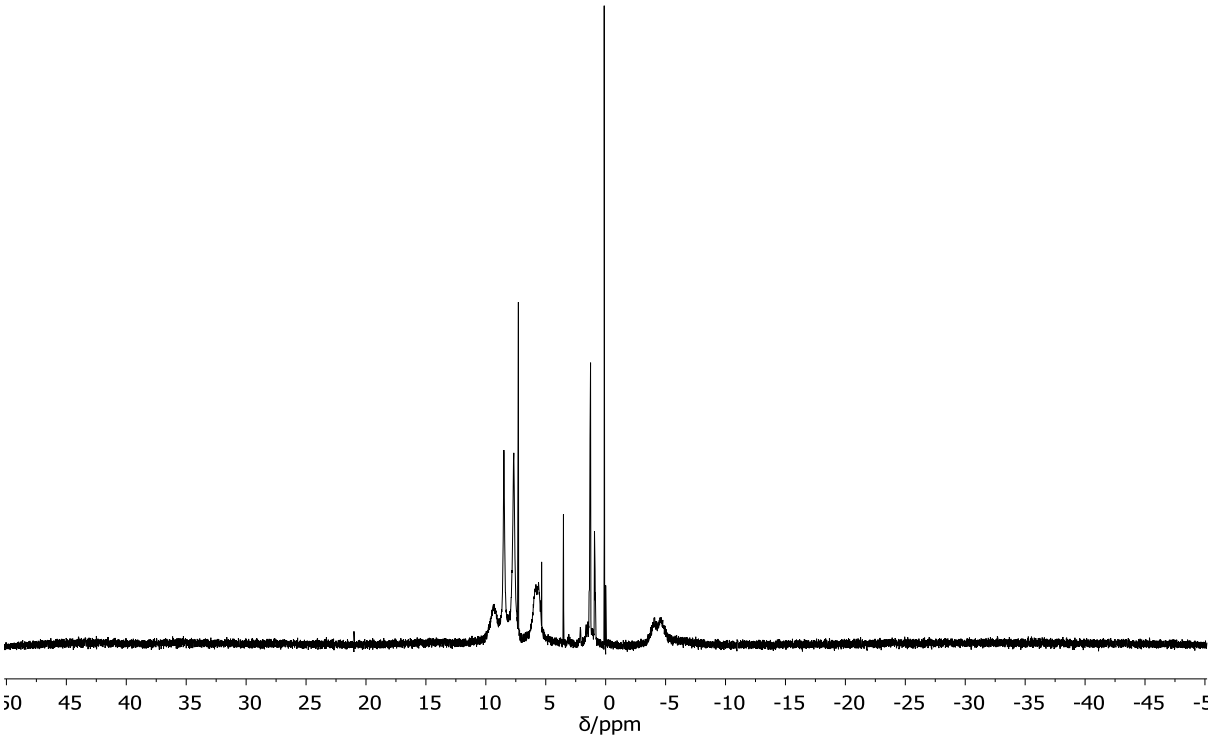

Figure S5. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Ni complex **5** after filtration**.**

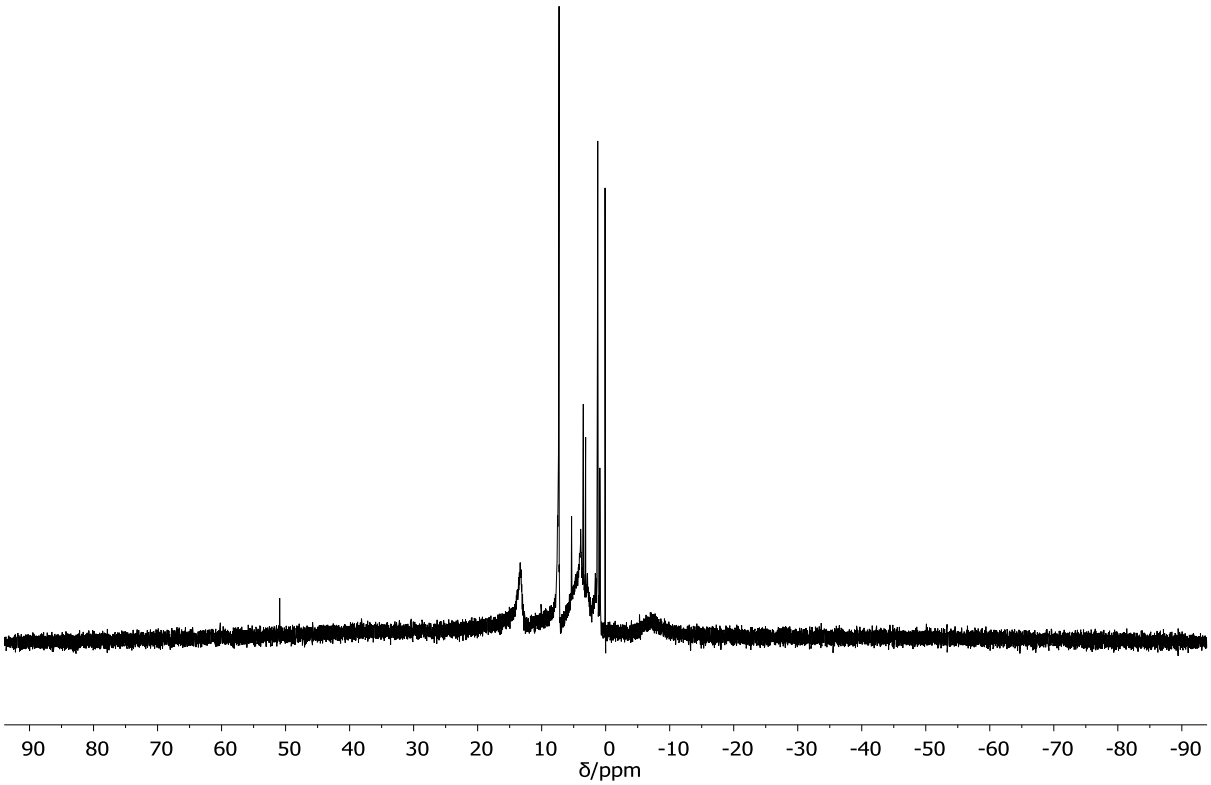

Figure S6. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Cu complex **6** after filtration**.**

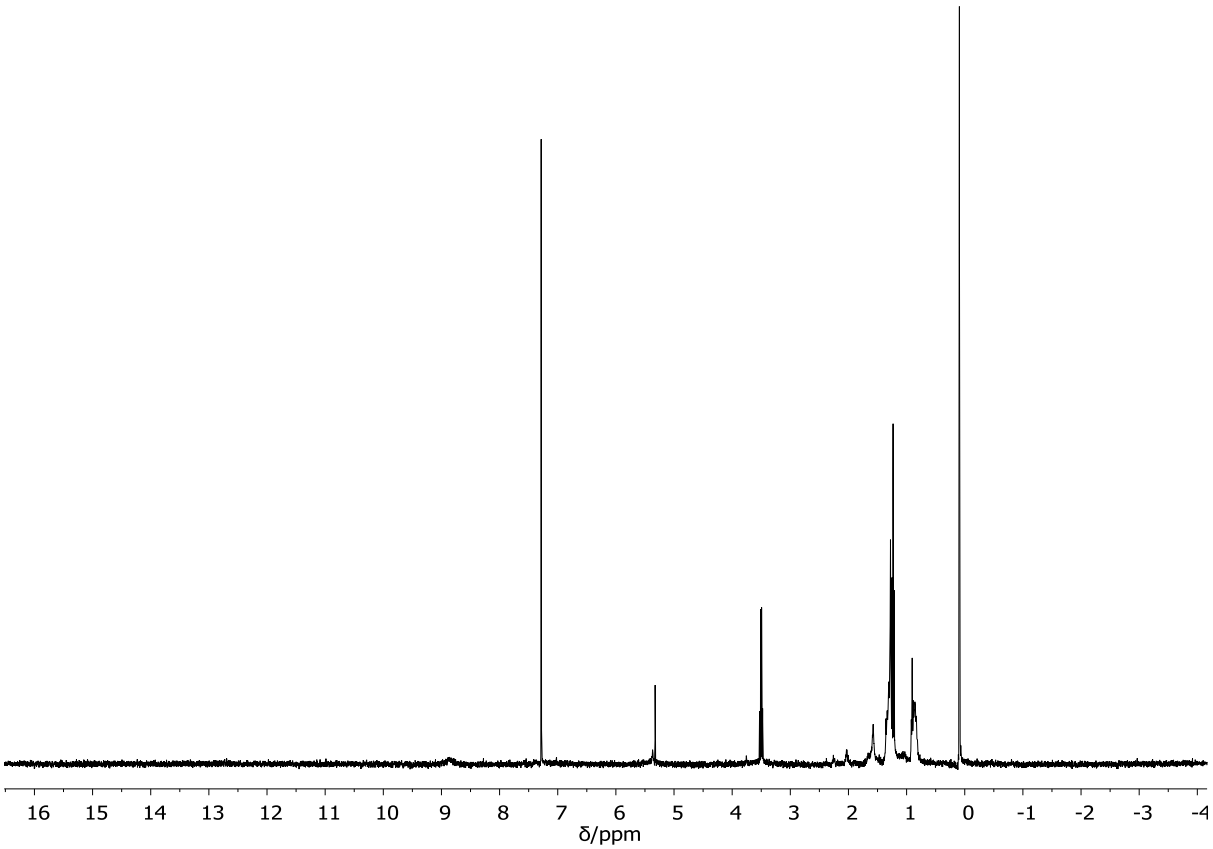

Figure S7. ^{1}H NMR (rd = 1s, 400 MHz, $CDCl_3$) spectrum of Cu complex **7** after filtration**.**

