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The Crystal and Molecular Structure of Di-(3-aminopropyl)aminedi-isothiocyanatecadmium(II)

M. CANNAS, A. CRISTINI and G. MARONGIU
Istituto Chimico, Università di Cagliari, 09100 Cagliari, Italy

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The crystal structure of the title compound has been determined from three dimensional X-ray data. Crystals are monoclinic, space group $P2_1/c$, with Z = 4 in a unit cell of dimensions: a = 7.77(1), b = 14.44(2), c = 13.54(2) Å, β = 112.2(3)°. The structure was solved by the heavy-atom method and refined by least-squares techniques to R 0.076 for 1760 observed reflections measured by diffractometer. The coordination polyhedron is square-pyramidal, with the basal plane occupied by the amine [Cd–N 2.20–2.33 Å] and thiocyanate nitrogen [Cd–N 2.36 Å] atoms; the apical position is filled by the nitrogen atom of the second thiocyanate group [Cd–N 2.17 Å]. The nitrogen atom of the basal thiocyanate group completes the geometry of centrosymmetrically related molecules to a distorted octahedron [Cd–N 3.08 Å].

Introduction

We have recently reported the unusual co-ordination of the terdentate ligand bis(2-aminoethyl)amine (*den*) in Cd(*den*)$(NCS)_2$ [1]. In this compound the ligand molecule is bonded by two nitrogen atoms to the same cation and by the remaining one to the nearest cation, giving rise to a polymeric structure; this consists of zig-zag Cd–SCN–Cd chains running along the *a* axis and held together by the non-chelating arm of the amine. We suggested that this type of structure is possible because the amine arm in *den* ligand has the right length to bridge the Cd–SCN–Cd chains. In order to gain further support to this hypothesis, we have prepared the title compound, where the ligand (*dpt*) contains propylenic instead of ethylenic chains and we report herewith the results of the single-crystal structure analysis.

Experimental

The compound, prepared by dropwise addition of the ligand to an hot alcohol solution of $Cd(SCN)_2$, was characterized by elemental analysis; colourless prismatic crystals were obtained by evaporation of a concentrated methyl alcohol solution, containing a few drops of water.

Crystal Data

$C_8H_{17}N_5CdS_2$, M = 359.79, Monoclinic, *a* = 7.77(1), *b* = 14.44(2), *c* = 13.54(2) Å, β = 112.2(3)°, U = 1406.5 Å^3, D_m (flotation) 1.68 g cm^{-3}, Z = 4, D_c = 1.70 g cm^{-3}, F(000) = 720. Space group $P2_1/c$ from systematic absences. MoKα radiation, λ = 0.7107 Å, μ(MoKα) = 18.02 cm^{-1}. Unit-cell parameters and their estimated standard deviations were determined by a least-squares fit to 16 values of θ, χ, φ, accurately measured by use of a very narrow counter aperture.

Intensity Measurements

A crystal of dimensions 0.015 × 0.02 × 0.10 cm was mounted on a Siemens automatic single-crystal AED diffractometer with the *c* axis nearly coincident with the polar φ axis of the goniostat. A total of 2405 independent intensities up to $2\theta \leqslant 50°$ was recorded, by a procedure similar to that described previously [1], using the θ–2θ scan technique. The values of I and σ(I) (from counting statistics) were corrected for Lorentz-polarization effects but not for absorption or extinction. 241 reflections had a negative net intensity count and were reset to zero; 1760 obey the condition $F_o \geqslant 2\sigma(F_o)$ and were used in subsequent calculations.

Solution and Refinement of the Structure

The positions of the cadmium and sulphur atoms were determined by a three-dimensional Patterson synthesis; a successive three-dimensional Fourier map gave the positions of all the remaining non-hydrogen atoms. The R factor, obtained by use of the overall and scale factors derived from a Wilson plot, was 0.16 for 1760 observed reflections. Refinement of the structure was carried out by block-diagonal least-squares method. Throughout the refinement the quantity minimized was $\Sigma w(\Delta F)^2$, where $w = 4F_o^2/[\sigma^2(F_o^2) + (0.12 F_o^2)^2]$. Atomic scattering factors for Cd, S, N and C were taken from Cromer and Waber [2], that for hydrogen from Stewart, Davidson and Simpson [3].

