

Supplementary Material

Synthesis and Characterization of $[(en)_2Co]^{3+}$ Complexes Coordinated by Substituted Thiourea Ligands.

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Table S1. Selected bond lengths for the cation [Co-4a]²⁺ (*endo* isomer). Bond lengths are in units of Å. Standard deviations are in parentheses. Refer to Figure 7 for the numbering scheme.

Coordination Sphere

Co(1)-N(2)	1.934(3)	Co(1)-N(5)	1.957(2)
Co(1)-N(3)	1.957(3)	Co(1)-N(6)	1.962(2)
Co(1)-N(4)	1.976(3)	Co(1)-S(1)	2.2848(10)

Thiourea Ligand

S(1)-C(1)	1.740(3)	N(1)-C(1)	1.329(4)
N(1)-C(2)	1.453(4)	N(2)-C(1)	1.317(4)
N(2)-C(3)	1.427(4)	C(3)-C(4)	1.392(5)
C(4)-C(5)	1.390(5)	C(5)-C(6)	1.381(6)
C(6)-C(7)	1.379(6)	C(7)-C(8)	1.384(5)
C(3)-C(8)	1.390(5)		

Ethylenediamine Ligands

N(5)-C(11)	1.478(4)	N(6)-C(12)	1.486(4)
N(3)-C(9)	1.483(4)	N(4)-C(10)	1.480(4)
C(9)-C(10)	1.510(5)	C(11)-C(12)	1.502(4)

Table S2. Selected bond angles for the cation [Co-4a]²⁺ (*endo* isomer). Bond angles are in degrees.

Standard deviations are in parentheses. Refer to Figure 7 for the numbering scheme.

Coordination Sphere

N(2)-Co(1)-N(5)	91.56(11)	N(2)-Co(1)-N(3)	90.88(11)
N(5)-Co(1)-N(3)	177.15(11)	N(2)-Co(1)-N(6)	169.44(11)
N(5)-Co(1)-N(6)	85.28(10)	N(3)-Co(1)-N(6)	92.57(11)
N(2)-Co(1)-N(4)	96.45(11)	N(5)-Co(1)-N(4)	92.86(11)
N(3)-Co(1)-N(4)	85.41(11)	N(6)-Co(1)-N(4)	93.77(11)
N(2)-Co(1)-S(1)	72.26(8)	N(5)-Co(1)-S(1)	90.65(9)
N(3)-Co(1)-S(1)	91.49(8)	N(6)-Co(1)-S(1)	97.66(8)
N(4)-Co(1)-S(1)	168.28(8)		

Thiourea Ligand

C(1)-S(1)-Co(1)	77.14(12)	C(1)-N(1)-C(2)	122.7(3)
C(1)-N(2)-C(3)	124.5(3)	C(1)-N(2)-Co(1)	101.4(2)
C(3)-N(2)-Co(1)	133.8(2)	N(2)-C(1)-N(1)	127.0(3)
N(2)-C(1)-S(1)	109.2(2)	N(1)-C(1)-S(1)	123.8(3)
C(8)-C(3)-C(4)	119.7(3)	C(8)-C(3)-N(2)	119.3(3)
C(4)-C(3)-N(2)	120.9(3)	C(5)-C(4)-C(3)	119.1(4)
C(6)-C(5)-C(4)	120.9(4)	C(7)-C(6)-C(5)	119.8(4)
C(6)-C(7)-C(8)	120.0(4)	C(7)-C(8)-C(3)	120.4(4)