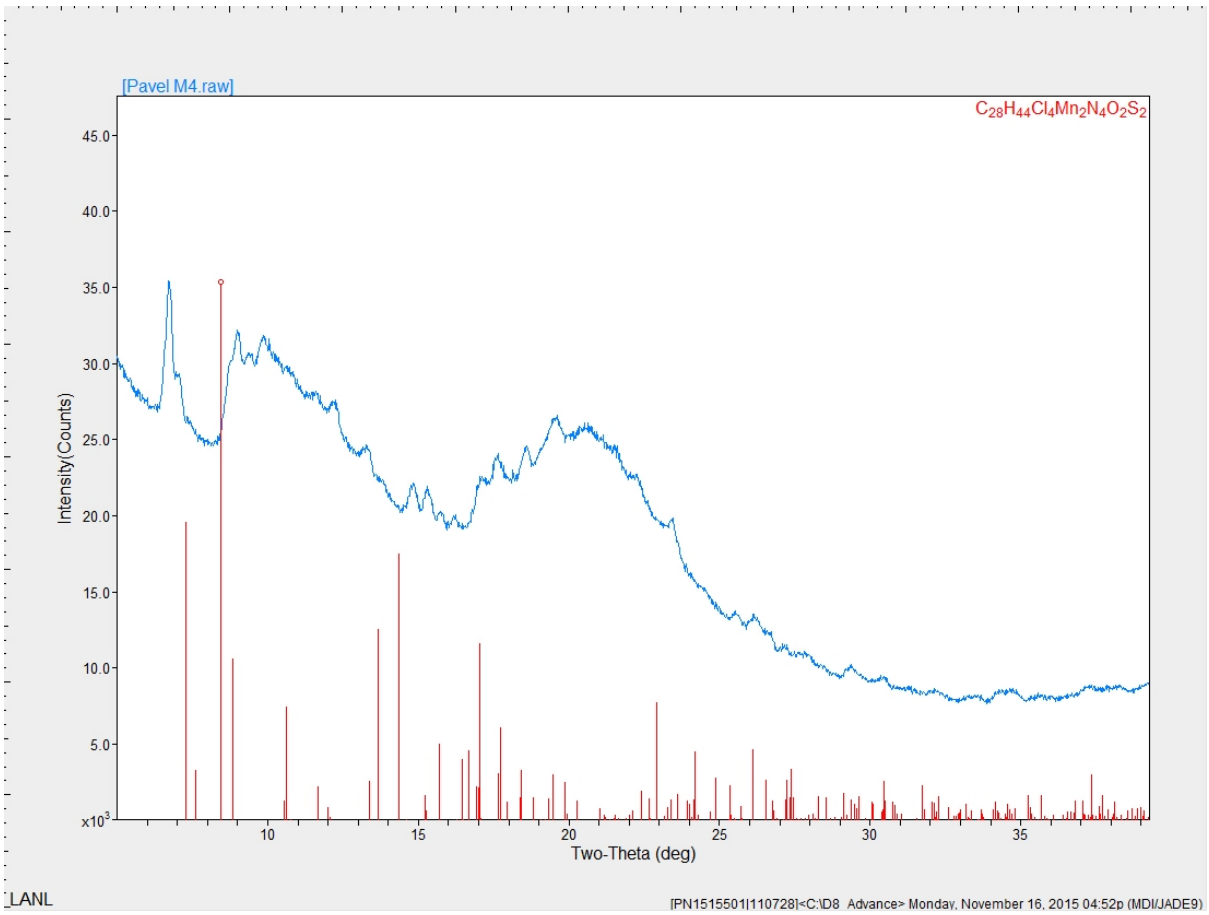

Figure S8. X-Ray powder diffraction (XRD) pattern observed for **1** (blue) and predicted for **1'** (red).

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For complex **1'**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	5939(1)	11012(1)	9662(1)	12(1)
Mn(2)	7102(1)	8512(1)	9321(1)	13(1)
S(1)	8496(1)	11597(1)	11967(1)	17(1)
S(2)	10054(1)	5951(1)	10697(1)	22(1)
Cl(1)	5457(1)	9682(1)	8841(1)	15(1)
Cl(2)	7941(1)	10554(1)	9622(1)	15(1)
Cl(3)	6110(1)	9001(1)	10234(1)	14(1)
Cl(4)	6200(1)	6655(1)	9169(1)	21(1)
N(1)	6372(2)	11988(2)	10461(1)	13(1)
N(2)	5762(2)	12904(2)	9336(1)	15(1)
N(3)	8615(2)	7729(2)	9879(1)	16(1)
N(4)	8266(2)	8221(2)	8670(1)	16(1)
O(1)	5850(2)	13021(2)	8172(1)	28(1)
O(2)	7455(2)	9374(2)	7623(1)	23(1)
C(1)	8618(2)	10084(2)	12071(1)	15(1)
C(2)	7957(2)	9252(2)	11757(1)	18(1)
C(3)	8125(2)	8092(2)	11886(1)	21(1)
C(4)	8937(2)	7749(2)	12328(1)	22(1)
C(5)	9603(2)	8578(2)	12642(1)	22(1)
C(6)	9462(2)	9737(2)	12510(1)	18(1)
C(7)	7217(2)	11802(2)	11468(1)	16(1)
C(8)	7351(2)	11582(2)	10871(1)	17(1)
C(9)	6429(2)	13232(2)	10342(1)	19(1)
C(10)	5595(2)	13565(2)	9833(1)	21(1)
C(11)	6754(2)	13347(2)	9130(1)	19(1)
C(12)	6824(2)	12809(3)	8580(1)	26(1)
C(13)	4885(2)	12598(3)	8352(1)	27(1)
C(14)	4764(2)	13146(2)	8894(1)	22(1)
C(15)	9458(2)	5419(2)	11254(1)	17(1)
C(16)	10168(2)	5053(2)	11734(1)	21(1)
C(17)	9715(3)	4609(2)	12170(1)	25(1)
C(18)	8569(3)	4544(2)	12129(1)	30(1)
C(19)	7861(3)	4911(2)	11650(1)	28(1)
C(20)	8298(2)	5340(2)	11209(1)	24(1)

C(21)	9969(2)	7506(2)	10794(1)	19(1)
C(22)	8911(2)	8068(2)	10468(1)	18(1)
C(23)	9545(2)	7841(2)	9574(1)	20(1)
C(24)	9149(2)	7460(2)	8983(1)	19(1)
C(25)	8794(2)	9284(2)	8493(1)	20(1)
C(26)	7940(2)	9995(2)	8106(1)	21(1)
C(27)	6925(2)	8360(2)	7779(1)	20(1)
C(28)	7750(2)	7595(2)	8153(1)	20(1)

Table S2. Bond lengths [Å] and angles [°] for complex **1'**.

Mn(1)-N(1)	2.247(2)
Mn(1)-N(2)	2.333(2)
Mn(1)-Cl(2)	2.5143(9)
Mn(1)-Cl(1)	2.5245(8)
Mn(1)-Cl(3)#1	2.5546(9)
Mn(1)-Cl(3)	2.7116(8)
Mn(2)-N(3)	2.269(2)
Mn(2)-N(4)	2.359(2)
Mn(2)-Cl(4)	2.4143(9)
Mn(2)-Cl(1)	2.5204(8)
Mn(2)-Cl(2)	2.6283(8)
Mn(2)-Cl(3)	2.8052(8)
S(1)-C(1)	1.775(3)
S(1)-C(7)	1.809(3)
S(2)-C(15)	1.780(3)
S(2)-C(21)	1.824(3)
Cl(3)-Mn(1)#1	2.5546(9)
N(1)-C(9)	1.476(3)
N(1)-C(8)	1.485(3)
N(2)-C(11)	1.488(3)
N(2)-C(10)	1.490(3)
N(2)-C(14)	1.498(3)
N(3)-C(23)	1.478(3)
N(3)-C(22)	1.481(3)
N(4)-C(24)	1.489(3)
N(4)-C(25)	1.493(3)
N(4)-C(28)	1.498(3)

O(1)-C(13)	1.420(3)
O(1)-C(12)	1.424(3)
O(2)-C(26)	1.421(3)
O(2)-C(27)	1.428(3)
C(1)-C(2)	1.393(4)
C(1)-C(6)	1.404(4)
C(2)-C(3)	1.388(4)
C(3)-C(4)	1.383(4)
C(4)-C(5)	1.393(4)
C(5)-C(6)	1.386(4)
C(7)-C(8)	1.533(3)
C(9)-C(10)	1.509(4)
C(11)-C(12)	1.509(4)
C(13)-C(14)	1.511(4)
C(15)-C(16)	1.392(4)
C(15)-C(20)	1.398(4)
C(16)-C(17)	1.396(4)
C(17)-C(18)	1.381(4)
C(18)-C(19)	1.390(4)
C(19)-C(20)	1.392(4)
C(21)-C(22)	1.528(4)
C(23)-C(24)	1.511(4)
C(25)-C(26)	1.514(4)
C(27)-C(28)	1.513(4)

N(1)-Mn(1)-N(2)	79.59(8)
N(1)-Mn(1)-Cl(2)	94.18(5)
N(2)-Mn(1)-Cl(2)	102.23(5)
N(1)-Mn(1)-Cl(1)	172.51(6)
N(2)-Mn(1)-Cl(1)	107.83(6)
Cl(2)-Mn(1)-Cl(1)	85.36(2)
N(1)-Mn(1)-Cl(3)#1	89.18(5)
N(2)-Mn(1)-Cl(3)#1	90.70(5)
Cl(2)-Mn(1)-Cl(3)#1	167.02(3)
Cl(1)-Mn(1)-Cl(3)#1	89.68(2)
N(1)-Mn(1)-Cl(3)	89.71(6)
N(2)-Mn(1)-Cl(3)	168.73(5)
Cl(2)-Mn(1)-Cl(3)	81.93(2)
Cl(1)-Mn(1)-Cl(3)	82.82(3)

Cl(3)#1-Mn(1)-Cl(3)	85.56(2)
N(3)-Mn(2)-N(4)	80.35(7)
N(3)-Mn(2)-Cl(4)	91.72(6)
N(4)-Mn(2)-Cl(4)	94.64(6)
N(3)-Mn(2)-Cl(1)	168.99(6)
N(4)-Mn(2)-Cl(1)	106.43(6)
Cl(4)-Mn(2)-Cl(1)	96.27(3)
N(3)-Mn(2)-Cl(2)	87.84(6)
N(4)-Mn(2)-Cl(2)	93.98(6)
Cl(4)-Mn(2)-Cl(2)	171.17(3)
Cl(1)-Mn(2)-Cl(2)	83.09(3)
N(3)-Mn(2)-Cl(3)	91.04(6)
N(4)-Mn(2)-Cl(3)	168.65(6)
Cl(4)-Mn(2)-Cl(3)	93.00(2)
Cl(1)-Mn(2)-Cl(3)	81.02(2)
Cl(2)-Mn(2)-Cl(3)	78.19(2)
C(1)-S(1)-C(7)	105.39(12)
C(15)-S(2)-C(21)	101.59(12)
Mn(2)-Cl(1)-Mn(1)	84.74(2)
Mn(1)-Cl(2)-Mn(2)	82.73(2)
Mn(1)#1-Cl(3)-Mn(1)	94.44(2)
Mn(1)#1-Cl(3)-Mn(2)	131.03(3)
Mn(1)-Cl(3)-Mn(2)	76.07(2)
C(9)-N(1)-C(8)	112.5(2)
C(9)-N(1)-Mn(1)	109.27(15)
C(8)-N(1)-Mn(1)	117.45(15)
C(11)-N(2)-C(10)	110.5(2)
C(11)-N(2)-C(14)	106.58(19)
C(10)-N(2)-C(14)	106.5(2)
C(11)-N(2)-Mn(1)	114.50(15)
C(10)-N(2)-Mn(1)	102.61(15)
C(14)-N(2)-Mn(1)	115.83(16)
C(23)-N(3)-C(22)	114.1(2)
C(23)-N(3)-Mn(2)	105.54(15)
C(22)-N(3)-Mn(2)	120.42(15)
C(24)-N(4)-C(25)	109.4(2)
C(24)-N(4)-C(28)	107.5(2)
C(25)-N(4)-C(28)	106.6(2)
C(24)-N(4)-Mn(2)	101.47(15)