Six cycles of isotropic refinement of non hydrogen atoms parameters reduced R to 0.09; refinement was terminated after four cycles using anisotropic thermal parameters for cadmium and sulphur atoms and

TABLE I. Atomic Coordinates (× 10^4) and Thermal Parameters

	x/a	y/b	z/c	B
Cd	1150(2)	313(1)	1648(1)	a
S(1)	−4811(7)	1715(4)	−801(4)	a
S(2)	605(11)	1893(5)	4754(6)	a
N(1)	−1466(24)	843(12)	190(14)	4.74(35)
N(2)	871(27)	1162(14)	2898(15)	5.78(42)
N(3)	3044(23)	1096(12)	1093(13)	4.66(34)
N(4)	3742(21)	−450(10)	2846(13)	3.61(28)
N(5)	−501(19)	−1009(10)	1706(11)	3.46(28)
C(1)	−2815(22)	1177(11)	−183(13)	2.81(30)
C(2)	855(27)	1461(14)	3709(16)	3.96(37)
C(3)	4690(40)	1490(20)	1920(25)	4.50(55)
C(4)	5896(38)	780(20)	2499(22)	6.92(59)
C(5)	5249(38)	215(18)	3286(23)	6.60(57)
C(6)	3421(30)	−940(16)	3706(17)	4.87(43)
C(7)	1899(35)	−1673(18)	3285(20)	5.96(53)
C(8)	−165(31)	−1349(16)	2757(17)	4.82(44)

[a]Anisotropic thermal parameters in the form: $\exp-1/4(B_{11}h^2a^{*2} + B_{22}k^2b^{*2} + B_{33}l^2c^{*2} + 2B_{12}hka^*b^* + 2B_{13}hla^*c^* + 2B_{23}Klb^*c^*)$.

	B_{11}	B_{22}	B_{33}
Cd	3.11(5)	3.37(5)	3.22(5)
S(1)	3.40(23)	5.26(27)	4.74(26)
S(2)	9.51(45)	6.99(37)	5.69(34)
	B_{12}	B_{13}	B_{23}
Cd	−0.13(10)	2.27(8)	0.43(11)
S(1)	1.39(41)	2.79(40)	0.56(43)
S(2)	−2.60(67)	9.47(67)	−2.91(58)

including the contribution of the hydrogen atoms held fixed at calculated positions (B = 4.5 Å²). The final R factor is 0.076 for 1760 refined reflections and 0.12 for 2405 measured ones. A difference electron density map, calculated from the final structure factors with no hydrogen contribution, showed some peaks ranging from 0.7 to 0.9 e/Å³ in height close to some of the positions calculated for the hydrogen atoms and a few others of comparable height close to the cadmium atom or scattered through the cell.

Final structural parameters are given in Table I; observed and calculated structure factors are listed in Table II.

Discussion

Differently from *den* in the analogous thiocyanate-cadmium(II) complex the *dpt* ligand in this compound is chelated to one metal atom, as usually found in the other known derivatives [4–7]. Since the only factor which differentiates the two compounds is the length of the amine arm, the hypothesis that it plays a determinant role in the formation of a polymeric structure in the *den* derivative seems to be confirmed. After this analysis was completed, the complex with (2-aminoethyl-3-aminopropyl)amine, which contains both ethylenic and propylenic chains, has been prepared and characterized by elemental analysis; its structure may also be formed by discrete molecules since the crystal data

TABLE II. Observed and Calculated Structure Factors.

2	14	0	38*	-37
2	15	0	36*	-2
2	16	0	23*	-22
2	1	1	630	-603
2	2	1	98	82
2	3	1	478	-453
2	4	1	257	-262
2	5	1	294	-260
2	6	1	382	-372
2	7	1	112	-92
2	8	1	326	-361
2	9	1	23*	-52
2	10	1	248	-250
2	11	1	180	171
2	12	1	81	-84
2	13	1	190	186
2	14	1	36*	-51
2	15	1	41	75
2	16	1	0*	-4
2	0	2	478	-493
2	1	2	380	342
2	2	2	917	-885
2	3	2	563	529
2	4	2	411	-415
2	5	2	252	253
2	6	2	48	28
2	7	2	162	148
2	8	2	140	-139
2	9	2	117	106
2	10	2	144	149
2	11	2	75	88
2	12	2	221	234
2	13	2	82	111
2	14	2	126	141
2	15	2	0*	11
2	16	2	120	139
2	1	3	83	-114
2	2	3	369	367
2	3	3	41	84
2	4	3	242	238
2	5	3	160	-194
2	6	3	511	538
2	7	3	0*	3
2	8	3	411	421
2	9	3	50	55
2	10	3	139	153
2	11	3	0*	29
2	12	3	205	225
2	13	3	15*	54
2	14	3	103	116
2	15	3	8*	20
2	16	3	35*	-24
2	0	4	535	558
2	1	4	192	184
2	2	4	392	384
2	3	4	144	148
2	3	4	148	148
2	4	4	303	342
2	4	4	306	342
2	5	4	143	133
2	6	4	115	121
2	7	4	325	345
2	8	4	63	-94
2	9	4	170	187
2	10	4	86	-64
2	11	4	65	53
2	12	4	165	-152
2	13	4	75	98
2	14	4	122	-128
2	15	4	56	53
2	1	5	432	421
2	2	5	31*	34
2	3	5	509	508
2	3	5	513	508
2	4	5	183	-185
2	4	5	186	-189
2	5	5	197	175
2	6	5	32*	-48
2	7	5	109	110
2	8	5	35*	8
2	9	5	24*	-57
2	10	5	123	-138
2	11	5	187	-197
2	12	5	51	-70
2	13	5	112	-115
2	14	5	36*	-3
2	15	5	128	-125
2	0	6	85	95
2	1	6	98	-95
2	2	6	114	98
2	3	6	238	-294
2	4	6	73	73
2	5	6	259	-274
2	5	6	145*	-274
2	6	6	31*	-58
2	7	6	214	-238
2	8	6	0*	19
2	9	6	329	-325
2	10	6	75	79
2	11	6	227	-217
2	12	6	35*	-32
2	13	6	76	-78
2	14	6	22*	-15
2	1	7	351	-346
2	2	7	183	-181
2	3	7	103	-103
2	4	7	127	-124
2	5	7	271	-277
2	5	7	91*	-277
2	6	7	0*	-201
2	6	7	202	-201
2	7	7	60	-58
2	8	7	244	-241
2	9	7	102	102
2	10	7	186	-175
2	11	7	0*	42
2	12	7	91	-93
2	13	7	118	118
2	0	8	340	-345
2	1	8	0*	-4
2	2	8	271	-290
2	3	8	65	54
2	4	8	163	-156
2	5	8	141	129
2	5	8	0*	129
2	6	8	107	-110
2	6	8	33*	-110
2	7	8	57	67
2	8	8	39*	-45
2	9	8	57	52
2	10	8	0*	54
2	11	8	62	68
2	12	8	100	87
2	1	9	112	-129
2	2	9	90	100
2	3	9	53	53
2	4	9	276	274
2	5	9	53	-49
2	6	9	217	197
2	7	9	31*	-37
2	9	9	48	27
2	10	9	166	182
2	11	9	0*	13
2	0	10	177	197
2	1	10	0*	4
2	2	10	125	126
2	3	10	76	80
2	4	10	74	101
2	5	10	160	157
2	6	10	80	88
2	7	10	104	103
2	8	10	0*	-6
2	9	10	95	92
2	10	10	45*	-45
2	1	11	254	244
2	2	11	113	-112
2	3	11	153	135
2	4	11	0*	1
2	5	11	97	88
2	6	11	0*	-38
2	7	11	40*	42
2	8	11	19*	-52
2	0	12	130	124
2	1	12	29*	-22
2	2	12	50	44
2	3	12	78	-86
2	4	12	0*	5
2	5	12	112	-114
2	6	12	0*	20
2	1	13	85	-86