C(25)-N(4)-Mn(2)	115.37(15)
C(28)-N(4)-Mn(2)	116.09(15)
C(13)-O(1)-C(12)	110.2(2)
C(26)-O(2)-C(27)	109.16(19)
C(2)-C(1)-C(6)	119.4(2)
C(2)-C(1)-S(1)	125.5(2)
C(6)-C(1)-S(1)	115.07(19)
C(3)-C(2)-C(1)	120.0(2)
C(4)-C(3)-C(2)	120.8(3)
C(3)-C(4)-C(5)	119.5(3)
C(6)-C(5)-C(4)	120.4(3)
C(5)-C(6)-C(1)	119.9(2)
C(8)-C(7)-S(1)	113.40(17)
N(1)-C(8)-C(7)	112.5(2)
N(1)-C(9)-C(10)	111.5(2)
N(2)-C(10)-C(9)	112.2(2)
N(2)-C(11)-C(12)	110.6(2)
O(1)-C(12)-C(11)	112.5(2)
O(1)-C(13)-C(14)	110.9(2)
N(2)-C(14)-C(13)	111.3(2)
C(16)-C(15)-C(20)	120.2(3)
C(16)-C(15)-S(2)	118.9(2)
C(20)-C(15)-S(2)	120.9(2)
C(15)-C(16)-C(17)	119.6(3)
C(18)-C(17)-C(16)	120.3(3)
C(17)-C(18)-C(19)	120.0(3)
C(18)-C(19)-C(20)	120.4(3)
C(19)-C(20)-C(15)	119.4(3)
C(22)-C(21)-S(2)	114.56(19)
N(3)-C(22)-C(21)	115.2(2)
N(3)-C(23)-C(24)	109.3(2)
N(4)-C(24)-C(23)	113.2(2)
N(4)-C(25)-C(26)	110.6(2)
O(2)-C(26)-C(25)	112.2(2)
O(2)-C(27)-C(28)	111.4(2)
N(4)-C(28)-C(27)	110.9(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+2

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **1'**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	8(1)	11(1)	18(1)	0(1)	1(1)	0(1)
Mn(2)	9(1)	11(1)	20(1)	0(1)	2(1)	1(1)
S(1)	14(1)	14(1)	21(1)	-1(1)	-3(1)	-1(1)
S(2)	20(1)	21(1)	26(1)	5(1)	7(1)	6(1)
Cl(1)	10(1)	14(1)	19(1)	0(1)	0(1)	1(1)
Cl(2)	9(1)	12(1)	23(1)	0(1)	3(1)	-1(1)
Cl(3)	8(1)	13(1)	20(1)	1(1)	2(1)	0(1)
Cl(4)	23(1)	14(1)	28(1)	-3(1)	7(1)	-5(1)
N(1)	6(1)	14(1)	19(1)	-1(1)	0(1)	0(1)
N(2)	14(1)	13(1)	20(1)	1(1)	3(1)	-1(1)
N(3)	10(1)	15(1)	22(1)	0(1)	4(1)	-1(1)
N(4)	12(1)	13(1)	22(1)	2(1)	2(1)	3(1)
O(1)	34(1)	28(1)	22(1)	8(1)	7(1)	3(1)
O(2)	23(1)	24(1)	23(1)	4(1)	5(1)	3(1)
C(1)	14(1)	14(1)	16(1)	-1(1)	5(1)	0(1)
C(2)	15(1)	20(1)	18(1)	-2(1)	0(1)	-1(1)
C(3)	20(1)	18(1)	27(2)	-4(1)	5(1)	-3(1)
C(4)	22(2)	12(1)	33(2)	1(1)	7(1)	3(1)
C(5)	19(2)	20(1)	27(2)	2(1)	3(1)	5(1)
C(6)	12(1)	18(1)	23(1)	-2(1)	0(1)	1(1)
C(7)	12(1)	16(1)	20(1)	0(1)	1(1)	2(1)
C(8)	10(1)	19(1)	21(1)	-1(1)	-1(1)	1(1)
C(9)	19(1)	13(1)	24(1)	-3(1)	3(1)	-2(1)
C(10)	19(2)	15(1)	29(2)	0(1)	7(1)	2(1)
C(11)	12(1)	14(1)	30(2)	5(1)	2(1)	-1(1)
C(12)	24(2)	23(2)	32(2)	7(1)	11(1)	5(1)
C(13)	26(2)	25(2)	26(2)	5(1)	-5(1)	-1(1)
C(14)	13(1)	22(2)	31(2)	12(1)	2(1)	3(1)
C(15)	18(1)	10(1)	24(1)	-1(1)	4(1)	0(1)
C(16)	20(1)	14(1)	28(2)	-3(1)	2(1)	1(1)
C(17)	35(2)	14(1)	25(2)	2(1)	6(1)	2(1)
C(18)	44(2)	12(1)	39(2)	-3(1)	26(2)	-4(1)
C(19)	22(2)	15(1)	53(2)	-3(1)	18(1)	-3(1)
C(20)	17(1)	17(1)	35(2)	-2(1)	1(1)	-1(1)

C(21)	14(1)	20(1)	23(1)	6(1)	1(1)	0(1)
C(22)	15(1)	15(1)	24(1)	2(1)	1(1)	-1(1)
C(23)	8(1)	24(2)	26(2)	4(1)	4(1)	2(1)
C(24)	13(1)	19(1)	26(1)	3(1)	5(1)	7(1)
C(25)	16(1)	20(1)	26(1)	3(1)	9(1)	0(1)
C(26)	19(1)	20(2)	26(2)	4(1)	6(1)	3(1)
C(27)	18(1)	22(2)	20(1)	-1(1)	2(1)	1(1)
C(28)	20(1)	18(1)	22(1)	-4(1)	6(1)	2(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex **1'**.

	x	y	z	U(eq)
H(1)	5771	11903	10629	16
H(3)	8469	6959	9883	19
H(2)	7403	9473	11462	22
H(3A)	7686	7540	11673	26
H(4)	9037	6971	12415	27
H(5)	10145	8351	12941	27
H(6)	9926	10284	12713	22
H(7A)	6649	11285	11556	20
H(7B)	6956	12586	11497	20
H(8A)	8018	11973	10805	20
H(8B)	7451	10762	10819	20
H(9A)	7178	13423	10290	23
H(9B)	6280	13671	10656	23
H(10A)	4844	13427	9897	25
H(10B)	5665	14383	9764	25
H(11A)	7429	13171	9395	23
H(11B)	6700	14179	9090	23
H(12A)	7472	13115	8453	31
H(12B)	6927	11983	8628	31
H(13A)	4943	11767	8397	32
H(13B)	4226	12764	8074	32
H(14A)	4675	13973	8844	27
H(14B)	4097	12848	9006	27

H(16)	10940	5105	11764	25
H(17)	10187	4356	12490	30
H(18)	8272	4254	12422	36
H(19)	7090	4870	11625	34
H(20)	7823	5572	10886	28
H(21A)	10008	7662	11184	23
H(21B)	10615	7865	10686	23
H(22A)	8289	7876	10646	22
H(22B)	9005	8899	10488	22
H(23A)	10171	7367	9747	23
H(23B)	9794	8636	9583	23
H(24A)	9783	7447	8797	23
H(24B)	8860	6680	8982	23
H(25A)	9399	9070	8307	24
H(25B)	9107	9740	8815	24
H(26A)	7353	10234	8299	26
H(26B)	8298	10685	8000	26
H(27A)	6595	7933	7450	24
H(27B)	6328	8580	7969	24
H(28A)	7368	6911	8248	23
H(28B)	8332	7351	7958	23

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For complex **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5430(1)	1386(1)	6664(1)	11(1)
Fe(2)	479(1)	4884(1)	6479(1)	12(1)
Cl(1)	7037(1)	1212(1)	7490(1)	16(1)
Cl(2)	6809(1)	1804(1)	5876(1)	15(1)
Cl(3)	1903(1)	4443(1)	5710(1)	19(1)
Cl(4)	2042(1)	5072(1)	7312(1)	17(1)
S(1)	8143(1)	-380(1)	5490(1)	17(1)
S(2)	3087(1)	6715(1)	5324(1)	24(1)
O(1)	2772(2)	3033(1)	7132(1)	23(1)
O(2)	-2250(3)	3239(1)	6945(1)	25(1)
N(1)	2556(3)	1735(1)	6757(1)	10(1)

N(2)	4038(3)	579(1)	6311(1)	10(1)
N(3)	-2401(3)	4537(1)	6573(1)	12(1)
N(4)	-897(3)	5694(1)	6131(1)	13(1)
C(1)	2096(4)	1941(1)	7360(1)	17(1)
C(2)	3192(4)	2526(1)	7518(1)	24(1)
C(3)	3250(4)	2856(1)	6556(1)	19(1)
C(4)	2164(3)	2280(1)	6367(1)	14(1)
C(5)	1310(3)	1201(1)	6591(1)	12(1)
C(6)	2188(3)	825(1)	6104(1)	13(1)
C(7)	5043(3)	229(1)	5855(1)	13(1)
C(8)	6846(3)	-66(1)	6097(1)	14(1)
C(9)	10117(3)	-758(1)	5809(1)	12(1)
C(10)	10546(4)	-752(1)	6397(1)	15(1)
C(11)	12148(4)	-1067(1)	6601(1)	16(1)
C(12)	13319(4)	-1380(1)	6221(1)	17(1)
C(13)	12894(4)	-1382(1)	5632(1)	16(1)
C(14)	11311(3)	-1074(1)	5424(1)	13(1)
C(15)	-2776(3)	4000(1)	6174(1)	15(1)
C(16)	-1718(4)	3419(1)	6372(1)	22(1)
C(17)	-1842(4)	3740(1)	7335(1)	22(1)
C(18)	-2905(4)	4332(1)	7170(1)	17(1)
C(19)	-3636(3)	5075(1)	6401(1)	13(1)
C(20)	-2749(3)	5451(1)	5916(1)	14(1)
C(21)	108(3)	6048(1)	5679(1)	16(1)
C(22)	1899(3)	6349(1)	5927(1)	16(1)
C(23)	5127(3)	7061(1)	5632(1)	15(1)
C(24)	6301(4)	7374(1)	5243(1)	19(1)
C(25)	7916(4)	7676(1)	5436(1)	24(1)
C(26)	8390(4)	7665(1)	6020(1)	24(1)
C(27)	7248(4)	7349(1)	6406(1)	19(1)
C(28)	5615(4)	7044(1)	6217(1)	16(1)

Table S6. Bond lengths [Å] and angles [°] for complex **2**.