2	2	13	59	-55
3	0	0	418	-393
3	1	0	305	-338
3	2	0	212	-205
3	3	0	256	-258
3	4	0	262	-276
3	5	0	180	-179
3	6	0	318	-305
3	7	0	324	-336
3	8	0	88	90
3	9	0	281	-306
3	10	0	124	137
3	11	0	215	-252
3	12	0	5*	1
3	13	0	81	-84
3	14	0	100	92
3	15	0	0*	-16
3	16	0	84	91
3	1	1	705	-720
3	2	1	246	228
3	3	1	275	-288
3	4	1	0*	0
3	5	1	421	-428
3	6	1	0*	80
3	7	1	66	-54
3	8	1	30*	48
3	9	1	208	214
3	10	1	0*	5
3	11	1	115	130
3	12	1	0*	15
3	13	1	160	162
3	14	1	12*	0
3	15	1	155	165
3	0	2	258	-225
3	1	2	10*	2
3	2	2	303	-272
3	3	2	183	222
3	4	2	245	-215
3	5	2	319	298
3	6	2	117	-107
3	7	2	256	243
3	8	2	75	70
3	9	2	286	328
3	10	2	92	105
3	11	2	172	185
3	12	2	0*	21
3	13	2	83	75
3	14	2	72	76
3	15	2	65	59
3	1	3	224	237
3	2	3	0*	23
3	3	3	320	332
3	4	3	455	393
3	5	3	0*	19
3	6	3	436	423
3	7	3	86	63
3	8	3	205	208
3	9	3	22*	10
3	10	3	189	205
3	11	3	173	-158
3	12	3	151	149
3	13	3	106	-103
3	14	3	63	61
3	15	3	61	-69
3	0	4	538	541
3	1	4	153	-174
3	2	4	366	333
3	3	4	76	57
3	4	4	384	351
3	5	4	173	172
3	6	4	284	292
3	7	4	68	-42
3	8	4	21*	-36
3	9	4	38*	37
3	10	4	132	-135
3	11	4	0*	-3
3	12	4	145	-162
3	13	4	32*	-52
3	14	4	129	-131
3	1	5	174	171
3	2	5	238	-222
3	3	5	148	142
3	4	5	234	-223
3	5	5	104	92
3	5	5	103	92
3	6	5	311	-280
3	7	5	62	80
3	8	5	269	-290
3	9	5	15*	-38
3	10	5	170	-174
3	11	5	21*	-45
3	12	5	130	-130
3	13	5	30*	-36
3	14	5	62	-66
3	0	6	89	-97
3	1	6	120	-120
3	2	6	237	-236
3	3	6	184	-181
3	4	6	157	-134
3	5	6	187	-205
3	6	6	0*	-26
3	7	6	289	-253
3	8	6	33*	-58
3	9	6	211	-205
3	10	6	91	84
3	11	6	118	-128
3	12	6	69	63
3	13	6	82	-74
3	1	7	246	-255
3	2	7	55	39
3	3	7	323	-318
3	4	7	48	22
3	5	7	138	-157
3	6	7	29*	6
3	7	7	31*	18
3	8	7	20*	16
3	9	7	17*	8
3	10	7	0*	-6
3	11	7	87	83
3	12	7	42*	-10
3	0	8	24*	-10
3	1	8	127	130
3	2	8	215	-208
3	3	8	195	200
3	4	8	179	-162
3	5	8	168	164
3	6	8	21*	21
3	7	8	180	172
3	8	8	0*	-19
3	9	8	120	127
3	10	8	54	48
3	11	8	85	104
3	1	9	85	101
3	2	9	151	158
3	3	9	66	81
3	4	9	105	122
3	5	9	30*	32
3	6	9	132	126
3	7	9	0*	25
3	8	9	148	141
3	9	9	0*	-9
3	10	9	96	96
3	0	10	282	271
3	1	10	0*	22
3	2	10	198	185
3	3	10	5*	-23
3	4	10	131	123
3	5	10	15*	-5
3	6	10	101	85
3	7	10	54	47
3	8	10	28*	-3
3	1	11	88	90
3	2	11	0*	-37
3	3	11	99	100
3	4	11	91	-102
3	5	11	34*	17
3	6	11	93	-93
3	0	12	56	-81
3	1	12	0*	14
3	2	12	64	-56
4	0	0	462	-424
4	1	0	304	-317
4	2	0	650	-616
4	3	0	154	-144
4	4	0	407	-402
4	5	0	20*	-5
4	6	0	0*	3
4	7	0	173	-153
4	8	0	46*	16
4	9	0	21*	-8
4	10	0	90	100
4	11	0	41*	-62
4	12	0	151	171
4	13	0	42*	-64
4	14	0	124	125
4	15	0	20*	6
4	1	1	334	-311
4	2	1	213	220
4	3	1	483	-477
4	4	1	75	48
4	5	1	87	-56
4	6	1	218	227
4	7	1	0*	29
4	8	1	269	262
4	9	1	38*	-31
4	10	1	160	176
4	11	1	128	119
4	12	1	82	100
4	13	1	115	108
4	14	1	0*	22
4	0	2	310	299
4	1	2	127	112
4	2	2	91	77
4	3	2	351	356
4	4	2	49	39
4	5	2	366	353
4	6	2	107	105
4	7	2	304	297
4	8	2	62	-52
4	9	2	249	282
4	10	2	27*	-29
4	11	2	186	189
4	12	2	40*	-26
4	13	2	126	124
4	14	2	63	-68
4	1	3	323	321
4	2	3	155	151
4	3	3	348	365
4	4	3	38*	6
4	5	3	260	264
4	6	3	80	139
4	7	3	73	86
4	8	3	72	87
4	9	3	72	-69
4	10	3	0*	16
4	11	3	100	-104
4	12	3	97	88
4	13	3	140	-132
4	14	3	34*	11
4	0	4	208	229
4	1	4	52	45
4	2	4	148	158
4	3	4	144	-126
4	4	4	196	206
4	5	4	347	-330
4	6	4	147	166
4	7	4	174	-191
4	8	4	0*	-17
4	9	4	123	-125
4	10	4	37*	-66
4	11	4	115	-130
4	12	4	85	-91
4	13	4	40*	-39
4	1	5	86	-111
4	2	5	0*	35
4	3	5	26*	13
4	4	5	298	-295
4	5	5	24*	-53
4	6	5	254	-272
4	7	5	15*	11
4	8	5	194	-210
4	9	5	52	21
4	10	5	201	-197
4	11	5	0*	-26
4	12	5	65	-72
4	0	6	332	-296
4	1	6	21*	-5
4	2	6	222	-238
4	3	6	40*	-30
4	4	6	142	-154
4	5	6	68	-61
4	6	6	124	-117
4	7	6	43*	-53
4	8	6	25*	17
4	9	6	71	-44
4	10	6	78	90
4	11	6	55	-44
4	1	7	243	-211
4	2	7	78	75
4	3	7	164	-135
4	4	7	95	105
4	5	7	185	-185
4	6	7	114	139
4	7	7	55*	-14
4	8	7	117	114
4	9	7	61	77
4	10	7	83	86
4	0	8	0*	-2
4	1	8	19*	35
4	2	8	47	46
4	3	8	145	145
4	4	8	42*	52
4	5	8	168	167
4	6	8	0*	-18
4	7	8	112	111
4	8	8	0*	14
4	9	8	138	133
4	1	9	157	150
4	2	9	29*	34
4	3	9	215	213
4	4	9	87	72
4	5	9	85	81
4	6	9	27*	29
4	7	9	0*	23
4	0	10	126	121
4	1	10	39*	-40
4	2	10	98	92
4	3	10	40	-40
4	4	10	83	85
4	5	10	27*	-43
5	0	0	536	-542
5	1	0	0*	-97
5	2	0	272	-281
5	3	0	41	17
5	4	0	107	-131
5	5	0	102	126
5	6	0	194	-182
5	7	0	151	165
5	8	0	35*	-16
5	9	0	140	143
5	10	0	70	59
5	11	0	76	69
5	12	0	90	56
5	13	0	33*	47
5	1	1	26*	-27
5	2	1	271	294
5	3	1	116	112
5	4	1	164	171
5	5	1	88	-55
5	6	1	258	287
5	7	1	50	-52
5	8	1	259	311
5	9	1	30*	42
5	10	1	222	223
5	11	1	13*	-7
5	12	1	131	134
5	13	1	0*	6
5	0	2	106	141
5	1	2	26*	-22
5	2	2	263	283
5	3	2	128	158
5	4	2	215	234
5	5	2	172	170
5	6	2	0*	38
5	7	2	81	66
5	8	2	68	52
5	9	2	146	155
5	10	2	37*	-35
5	11	2	125	110
5	12	2	107	-112
5	13	2	0*	30
5	1	3	244	236
5	2	3	105	-86
5	3	3	298	276
5	4	3	71	-91
5	5	3	123	134
5	6	3	94	-108
5	7	3	32*	33
5	8	3	136	-142
5	9	3	0*	-29
5	10	3	52	-49
5	11	3	55	-91
5	12	3	15*	-25
5	0	4	85	74