Fe(1)-N(2)	2.135(2)
Fe(1)-N(1)	2.1689(19)
Fe(1)-Cl(1)	2.2401(7)
Fe(1)-Cl(2)	2.2456(7)

Fe(2)-N(4)	2.131(2)
Fe(2)-N(3)	2.172(2)
Fe(2)-Cl(4)	2.2433(7)
Fe(2)-Cl(3)	2.2443(7)
S(1)-C(9)	1.765(2)
S(1)-C(8)	1.802(2)
S(2)-C(23)	1.761(2)
S(2)-C(22)	1.802(2)
O(1)-C(3)	1.420(3)
O(1)-C(2)	1.426(3)
O(2)-C(17)	1.420(3)
O(2)-C(16)	1.425(3)
N(1)-C(5)	1.483(3)
N(1)-C(4)	1.491(3)
N(1)-C(1)	1.491(3)
N(2)-C(7)	1.472(3)
N(2)-C(6)	1.483(3)
N(3)-C(18)	1.486(3)
N(3)-C(19)	1.490(3)
N(3)-C(15)	1.488(3)
N(4)-C(21)	1.468(3)
N(4)-C(20)	1.487(3)
C(1)-C(2)	1.507(4)
C(3)-C(4)	1.507(3)
C(5)-C(6)	1.510(3)
C(7)-C(8)	1.520(3)
C(9)-C(10)	1.384(3)
C(9)-C(14)	1.397(3)
C(10)-C(11)	1.393(3)
C(11)-C(12)	1.376(3)
C(12)-C(13)	1.388(3)
C(13)-C(14)	1.378(3)
C(15)-C(16)	1.511(3)
C(17)-C(18)	1.513(4)
C(19)-C(20)	1.509(3)
C(21)-C(22)	1.525(3)
C(23)-C(28)	1.391(3)
C(23)-C(24)	1.391(4)
C(24)-C(25)	1.379(4)

C(25)-C(26)	1.383(4)
C(26)-C(27)	1.376(4)
C(27)-C(28)	1.390(3)

N(2)-Fe(1)-N(1)	83.30(8)
N(2)-Fe(1)-Cl(1)	114.84(6)
N(1)-Fe(1)-Cl(1)	116.21(5)
N(2)-Fe(1)-Cl(2)	102.15(6)
N(1)-Fe(1)-Cl(2)	110.70(5)
Cl(1)-Fe(1)-Cl(2)	122.14(3)
N(4)-Fe(2)-N(3)	83.52(8)
N(4)-Fe(2)-Cl(4)	113.48(6)
N(3)-Fe(2)-Cl(4)	115.60(5)
N(4)-Fe(2)-Cl(3)	104.20(6)
N(3)-Fe(2)-Cl(3)	111.03(6)
Cl(4)-Fe(2)-Cl(3)	121.89(3)
C(9)-S(1)-C(8)	104.33(11)
C(23)-S(2)-C(22)	104.62(12)
C(3)-O(1)-C(2)	109.35(19)
C(17)-O(2)-C(16)	109.3(2)
C(5)-N(1)-C(4)	109.28(17)
C(5)-N(1)-C(1)	109.50(18)
C(4)-N(1)-C(1)	106.89(19)
C(5)-N(1)-Fe(1)	105.47(14)
C(4)-N(1)-Fe(1)	112.10(14)
C(1)-N(1)-Fe(1)	113.56(14)
C(7)-N(2)-C(6)	112.06(18)
C(7)-N(2)-Fe(1)	117.11(15)
C(6)-N(2)-Fe(1)	103.96(14)
C(18)-N(3)-C(19)	109.13(19)
C(18)-N(3)-C(15)	107.66(19)
C(19)-N(3)-C(15)	108.89(18)
C(18)-N(3)-Fe(2)	114.75(14)
C(19)-N(3)-Fe(2)	105.00(14)
C(15)-N(3)-Fe(2)	111.26(15)
C(21)-N(4)-C(20)	111.70(18)
C(21)-N(4)-Fe(2)	117.35(16)
C(20)-N(4)-Fe(2)	103.95(15)
N(1)-C(1)-C(2)	110.7(2)

O(1)-C(2)-C(1)	111.6(2)
O(1)-C(3)-C(4)	111.2(2)
N(1)-C(4)-C(3)	111.38(19)
N(1)-C(5)-C(6)	110.56(19)
N(2)-C(6)-C(5)	108.15(18)
N(2)-C(7)-C(8)	110.64(18)
C(7)-C(8)-S(1)	107.19(16)
C(10)-C(9)-C(14)	119.6(2)
C(10)-C(9)-S(1)	124.84(19)
C(14)-C(9)-S(1)	115.51(17)
C(9)-C(10)-C(11)	119.9(2)
C(12)-C(11)-C(10)	120.5(2)
C(11)-C(12)-C(13)	119.6(2)
C(14)-C(13)-C(12)	120.5(2)
C(13)-C(14)-C(9)	119.9(2)
N(3)-C(15)-C(16)	110.69(19)
O(2)-C(16)-C(15)	111.5(2)
O(2)-C(17)-C(18)	111.5(2)
N(3)-C(18)-C(17)	110.8(2)
N(3)-C(19)-C(20)	110.96(19)
N(4)-C(20)-C(19)	107.75(19)
N(4)-C(21)-C(22)	110.56(19)
C(21)-C(22)-S(2)	106.22(16)
C(28)-C(23)-C(24)	119.4(2)
C(28)-C(23)-S(2)	125.2(2)
C(24)-C(23)-S(2)	115.42(18)
C(25)-C(24)-C(23)	120.6(2)
C(26)-C(25)-C(24)	120.1(3)
C(27)-C(26)-C(25)	119.7(2)
C(26)-C(27)-C(28)	120.9(2)
C(23)-C(28)-C(27)	119.4(2)

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}

Fe(1)	9(1)	13(1)	10(1)	-1(1)	-1(1)	1(1)
Fe(2)	10(1)	14(1)	12(1)	0(1)	-1(1)	-1(1)
Cl(1)	15(1)	22(1)	12(1)	2(1)	-3(1)	-1(1)
Cl(2)	15(1)	16(1)	14(1)	1(1)	1(1)	-1(1)
Cl(3)	16(1)	26(1)	14(1)	-4(1)	0(1)	1(1)
Cl(4)	15(1)	23(1)	13(1)	-3(1)	-3(1)	2(1)
S(1)	17(1)	24(1)	11(1)	-2(1)	0(1)	9(1)
S(2)	22(1)	35(1)	14(1)	3(1)	-2(1)	-14(1)
O(1)	22(1)	14(1)	33(1)	-8(1)	0(1)	3(1)
O(2)	22(1)	15(1)	37(1)	8(1)	-5(1)	-5(1)
N(1)	10(1)	8(1)	12(1)	-1(1)	0(1)	1(1)
N(2)	10(1)	11(1)	10(1)	0(1)	-1(1)	2(1)
N(3)	14(1)	12(1)	12(1)	-1(1)	0(1)	0(1)
N(4)	12(1)	15(1)	13(1)	2(1)	-1(1)	-4(1)
C(1)	16(1)	21(2)	13(1)	-4(1)	3(1)	4(1)
C(2)	24(2)	26(2)	22(2)	-8(1)	-2(1)	8(1)
C(3)	12(1)	13(1)	30(2)	2(1)	1(1)	1(1)
C(4)	10(1)	14(1)	17(1)	4(1)	-1(1)	4(1)
C(5)	7(1)	12(1)	17(1)	3(1)	1(1)	0(1)
C(6)	10(1)	14(1)	15(1)	3(1)	-4(1)	-2(1)
C(7)	12(1)	14(1)	12(1)	-2(1)	0(1)	0(1)
C(8)	15(1)	13(1)	13(1)	-2(1)	-1(1)	3(1)
C(9)	12(1)	9(1)	16(1)	1(1)	1(1)	-2(1)
C(10)	20(1)	12(1)	13(1)	-2(1)	1(1)	0(1)
C(11)	22(1)	12(1)	14(1)	1(1)	-6(1)	-1(1)
C(12)	14(1)	10(1)	26(2)	2(1)	-4(1)	4(1)
C(13)	18(1)	11(1)	19(1)	-2(1)	5(1)	2(1)
C(14)	14(1)	14(1)	11(1)	2(1)	-1(1)	-2(1)
C(15)	12(1)	13(1)	20(1)	-4(1)	-2(1)	-2(1)
C(16)	15(1)	13(2)	37(2)	-2(1)	-2(1)	0(1)
C(17)	18(1)	25(2)	24(2)	7(1)	-4(1)	-5(1)
C(18)	16(1)	21(2)	15(1)	4(1)	2(1)	-4(1)
C(19)	9(1)	11(1)	20(1)	-4(1)	-1(1)	2(1)
C(20)	12(1)	13(1)	18(1)	1(1)	-3(1)	0(1)
C(21)	16(1)	14(1)	18(1)	3(1)	-1(1)	-1(1)
C(22)	15(1)	19(2)	15(1)	3(1)	0(1)	-4(1)
C(23)	15(1)	13(1)	18(1)	1(1)	-3(1)	-1(1)
C(24)	21(2)	20(2)	16(1)	7(1)	-3(1)	0(1)
C(25)	19(2)	22(2)	31(2)	13(1)	-1(1)	-6(1)

C(26)	21(2)	19(2)	32(2)	3(1)	-12(1)	-6(1)
C(27)	22(2)	17(2)	18(1)	2(1)	-7(1)	0(1)
C(28)	19(1)	15(1)	14(1)	2(1)	1(1)	0(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) For complex **2**.

	x	y	z	U(eq)
H(1A)	2407	1607	7631	20
H(1B)	748	2025	7388	20
H(2A)	2882	2649	7912	29
H(2B)	4540	2436	7504	29
H(3A)	4600	2771	6536	22
H(3B)	2969	3201	6294	22
H(4A)	817	2372	6370	16
H(4B)	2516	2172	5973	16
H(5A)	85	1361	6467	14
H(5B)	1114	931	6925	14
H(6A)	1360	480	5996	16
H(6B)	2370	1091	5766	16
H(7A)	5360	512	5539	15
H(7B)	4223	-99	5702	15
H(8A)	6538	-399	6369	17
H(8B)	7599	248	6298	17
H(10)	9766	-538	6655	18
H(11)	12428	-1066	6996	19
H(12)	14389	-1589	6359	20
H(13)	13684	-1593	5375	19
H(14)	11037	-1076	5029	16
H(15A)	-2381	4110	5784	18
H(15B)	-4126	3912	6163	18
H(16A)	-1982	3076	6106	26
H(16B)	-366	3502	6363	26
H(17A)	-490	3824	7333	27
H(17B)	-2192	3616	7726	27
H(18A)	-4259	4255	7190	21