5	1	4	118	-121
5	2	4	70	47
5	3	4	132	-108
5	4	4	54	36
5	5	4	180	-170
5	6	4	47	35
5	7	4	301	-255
5	8	4	13*	-7
5	9	4	160	-155
5	10	4	25*	-44
5	11	4	83	-100
5	1	5	275	-247
5	2	5	152	-131
5	3	5	187	-154
5	4	5	78	-73
5	5	5	77	-79
5	6	5	115	-93
5	7	5	29*	-18
5	8	5	135	-124
5	9	5	22*	11
5	10	5	21*	-48
5	0	6	230	-216
5	1	6	66	-63
5	2	6	259	-241
5	3	6	37*	6
5	4	6	156	-135
5	5	6	105	85
5	6	6	39*	-39
5	7	6	45	65
5	8	6	44*	-33
5	9	6	96	88
5	1	7	20*	-5
5	2	7	69	64
5	3	7	61	-41
5	4	7	131	108
5	5	7	23*	17
5	6	7	146	163
5	7	7	0*	14
5	8	7	148	148
5	0	8	165	174
5	1	8	0*	23
5	2	8	94	102
5	3	8	61	63
5	4	8	80	94
5	5	8	76	77
5	6	8	74	76
5	1	9	113	121
5	2	9	0*	11
6	0	0	86	-71
6	1	0	0*	-14
6	2	0	125	-106
6	3	0	159	156
6	4	0	97	-88
6	5	0	254	258
6	6	0	18*	-5
6	7	0	216	212
6	8	0	0*	-17
6	9	0	224	222
6	10	0	26*	14
6	11	0	98	112
6	12	0	55	70
6	1	1	238	234
6	2	1	88	106
6	3	1	7*	11
6	4	1	131	122
6	5	1	74	90
6	6	1	188	179
6	7	1	55	59
6	8	1	178	177
6	9	1	67	-49
6	10	1	128	128
6	11	1	0*	-18
6	0	2	431	403
6	1	2	87	-85
6	2	2	263	249
6	3	2	83	-71
6	4	2	153	124
6	5	2	18*	-9
6	6	2	115	90
6	7	2	5*	-18
6	8	2	0*	-22
6	9	2	30*	-17
6	10	2	[illegible]	-46
6	11	2	6*	-24
6	1	3	157	144
6	2	3	53	-60
6	3	3	35*	62
6	4	3	211	-211
6	5	3	70	72
6	6	3	154	-128
6	7	3	0*	-1
6	8	3	131	-135
6	9	3	36*	-36
6	10	3	155	-185
6	0	4	174	-185
6	1	4	16*	-12
6	2	4	166	-149
6	3	4	101	-100
6	4	4	92	-84
6	5	4	165	-155
6	6	4	0*	-15
6	7	4	85	-52
6	8	4	0*	4
6	9	4	116	-106
6	1	5	153	-208
6	2	5	0*	18
6	3	5	128	-144
6	4	5	65	-58
6	5	5	78	-96
6	6	5	32*	37
6	7	5	36*	-34
6	8	5	42*	45
6	0	6	84	-81
6	1	6	21*	30
6	2	6	49	-48
6	3	6	45*	54
6	4	6	13*	-26
6	5	6	57	92
6	6	6	74	-35
6	1	7	41*	65
6	2	7	21*	27
6	3	7	69	68
7	0	0	32*	11
7	1	0	72	56
7	2	0	104	103
7	3	0	100	90
7	4	0	63	53
7	5	0	108	134
7	6	0	30*	-28
7	7	0	208	205
7	8	0	32*	39
7	9	0	121	136
7	1	1	245	248
7	2	1	36*	0
7	3	1	218	155
7	4	1	30*	-21
7	5	1	59	61
7	6	1	41*	45
7	7	1	23*	21
7	8	1	40*	51
7	9	1	18*	15
7	0	2	117	108
7	1	2	45	-46
7	2	2	161	167
7	3	2	36*	-70
7	4	2	73	86
7	5	2	55	-85
7	6	2	0*	-26
7	7	2	105	-113
7	8	2	25*	26
7	1	3	71	-74
7	2	3	75	-53
7	3	3	0*	-31
7	4	3	99	-103
7	5	3	31*	-45
7	6	3	130	-132
7	7	3	39*	-14
7	0	4	144	-139
7	1	4	55	-47
7	2	4	118	-127
7	3	4	0*	-12
7	4	4	104	-121
7	5	4	13*	-10
7	1	5	112	-85
8	0	0	166	154
8	1	0	27*	2
8	2	0	132	146
8	3	0	70	61
8	4	0	96	111
8	5	0	94	65
8	6	0	67	64
8	1	1	172	171
8	2	1	0*	-19
8	3	1	48	47
8	4	1	14*	-25
8	0	2	41*	12
8	1	2	0*	-24