H(18B)	-2597	4664	7443	21
H(19A)	-3834	5346	6735	16
H(19B)	-4861	4918	6275	16
H(20A)	-2560	5185	5579	17
H(20B)	-3571	5797	5807	17
H(21A)	-717	6373	5524	19
H(21B)	443	5766	5364	19
H(22A)	2706	6032	6105	19
H(22B)	1579	6660	6219	19
H(24)	5995	7380	4850	23
H(25)	8686	7888	5174	29
H(26)	9476	7870	6151	28
H(27)	7574	7340	6798	23
H(28)	4856	6830	6481	19
H(4)	-1120(50)	5978(18)	6412(15)	80
H(2)	3850(50)	333(19)	6576(15)	80

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For complex **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	4561(1)	7116(1)	-658(1)	12(1)
S(1)	3711(1)	8927(1)	3384(1)	20(1)
Cl(1)	2919(1)	8685(1)	-1073(1)	21(1)
Cl(2)	2552(1)	5417(1)	-967(1)	18(1)
N(1)	6959(3)	7028(2)	-1361(2)	11(1)
N(2)	6637(3)	7586(2)	1100(2)	16(1)
O(1)	5522(2)	6516(2)	-4052(2)	19(1)
C(1)	6983(3)	5832(2)	-2100(2)	15(1)
C(2)	5324(3)	5611(2)	-3333(2)	18(1)
C(3)	7080(3)	7960(2)	-2141(2)	14(1)
C(4)	5435(3)	7667(2)	-3381(2)	18(1)
C(5)	8729(3)	7267(2)	-207(2)	13(1)
C(6)	8357(3)	8151(2)	799(2)	16(1)
C(7)	6127(3)	8401(2)	2057(2)	18(1)
C(8)	4427(3)	7783(2)	2382(2)	18(1)
C(9)	2018(3)	8127(2)	3913(2)	15(1)

C(10)	1241(3)	6930(2)	3459(2)	18(1)
C(11)	-65(4)	6387(2)	3969(3)	26(1)
C(12)	-628(4)	7026(3)	4910(3)	29(1)
C(13)	120(4)	8225(3)	5346(2)	26(1)
C(14)	1431(4)	8778(2)	4858(2)	21(1)

Table S10. Bond lengths [Å] and angles [°] for complex **3**.

Co(1)-N(2)	2.069(2)
Co(1)-N(1)	2.1005(19)
Co(1)-Cl(1)	2.2227(8)
Co(1)-Cl(2)	2.2301(8)
S(1)-C(9)	1.757(2)
S(1)-C(8)	1.807(2)
N(1)-C(3)	1.488(3)
N(1)-C(1)	1.491(3)
N(1)-C(5)	1.497(3)
N(2)-C(7)	1.474(3)
N(2)-C(6)	1.496(3)
O(1)-C(2)	1.426(3)
O(1)-C(4)	1.427(3)
C(1)-C(2)	1.513(3)
C(3)-C(4)	1.513(3)
C(5)-C(6)	1.510(3)
C(7)-C(8)	1.524(3)
C(9)-C(10)	1.387(3)
C(9)-C(14)	1.404(3)
C(10)-C(11)	1.392(3)
C(11)-C(12)	1.384(4)
C(12)-C(13)	1.383(4)
C(13)-C(14)	1.382(4)

N(2)-Co(1)-N(1)	87.14(8)
N(2)-Co(1)-Cl(1)	108.09(6)
N(1)-Co(1)-Cl(1)	113.45(5)
N(2)-Co(1)-Cl(2)	115.40(6)
N(1)-Co(1)-Cl(2)	117.27(5)
Cl(1)-Co(1)-Cl(2)	112.77(3)

C(9)-S(1)-C(8)	103.94(11)
C(3)-N(1)-C(1)	107.96(17)
C(3)-N(1)-C(5)	109.26(16)
C(1)-N(1)-C(5)	109.10(16)
C(3)-N(1)-Co(1)	113.05(13)
C(1)-N(1)-Co(1)	114.07(13)
C(5)-N(1)-Co(1)	103.22(12)
C(7)-N(2)-C(6)	111.18(18)
C(7)-N(2)-Co(1)	118.28(15)
C(6)-N(2)-Co(1)	101.10(13)
C(2)-O(1)-C(4)	109.45(17)
N(1)-C(1)-C(2)	110.57(18)
O(1)-C(2)-C(1)	110.79(18)
N(1)-C(3)-C(4)	110.59(18)
O(1)-C(4)-C(3)	111.44(18)
N(1)-C(5)-C(6)	110.67(17)
N(2)-C(6)-C(5)	107.21(18)
N(2)-C(7)-C(8)	109.98(18)
C(7)-C(8)-S(1)	105.81(16)
C(10)-C(9)-C(14)	119.3(2)
C(10)-C(9)-S(1)	124.79(18)
C(14)-C(9)-S(1)	115.89(18)
C(9)-C(10)-C(11)	119.5(2)
C(12)-C(11)-C(10)	121.1(2)
C(13)-C(12)-C(11)	119.3(2)
C(14)-C(13)-C(12)	120.5(2)
C(13)-C(14)-C(9)	120.3(2)

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	9(1)	15(1)	11(1)	0(1)	4(1)	-2(1)
S(1)	21(1)	15(1)	24(1)	3(1)	10(1)	-2(1)
Cl(1)	19(1)	14(1)	35(1)	5(1)	13(1)	3(1)
Cl(2)	15(1)	14(1)	25(1)	5(1)	8(1)	0(1)

N(1)	11(1)	12(1)	10(1)	2(1)	4(1)	0(1)
N(2)	15(1)	19(1)	15(1)	2(1)	6(1)	0(1)
O(1)	22(1)	24(1)	12(1)	2(1)	7(1)	1(1)
C(1)	18(1)	13(1)	16(1)	1(1)	8(1)	2(1)
C(2)	19(1)	19(1)	15(1)	-1(1)	8(1)	-1(1)
C(3)	14(1)	15(1)	14(1)	5(1)	6(1)	1(1)
C(4)	18(1)	22(1)	14(1)	5(1)	4(1)	4(1)
C(5)	10(1)	16(1)	13(1)	4(1)	3(1)	1(1)
C(6)	11(1)	23(1)	12(1)	1(1)	3(1)	-2(1)
C(7)	18(1)	20(1)	16(1)	0(1)	8(1)	-1(1)
C(8)	19(1)	21(1)	14(1)	-2(1)	9(1)	-3(1)
C(9)	12(1)	19(1)	14(1)	4(1)	1(1)	2(1)
C(10)	18(1)	18(1)	19(1)	1(1)	7(1)	0(1)
C(11)	23(1)	27(1)	28(1)	4(1)	11(1)	-4(1)
C(12)	22(1)	45(2)	26(1)	11(1)	13(1)	2(1)
C(13)	22(1)	42(2)	17(1)	3(1)	9(1)	12(1)
C(14)	19(1)	23(1)	16(1)	-2(1)	1(1)	5(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) For complex **3**.

	x	y	z	U(eq)
H(2)	6975	6901	1400	20
H(1A)	6830	5204	-1629	18
H(1B)	8249	5804	-2250	18
H(2A)	5353	4827	-3797	21
H(2B)	4057	5612	-3182	21
H(3A)	8355	7999	-2283	16
H(3B)	6973	8741	-1703	16
H(4A)	4162	7674	-3238	22
H(4B)	5546	8279	-3877	22
H(5A)	9875	7589	-401	16
H(5B)	9013	6518	93	16
H(6A)	9523	8321	1535	19
H(6B)	8053	8901	505	19
H(7A)	5739	9131	1746	22

H(7B)	7276	8621	2800	22
H(8A)	4859	7122	2812	22
H(8B)	3323	7471	1633	22
H(10)	1590	6494	2818	22
H(11)	-568	5580	3674	31
H(12)	-1500	6653	5245	35
H(13)	-261	8662	5972	31
H(14)	1926	9585	5157	25

Table S13. Crystal data and structure refinement for complex **4**.

Identification code	dq0237	
Empirical formula	C_{15} H_{24} Cl_2 Co N_2 O S	
Formula weight	410.25	
Temperature	100(1) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	A ba2	
Unit cell dimensions	a = 19.144(4) Å	α= 90°.
	b = 28.417(5) Å	β= 90°.
	c = 6.7820(13) Å	γ = 90°.
Volume	3689.5(12) $Å^3$	
Z	8	
Density (calculated)	1.477 Mg/m^3	
Absorption coefficient	1.335 mm^{-1}	
F(000)	1704	
Crystal size	0.60 x 0.36 x 0.06 mm^3	
Theta range for data collection	2.57 to 29.57°.	
Index ranges	-26<=h<=26, -39<=k<=39, -9<=l<=9	
Reflections collected	23031	
Independent reflections	5178 [R(int) = 0.0580]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9242 and 0.5014	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5178 / 25 / 200	
Goodness-of-fit on F^2	1.466	
Final R indices [I>2sigma(I)]	R1 = 0.1158, wR2 = 0.3065	
R indices (all data)	R1 = 0.1162, wR2 = 0.3067	

Absolute structure parameter	0.55(6)
Largest diff. peak and hole	1.532 and -2.171 e.Å^{-3}

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for complex **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	6307(1)	8324(1)	8869(2)	18(1)
Cl(1)	5195(1)	8164(1)	9923(4)	24(1)
Cl(2)	7078(1)	8423(1)	11425(4)	15(1)
S(1)	6690(1)	7448(1)	8669(5)	27(1)
N(1)	6238(5)	8219(3)	5897(13)	15(2)
N(2)	6112(5)	9098(4)	7895(13)	18(2)
O(1)	5894(5)	9770(3)	11083(15)	31(2)
C(1)	6241(6)	6569(4)	9944(18)	22(2)
C(2)	6679(9)	6432(8)	11480(30)	54(5)
C(3)	6896(10)	5975(6)	11660(30)	50(4)
C(4)	6687(10)	5653(7)	10330(30)	47(4)
C(5)	6258(9)	5768(5)	8740(30)	48(4)
C(6)	6032(7)	6238(5)	8570(20)	31(3)
C(7)	6008(7)	7070(5)	9770(20)	29(3)
C(8)	6505(6)	7365(4)	6048(17)	24(3)
C(9)	5998(7)	7725(5)	5348(16)	25(3)
C(10)	5818(7)	8587(5)	5063(19)	28(3)
C(11)	6132(7)	9062(5)	5716(17)	26(3)
C(12)	6634(7)	9463(5)	8520(30)	34(3)
C(13)	6573(6)	9596(4)	10660(18)	22(2)
C(14)	5410(6)	9301(4)	8389(17)	25(3)
C(15)	5385(7)	9421(5)	10536(17)	27(3)

Table S15. Bond lengths [Å] and angles [°] for complex **4**.