TABLE III. Bond Distances (Å) and Angles (°) in Cd(dpt)-$(NCS)_2$ with Calculated e.s.d.'s in Parentheses.

Distances			
Cd–N(1)	2.36(2)	Cd–N(4)	2.33(2)
Cd–N(2)	2.17(2)	Cd–N(5)	2.32(2)
Cd–N(3)	2.20(2)	Cd–N(1)^{I}	3.08(2)
S(1)–C(1)	1.65(2)	N(1)–C(1)	1.09(2)
S(2)–C(2)	1.62(2)	N(2)–C(2)	1.18(3)
N(3)–C(3)	1.46(2)	C(3)–C(4)	1.41(3)
N(4)–C(5)	1.46(3)	C(4)–C(5)	1.57(4)
N(4)–C(6)	1.46(3)	C(6)–C(7)	1.53(3)
N(5)–C(8)	1.43(3)	C(7)–C(8)	1.56(3)
Angles			
N(1)–Cd–N(2)	99.2(0.7)	Cd–N(1)–Cd^{I}	101.1(0.6)
N(1)–Cd–N(3)	91.4(0.6)	Cd–N(1)–C(1)^{I}	102.8(1.4)
N(1)–Cd–N(4)	168.2(0.6)	Cd–N(2)–C(2)	166.0(1.7)
N(1)–Cd–N(5)	89.0(0.6)	Cd–N(3)–C(3)	116.3(1.0)
N(1)–Cd–N(1)^{I}	78.9(0.6)	Cd–N(4)–C(5)	108.8(1.3)
N(2)–Cd–N(3)	104.7(0.7)	Cd–N(4)–C(6)	114.8(1.2)
N(2)–Cd–N(4)	92.3(0.7)	C(5)–N(4)–C(6)	110.3(1.7)
N(2)–Cd–N(5)	102.6(0.7)	Cd–N(5)–C(8)	114.9(1.2)
N(2)–Cd–N(1)^{I}	177.9(0.6)	S(1)–C(1)–N(1)	176.5(1.7)
N(3)–Cd–N(4)	88.1(0.6)	S(2)–C(2)–N(2)	174.1(1.9)
N(3)–Cd–N(5)	152.3(0.6)	N(3)–C(3)–C(4)	110.5(1.4)
N(3)–Cd–N(1)^{I}	74.6(0.6)	C(3)–C(4)–C(5)	116.1(2.1)
N(4)–Cd–N(5)	86.1(0.6)	N(4)–C(5)–C(4)	118.8(2.2)
N(4)–Cd–N(1)^{I}	89.6(0.6)	N(4)–C(6)–C(7)	112.3(1.8)
N(5)–Cd–N(1)^{I}	78.3(0.5)	C(6)–C(7)–C(8)	118.7(2.0)
Cd–N(1)–C(1)	154.8(1.5)	N(5)–C(8)–C(7)	109.2(1.8)

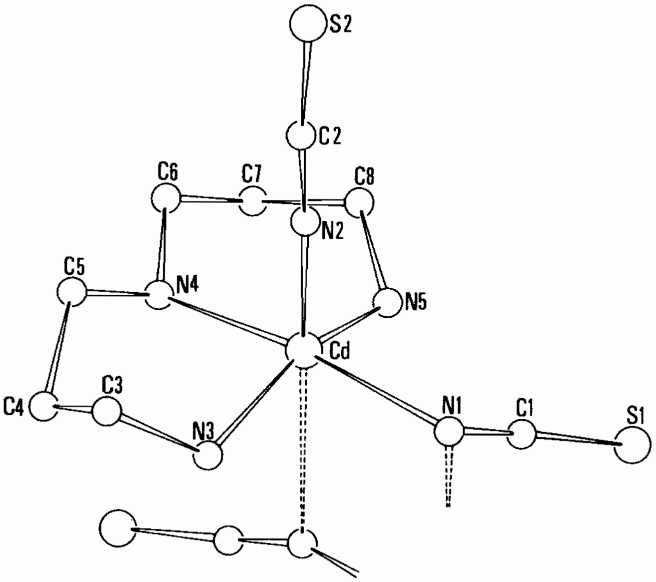

Figure 1. A view of the coordination polyhedron.

and the appearance of the Okl Weissenberg photograph are very similar to those of *dpt* complex.

A view of the co-ordination polyhedron is shown in Fig. 1; bond distances and angles are given in Table III.

The co-ordination polyhedron is very close to a square pyramid: the apical position is occupied by the nitrogen atom of a thiocyanate group, and the basal positions are occupied by the nitrogen atoms of the amine and by that of the second thiocyanate group. These atoms lie alternately 0.15 Å above [N(1), N(4)] and below [N(3), N(5)] the least-squares plane; cadmium is 0.39 Å above this plane towards the apical position. The nitrogen atom of the basal thiocyanate also fills the sixth position of the centrosymmetrically related molecule, so that the structure could also be considered as consisting of complex dimers formed by two octahedrons which share the N(1)–N(1)^{I} edge. Several other examples of centrosymmetric cations bridged by the thiocyanate nitrogen atom have been reported [8–10].

The two Cd–N_{prim} bond distances are significantly different, as also found in Cu(*dpt*)(OAc)ClO_4 [6]; in the other known structures containing this ligand the two bonds have been found equivalent. The Cd–N distances involving the thiocyanate nitrogen bridge are very different: the one in the base is an elongated covalent bond, about 0.2 Å longer than the apical one; the other is instead very close to the sum of the covalent radius of the metal in octahedral structrues (≅1.55 Å) and of the van der Waals radius of the nitrogen atom (≅1.50 Å). Nevertheless, its position is most probably a consequence of the tendency of cadmium(II) cation to be six-co-ordinate rather than of packing conditions. This is supported by a comparison with the structure of the analogous Cu(*dpt*)$(NCS)_2$ [7] compound, which is definitely five co-ordinate; in this last compound the basal planes of the square-pyramidal polyhedrons are faced one to the other, while in the compound reported here they are translated in order to allow the N-bridging of the basal thiocyanate group.

Bond lengths and angles in the ligands are close to the expected values. Atomic distances from the plane througt the amine nitrogen atoms show that the two fused chelated rings, which adopt the chair conformation, like that observed in the complexes of 1,3-diaminopropane, are almost related by a plane of symmetry through the Cd–N(4) bond.

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References

1 M. Cannas, G. Carta, A. Cristini and G. Marongiu, *Inorg. Chem.*, in press.
2 D. T. Cromer and J. T. Water, *Acta Cryst.*, *18*, 104 (1965).
3 R. F. Stewart, E. R. Davidson and W. T. Simpson, *J. Chem. Phys.*, *42*, 3175 (1965).
4 S. Biagini and M. Cannas, *J. Chem. Soc. A*, 2398 (1970).
5 P. R. Ireland, D. A. House and W. T. Robinson, *Inorg. Chim. Acta*, *4*, 137 (1970).
6 B. W. Skelton, T. N. Waters and N. F. Curtis, *J. Chem. Soc. Dalton*, 2134 (1972).
7 M. Cannas, G. Carta, A. Cristini and G. Marongiu, *J. Chem. Soc. Dalton*, 1278 (1974).
8 G. D. Andreetti, L. Coghi, M. Nardelli and P. Sgarabotto, *J. Cryst. Mol. Struct.*, *1*, 147 (1971).
9 M. Mercer and M. R. Truter, *J. Chem. Soc. Dalton*, 2469 (1973).
10 P. R. Mallinson, *J. Chem. Soc. Perkin II*, 261 (1975).