Co(1)-N(1)	2.042(9)
Co(1)-Cl(1)	2.292(3)
Co(1)-Cl(2)	2.294(3)
Co(1)-N(2)	2.325(10)

Co(1)-S(1)	2.599(3)
S(1)-C(8)	1.828(13)
S(1)-C(7)	1.846(15)
N(1)-C(10)	1.435(16)
N(1)-C(9)	1.524(14)
N(1)-H(1)	0.9100
N(2)-C(11)	1.481(15)
N(2)-C(14)	1.501(14)
N(2)-C(12)	1.501(17)
O(1)-C(13)	1.420(15)
O(1)-C(15)	1.439(17)
C(1)-C(6)	1.384(19)
C(1)-C(2)	1.395(18)
C(1)-C(7)	1.496(17)
C(2)-C(3)	1.37(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.35(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.39(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.408(18)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.49(2)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.542(18)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.51(2)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9700

C(13)-H(13B)	0.9700
C(14)-C(15)	1.496(16)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700

N(1)-Co(1)-Cl(1)	102.6(3)
N(1)-Co(1)-Cl(2)	143.7(3)
Cl(1)-Co(1)-Cl(2)	112.72(12)
N(1)-Co(1)-N(2)	81.2(3)
Cl(1)-Co(1)-N(2)	97.3(3)
Cl(2)-Co(1)-N(2)	101.7(3)
N(1)-Co(1)-S(1)	80.0(3)
Cl(1)-Co(1)-S(1)	95.03(11)
Cl(2)-Co(1)-S(1)	88.57(10)
N(2)-Co(1)-S(1)	159.4(3)
C(8)-S(1)-C(7)	100.4(5)
C(8)-S(1)-Co(1)	96.9(4)
C(7)-S(1)-Co(1)	109.7(4)
C(10)-N(1)-C(9)	114.0(9)
C(10)-N(1)-Co(1)	108.6(7)
C(9)-N(1)-Co(1)	113.3(7)
C(10)-N(1)-H(1)	106.8
C(9)-N(1)-H(1)	106.8
Co(1)-N(1)-H(1)	106.8
C(11)-N(2)-C(14)	105.8(9)
C(11)-N(2)-C(12)	108.1(11)
C(14)-N(2)-C(12)	105.5(9)
C(11)-N(2)-Co(1)	102.4(7)
C(14)-N(2)-Co(1)	116.4(7)
C(12)-N(2)-Co(1)	117.8(8)
C(13)-O(1)-C(15)	109.1(8)
C(6)-C(1)-C(2)	119.0(13)
C(6)-C(1)-C(7)	120.6(11)
C(2)-C(1)-C(7)	120.4(14)
C(3)-C(2)-C(1)	121.1(19)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5

C(4)-C(3)-C(2)	119.5(18)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(3)-C(4)-C(5)	122.4(17)
C(3)-C(4)-H(4)	118.8
C(5)-C(4)-H(4)	118.8
C(4)-C(5)-C(6)	117.7(19)
C(4)-C(5)-H(5)	121.2
C(6)-C(5)-H(5)	121.2
C(1)-C(6)-C(5)	120.3(14)
C(1)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(1)-C(7)-S(1)	112.1(8)
C(1)-C(7)-H(7A)	109.2
S(1)-C(7)-H(7A)	109.2
C(1)-C(7)-H(7B)	109.2
S(1)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9
C(9)-C(8)-S(1)	110.4(8)
C(9)-C(8)-H(8A)	109.6
S(1)-C(8)-H(8A)	109.6
C(9)-C(8)-H(8B)	109.6
S(1)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
C(8)-C(9)-N(1)	111.0(10)
C(8)-C(9)-H(9A)	109.4
N(1)-C(9)-H(9A)	109.4
C(8)-C(9)-H(9B)	109.4
N(1)-C(9)-H(9B)	109.4
H(9A)-C(9)-H(9B)	108.0
N(1)-C(10)-C(11)	107.8(10)
N(1)-C(10)-H(10A)	110.1
C(11)-C(10)-H(10A)	110.1
N(1)-C(10)-H(10B)	110.1
C(11)-C(10)-H(10B)	110.1
H(10A)-C(10)-H(10B)	108.5
N(2)-C(11)-C(10)	109.7(10)
N(2)-C(11)-H(11A)	109.7
C(10)-C(11)-H(11A)	109.7

N(2)-C(11)-H(11B)	109.7
C(10)-C(11)-H(11B)	109.7
H(11A)-C(11)-H(11B)	108.2
N(2)-C(12)-C(13)	113.1(11)
N(2)-C(12)-H(12A)	109.0
C(13)-C(12)-H(12A)	109.0
N(2)-C(12)-H(12B)	109.0
C(13)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
O(1)-C(13)-C(12)	110.7(10)
O(1)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13A)	109.5
O(1)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1
C(15)-C(14)-N(2)	109.5(9)
C(15)-C(14)-H(14A)	109.8
N(2)-C(14)-H(14A)	109.8
C(15)-C(14)-H(14B)	109.8
N(2)-C(14)-H(14B)	109.8
H(14A)-C(14)-H(14B)	108.2
O(1)-C(15)-C(14)	112.7(11)
O(1)-C(15)-H(15A)	109.1
C(14)-C(15)-H(15A)	109.1
O(1)-C(15)-H(15B)	109.1
C(14)-C(15)-H(15B)	109.1
H(15A)-C(15)-H(15B)	107.8

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	16(1)	24(1)	13(1)	-2(1)	-2(1)	0(1)
Cl(1)	15(1)	34(2)	22(1)	-8(1)	4(1)	-3(1)
Cl(2)	21(1)	10(1)	13(1)	-4(1)	-1(1)	6(1)

S(1)	20(1)	27(1)	33(2)	-12(1)	-5(1)	-3(1)
N(1)	19(4)	11(4)	14(4)	-5(3)	-3(3)	4(3)
N(2)	19(4)	29(5)	8(4)	1(3)	0(3)	8(4)
O(1)	42(5)	17(4)	34(5)	-11(4)	-1(4)	12(4)
C(1)	25(4)	18(4)	23(4)	6(3)	2(3)	9(3)
C(2)	45(9)	88(14)	30(7)	31(9)	-12(7)	14(9)
C(3)	51(6)	51(6)	49(6)	10(4)	-2(4)	6(4)
C(4)	47(5)	44(5)	49(5)	9(4)	1(4)	10(4)
C(5)	53(9)	25(6)	65(11)	24(9)	12(10)	10(6)
C(6)	27(6)	39(7)	27(7)	14(6)	-6(5)	2(5)
C(7)	23(5)	35(7)	28(6)	-13(6)	3(5)	9(5)
C(8)	19(5)	33(6)	22(6)	-11(5)	14(4)	-19(5)
C(9)	36(6)	30(6)	10(5)	-1(4)	1(4)	-17(5)
C(10)	27(6)	36(7)	19(5)	-15(5)	0(5)	-1(5)
C(11)	35(7)	28(6)	14(5)	8(4)	3(5)	5(5)
C(12)	24(5)	22(5)	55(10)	-6(6)	13(6)	4(4)
C(13)	26(4)	13(4)	28(4)	2(3)	-3(3)	1(3)
C(14)	21(5)	27(6)	26(6)	-2(4)	-6(4)	13(4)
C(15)	31(6)	31(7)	20(6)	-11(5)	8(5)	13(5)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for complex **4**.

	x	y	z	U(eq)
H(1)	6676	8255	5399	18
H(2)	6828	6654	12396	65
H(3)	7184	5887	12705	60
H(4)	6836	5343	10467	56
H(5)	6125	5542	7819	57
H(6)	5742	6325	7536	37
H(7A)	5890	7189	11065	34
H(7B)	5592	7084	8956	34
H(8A)	6935	7391	5300	29
H(8B)	6314	7053	5835	29
H(9A)	5544	7665	5932	30
H(9B)	5950	7702	3927	30

H(10A)	5340	8560	5524	33
H(10B)	5818	8564	3636	33
H(11A)	6610	9086	5259	31
H(11B)	5866	9318	5139	31
H(12A)	6570	9742	7715	40
H(12B)	7101	9344	8271	40
H(13A)	6667	9323	11475	27
H(13B)	6917	9835	10973	27
H(14A)	5329	9582	7609	29
H(14B)	5047	9075	8080	29
H(15A)	4922	9536	10859	33
H(15B)	5466	9137	11301	33

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For complex **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	9166(1)	2785(1)	2929(1)	16(1)
Cl(1)	11174(2)	1207(2)	2379(1)	24(1)
Cl(2)	7012(2)	4396(2)	3372(1)	20(1)
S(1)	9433(2)	3955(2)	1841(1)	24(1)
N(1)	12032(6)	4602(5)	3370(2)	20(1)
N(2)	9897(6)	2015(5)	3993(2)	18(1)
O(1)	6474(6)	-689(4)	4209(2)	25(1)
O(2)	6096(5)	1140(4)	2447(2)	18(1)
C(1)	7501(9)	5066(7)	1653(3)	29(1)
C(2)	7901(8)	5834(7)	1016(3)	25(1)
C(3)	7407(9)	4931(7)	324(3)	28(1)
C(4)	7802(9)	5630(8)	-261(3)	34(2)
C(5)	8685(10)	7258(8)	-156(4)	42(2)
C(6)	9186(10)	8186(8)	524(4)	38(2)
C(7)	8825(9)	7475(7)	1113(3)	28(1)
C(8)	11931(8)	5582(7)	2255(3)	29(1)
C(9)	12154(9)	6029(7)	3065(3)	30(1)
C(10)	12305(8)	4801(6)	4156(3)	25(1)
C(11)	12100(8)	3177(6)	4331(3)	25(1)

C(12)	8355(8)	2154(6)	4483(3)	20(1)
C(13)	6181(9)	842(7)	4245(3)	26(1)
C(14)	10101(8)	393(6)	3955(3)	24(1)
C(15)	7887(8)	-875(6)	3727(3)	24(1)
C(16)	5376(9)	-224(7)	1844(3)	26(1)
C(17)	5255(10)	280(8)	1125(3)	39(2)

Table S19. Bond lengths [Å] and angles [°] for complex **5**.

Ni(1)-N(1)	2.054(4)
Ni(1)-O(2)	2.089(4)
Ni(1)-N(2)	2.259(4)
Ni(1)-Cl(1)	2.4038(15)
Ni(1)-Cl(2)	2.4192(15)
Ni(1)-S(1)	2.4588(18)
S(1)-C(8)	1.818(6)
S(1)-C(1)	1.830(5)
N(1)-C(10)	1.457(7)
N(1)-C(9)	1.463(7)
N(2)-C(14)	1.482(6)
N(2)-C(12)	1.485(6)
N(2)-C(11)	1.491(6)
O(1)-C(15)	1.416(6)
O(1)-C(13)	1.424(6)
O(2)-C(16)	1.457(6)
C(1)-C(2)	1.499(8)
C(2)-C(3)	1.379(7)
C(2)-C(7)	1.389(7)
C(3)-C(4)	1.376(8)
C(4)-C(5)	1.374(8)
C(5)-C(6)	1.369(9)
C(6)-C(7)	1.385(8)
C(8)-C(9)	1.508(8)
C(10)-C(11)	1.509(7)
C(12)-C(13)	1.512(7)
C(14)-C(15)	1.511(7)
C(16)-C(17)	1.501(8)

N(1)-Ni(1)-O(2)	173.38(15)
N(1)-Ni(1)-N(2)	82.72(16)
O(2)-Ni(1)-N(2)	101.77(15)
N(1)-Ni(1)-Cl(1)	90.53(12)
O(2)-Ni(1)-Cl(1)	94.22(10)
N(2)-Ni(1)-Cl(1)	91.08(11)
N(1)-Ni(1)-Cl(2)	91.29(12)
O(2)-Ni(1)-Cl(2)	83.60(10)
N(2)-Ni(1)-Cl(2)	94.01(11)
Cl(1)-Ni(1)-Cl(2)	174.78(5)
N(1)-Ni(1)-S(1)	83.50(13)
O(2)-Ni(1)-S(1)	92.54(11)
N(2)-Ni(1)-S(1)	164.72(11)
Cl(1)-Ni(1)-S(1)	82.48(5)
Cl(2)-Ni(1)-S(1)	92.86(5)
C(8)-S(1)-C(1)	100.7(3)
C(8)-S(1)-Ni(1)	95.45(19)
C(1)-S(1)-Ni(1)	114.33(19)
C(10)-N(1)-C(9)	116.9(4)
C(10)-N(1)-Ni(1)	107.1(3)
C(9)-N(1)-Ni(1)	112.6(3)
C(14)-N(2)-C(12)	106.4(4)
C(14)-N(2)-C(11)	107.5(4)
C(12)-N(2)-C(11)	108.8(4)
C(14)-N(2)-Ni(1)	117.0(3)
C(12)-N(2)-Ni(1)	115.0(3)
C(11)-N(2)-Ni(1)	101.7(3)
C(15)-O(1)-C(13)	109.5(4)
C(16)-O(2)-Ni(1)	132.9(3)
C(2)-C(1)-S(1)	110.4(4)
C(3)-C(2)-C(7)	118.4(5)
C(3)-C(2)-C(1)	121.0(5)
C(7)-C(2)-C(1)	120.6(5)
C(4)-C(3)-C(2)	121.2(6)
C(5)-C(4)-C(3)	119.6(6)
C(6)-C(5)-C(4)	120.6(6)
C(5)-C(6)-C(7)	119.6(6)
C(6)-C(7)-C(2)	120.6(6)
C(9)-C(8)-S(1)	111.8(4)

N(1)-C(9)-C(8)	108.5(5)
N(1)-C(10)-C(11)	106.7(4)
N(2)-C(11)-C(10)	111.6(4)
N(2)-C(12)-C(13)	112.5(4)
O(1)-C(13)-C(12)	111.2(4)
N(2)-C(14)-C(15)	111.6(4)
O(1)-C(15)-C(14)	112.2(4)
O(2)-C(16)-C(17)	111.9(5)

Symmetry transformations used to generate equivalent atoms:

Table S20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	6(1)	19(1)	21(1)	0(1)	3(1)	4(1)
Cl(1)	11(1)	29(1)	28(1)	-5(1)	4(1)	8(1)
Cl(2)	9(1)	21(1)	30(1)	1(1)	5(1)	6(1)
S(1)	14(1)	30(1)	28(1)	7(1)	7(1)	8(1)
N(1)	3(2)	20(3)	33(3)	-2(2)	2(2)	4(2)
N(2)	5(2)	24(3)	24(2)	-1(2)	4(2)	6(2)
O(1)	20(2)	29(2)	31(2)	10(2)	11(2)	10(2)
O(2)	8(2)	17(2)	23(2)	-6(2)	0(2)	3(2)
C(1)	13(3)	37(4)	37(3)	7(3)	6(2)	9(3)
C(2)	11(3)	31(3)	32(3)	4(3)	4(2)	8(3)
C(3)	18(3)	24(3)	38(4)	6(3)	3(3)	4(3)
C(4)	26(4)	49(4)	31(3)	9(3)	6(3)	16(3)
C(5)	38(4)	50(5)	62(5)	34(4)	27(3)	29(4)
C(6)	35(4)	27(4)	62(5)	16(3)	19(3)	15(3)
C(7)	21(3)	21(3)	43(4)	1(3)	8(3)	8(3)
C(8)	10(3)	36(4)	43(4)	13(3)	7(2)	5(3)
C(9)	8(3)	30(4)	53(4)	8(3)	6(3)	7(3)
C(10)	8(3)	31(3)	28(3)	-10(3)	-2(2)	3(3)
C(11)	6(3)	34(4)	29(3)	0(3)	-4(2)	2(3)
C(12)	19(3)	32(3)	13(3)	4(2)	7(2)	14(3)
C(13)	20(3)	43(4)	22(3)	12(3)	10(2)	16(3)
C(14)	17(3)	31(3)	28(3)	6(3)	10(2)	11(3)

C(15)	19(3)	23(3)	31(3)	5(3)	4(2)	10(3)
C(16)	15(3)	27(3)	30(3)	-8(3)	2(2)	7(3)
C(17)	38(4)	49(4)	28(3)	-3(3)	3(3)	18(3)

Table S21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex **5**.

	x	y	z	U(eq)
H(1)	13140	4246	3247	24
H(1A)	6010	4347	1552	34
H(1B)	7671	5878	2076	34
H(3)	6796	3830	251	33
H(4)	7474	5005	-724	41
H(5)	8943	7733	-551	51
H(6)	9766	9288	591	46
H(7)	9204	8102	1577	34
H(8A)	13189	5270	2153	35
H(8B)	11919	6504	2043	35
H(9A)	13548	6843	3276	37
H(9B)	10986	6449	3174	37
H(10A)	11183	5204	4321	30
H(10B)	13732	5547	4391	30
H(11A)	13223	2787	4158	30
H(11B)	12338	3265	4853	30
H(12A)	8099	3178	4499	23
H(12B)	9021	2120	4970	23
H(13A)	5240	977	4584	31
H(13B)	5464	915	3771	31
H(14A)	10817	308	4426	28
H(14B)	11012	218	3610	28
H(15A)	7208	-827	3244	29
H(15B)	8087	-1917	3706	29
H(16A)	3941	-903	1870	31
H(16B)	6390	-840	1885	31
H(17A)	4300	928	1091	58
H(17B)	4691	-648	742	58

H(17C)	6695	882	1081	58
H(2)	5110(130)	1520(90)	2450(40)	80

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for complex **7**·hexane. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	4257(1)	563(1)	7270(1)	12(1)
Cl(1)	4038(1)	2391(1)	6985(1)	16(1)
Cl(2)	6084(1)	153(1)	7140(1)	15(1)
S(1)	4481(1)	1245(1)	8097(1)	15(1)
N(1)	3624(1)	-196(2)	6636(1)	13(1)
N(2)	4077(1)	-1004(2)	7590(1)	12(1)
O(1)	2725(1)	167(2)	5658(1)	24(1)
C(1)	4205(2)	153(2)	6185(1)	16(1)
C(2)	3726(2)	-270(2)	5706(1)	23(1)
C(3)	2125(2)	-220(2)	6069(1)	24(1)
C(4)	2562(2)	183(2)	6566(1)	17(1)
C(5)	3702(2)	-1465(2)	6733(1)	18(1)
C(6)	3423(2)	-1721(2)	7266(1)	16(1)
C(7)	3763(2)	-986(2)	8119(1)	16(1)
C(8)	4448(2)	-160(2)	8396(1)	17(1)
C(9)	3249(2)	1861(2)	8246(1)	16(1)
C(10)	3143(2)	2151(2)	8790(1)	16(1)
C(11)	2802(2)	1333(2)	9132(1)	23(1)
C(12)	2744(2)	1599(2)	9637(1)	28(1)
C(13)	3003(2)	2688(2)	9806(1)	27(1)
C(14)	3323(2)	3506(2)	9469(1)	23(1)
C(15)	3398(2)	3244(2)	8964(1)	18(1)

Table S23. Bond lengths [Å] and angles [°] for complex **7**·hexane.

Cu(1)-N(2)	2.0135(18)
Cu(1)-N(1)	2.0838(18)
Cu(1)-Cl(1)	2.2619(6)
Cu(1)-S(1)	2.3627(7)

Cu(1)-Cl(2)	2.4974(7)
S(1)-C(8)	1.807(2)
S(1)-C(9)	1.828(2)
N(1)-C(1)	1.485(3)
N(1)-C(4)	1.489(3)
N(1)-C(5)	1.491(3)
N(2)-C(7)	1.473(3)
N(2)-C(6)	1.478(3)
O(1)-C(3)	1.427(3)
O(1)-C(2)	1.428(3)
C(1)-C(2)	1.509(3)
C(3)-C(4)	1.521(3)
C(5)-C(6)	1.500(3)
C(7)-C(8)	1.511(3)
C(9)-C(10)	1.495(3)
C(10)-C(15)	1.387(3)
C(10)-C(11)	1.390(3)
C(11)-C(12)	1.385(3)
C(12)-C(13)	1.379(4)
C(13)-C(14)	1.371(3)
C(14)-C(15)	1.384(3)

N(2)-Cu(1)-N(1)	85.39(7)
N(2)-Cu(1)-Cl(1)	164.80(5)
N(1)-Cu(1)-Cl(1)	93.81(5)
N(2)-Cu(1)-S(1)	85.28(5)
N(1)-Cu(1)-S(1)	161.87(5)
Cl(1)-Cu(1)-S(1)	91.15(2)
N(2)-Cu(1)-Cl(2)	90.27(5)
N(1)-Cu(1)-Cl(2)	101.51(5)
Cl(1)-Cu(1)-Cl(2)	104.74(2)
S(1)-Cu(1)-Cl(2)	94.05(2)
C(8)-S(1)-C(9)	103.35(11)
C(8)-S(1)-Cu(1)	96.34(8)
C(9)-S(1)-Cu(1)	102.70(7)
C(1)-N(1)-C(4)	108.15(16)
C(1)-N(1)-C(5)	111.82(17)
C(4)-N(1)-C(5)	112.14(17)
C(1)-N(1)-Cu(1)	109.56(13)

C(4)-N(1)-Cu(1)	111.14(13)
C(5)-N(1)-Cu(1)	104.01(13)
C(7)-N(2)-C(6)	113.67(17)
C(7)-N(2)-Cu(1)	115.33(14)
C(6)-N(2)-Cu(1)	108.94(13)
C(3)-O(1)-C(2)	109.89(17)
N(1)-C(1)-C(2)	112.29(18)
O(1)-C(2)-C(1)	110.76(19)
O(1)-C(3)-C(4)	111.21(18)
N(1)-C(4)-C(3)	112.40(19)
N(1)-C(5)-C(6)	110.03(18)
N(2)-C(6)-C(5)	107.37(18)
N(2)-C(7)-C(8)	107.88(17)
C(7)-C(8)-S(1)	111.40(15)
C(10)-C(9)-S(1)	112.48(15)
C(15)-C(10)-C(11)	118.4(2)
C(15)-C(10)-C(9)	120.5(2)
C(11)-C(10)-C(9)	121.1(2)
C(12)-C(11)-C(10)	120.5(2)
C(13)-C(12)-C(11)	120.4(2)
C(14)-C(13)-C(12)	119.4(2)
C(13)-C(14)-C(15)	120.6(2)
C(14)-C(15)-C(10)	120.6(2)

Symmetry transformations used to generate equivalent atoms:

Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for complex **7**·hexane. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	13(1)	11(1)	11(1)	0(1)	0(1)	-1(1)
Cl(1)	18(1)	11(1)	19(1)	0(1)	0(1)	-1(1)
Cl(2)	10(1)	18(1)	17(1)	0(1)	2(1)	0(1)
S(1)	14(1)	17(1)	14(1)	-2(1)	1(1)	-1(1)
N(1)	14(1)	12(1)	13(1)	2(1)	0(1)	-2(1)
N(2)	10(1)	14(1)	12(1)	0(1)	0(1)	1(1)
O(1)	23(1)	36(1)	15(1)	5(1)	-5(1)	-4(1)

C(1)	15(1)	19(1)	14(1)	2(1)	2(1)	0(1)
C(2)	30(1)	25(1)	14(1)	0(1)	2(1)	-2(1)
C(3)	19(1)	31(2)	20(1)	5(1)	-5(1)	-5(1)
C(4)	12(1)	20(1)	17(1)	5(1)	-2(1)	1(1)
C(5)	25(1)	12(1)	17(1)	0(1)	-4(1)	-2(1)
C(6)	19(1)	11(1)	17(1)	1(1)	-5(1)	-4(1)
C(7)	15(1)	18(1)	13(1)	3(1)	3(1)	1(1)
C(8)	19(1)	20(1)	13(1)	0(1)	-2(1)	5(1)
C(9)	13(1)	15(1)	19(1)	-1(1)	0(1)	2(1)
C(10)	13(1)	16(1)	17(1)	-2(1)	1(1)	4(1)
C(11)	24(1)	19(1)	26(1)	-1(1)	6(1)	-4(1)
C(12)	32(2)	31(2)	21(1)	3(1)	11(1)	-3(1)
C(13)	29(2)	37(2)	15(1)	-5(1)	1(1)	8(1)
C(14)	29(1)	17(1)	22(1)	-8(1)	-5(1)	6(1)
C(15)	19(1)	17(1)	18(1)	1(1)	-2(1)	0(1)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for complex **7**·hexane.

	x	y	z	U(eq)
H(2)	4694	-1347	7585	15
H(1A)	4882	-157	6209	19
H(1B)	4255	991	6175	19
H(2A)	4126	-19	5422	27
H(2B)	3710	-1111	5705	27
H(3A)	2089	-1059	6065	28
H(3B)	1446	80	6033	28
H(4A)	2531	1022	6582	20
H(4B)	2155	-123	6837	20
H(5A)	4386	-1723	6670	21
H(5B)	3256	-1881	6509	21
H(6A)	2721	-1533	7325	19
H(6B)	3524	-2537	7339	19
H(7A)	3814	-1757	8262	19
H(7B)	3069	-730	8146	19
H(8A)	5123	-479	8407	21

H(8B)	4213	-74	8738	21
H(9A)	3149	2558	8049	19
H(9B)	2729	1311	8153	19
H(11)	2611	601	9021	28
H(12)	2529	1039	9864	34
H(13)	2961	2866	10145	33
H(14)	3490	4245	9581	27
H(15)	3622	3805	8741	22

Computational Studies.

Example of an input file.

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%mem=30GB
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1       -4.828148000      1.503380000      0.386859000
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1        0.523364000      2.283095000      0.646095000
1        1.047825000      2.826378000     -0.965414000
6        1.827371000      0.891638000     -0.355190000
1        1.911173000      0.415805000     -1.336725000
1        1.577818000      0.132456000      0.389598000
6        4.530659000      0.296220000      0.070388000
6        4.157447000     -1.024774000     -0.170290000
1        3.128143000     -1.292836000     -0.370907000
6        5.119829000     -2.030202000     -0.148925000
1        4.815205000     -3.053711000     -0.336400000
6        6.449982000     -1.734622000      0.111244000
1        7.193155000     -2.523158000      0.127463000
6        6.819959000     -0.414931000      0.353156000
1        7.855473000     -0.168242000      0.559439000
6        5.870801000      0.594831000      0.333014000
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1       -0.309103000      1.053998000     -1.874456000

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S 1 1.00
0.1066920 1.0
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11.1736750 0.1889250
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G 1 1.00
2.7110000 1.0
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c h n o s cl 0
6-311++g**
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S-F
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2 10.610000 47.156846
P-F
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2 10.440000 35.233352
D-F
2
2 29.540000 -26.475333
2 10.180000 -1.825787
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Table of Energy Data

	E	E_{ZPVE}	$G°_{298K}$
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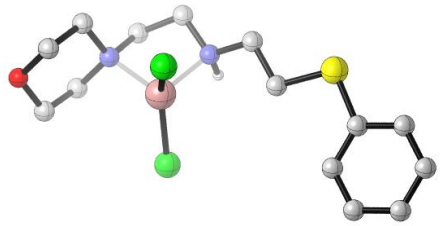
3B	-2196.04019	-2195.682414	-2195.73793
3C	-2196.038447	-2195.680395	-2195.73502
3D	-2196.039126	-2195.681417	-2195.7372
3E	-2196.022966	-2195.665773	-2195.72203
3F	-2196.023626	-2195.665735	-2195.72104
4A	-2235.353154	-2234.967013	-2235.02731
4B	-2235.360197	-2234.973795	-2235.0327
4C	-2235.355344	-2234.968667	-2235.02498

Cartesian Coordinates for structures

3A



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17	-0.834152000	0.026954000	2.216943000
17	-0.785368000	-2.005898000	-1.333221000
7	-3.218052000	0.426773000	-0.458904000
7	-0.497950000	1.374777000	-0.924466000
8	-5.211565000	-1.134830000	0.888571000
6	-4.057271000	-0.574920000	-1.157932000
1	-3.469335000	-1.009744000	-1.968843000
1	-4.945081000	-0.078033000	-1.574287000
6	-4.489693000	-1.669142000	-0.198476000
1	-5.149217000	-2.369878000	-0.710957000
1	-3.607939000	-2.222365000	0.157340000
6	-3.952916000	0.928686000	0.727735000
1	-4.827499000	1.502011000	0.388511000
1	-3.297635000	1.581456000	1.307670000
6	-4.410808000	-0.223722000	1.609409000
1	-3.539344000	-0.732673000	2.040678000
1	-5.021452000	0.164523000	2.425027000
6	-2.887410000	1.533315000	-1.383310000
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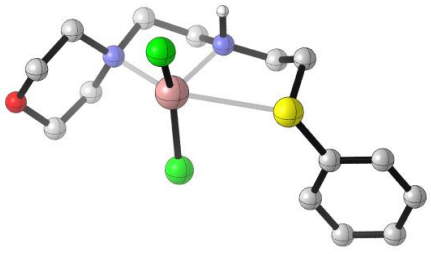

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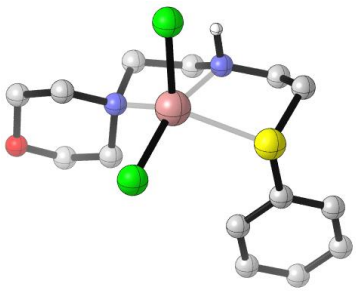

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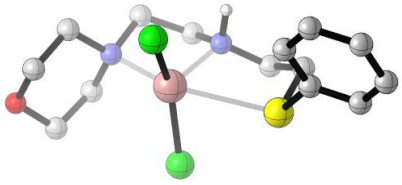

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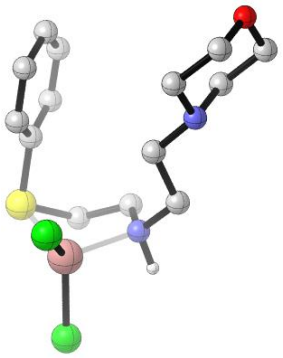

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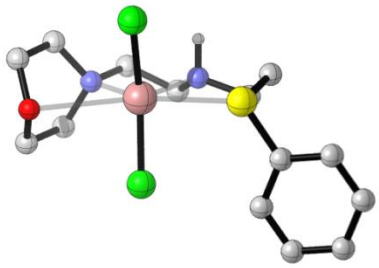

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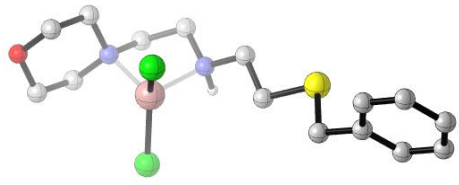

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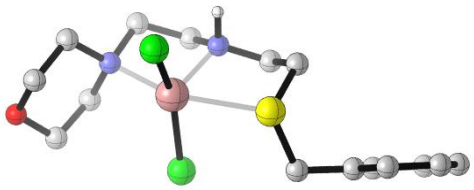

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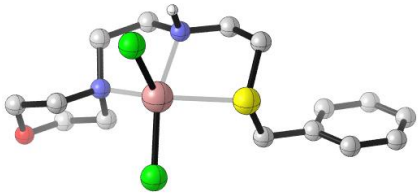
4C



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