Mercury(II)–Ethylenediamine Complexes. Crystal and Molecular Structure of Bis(ethylenediamine)mercury(II) Diperchlorate and Dithiocyanato-(ethylenediamine)mercury(II)

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Crystals of bis(ethylenediamine)mercury(II) diperchlorate, (I), are monoclinic, $a = 7.754(6)$, $b = 11.618(7)$, $c = 7.754(6)$ Å, $\beta = 100.38(3)°$, space group $P2_1$, $Z = 2$. In the complex cation the mercury ion is co-ordinated by four nitrogen atoms (Hg–N 2.30—2.33 Å) in a distorted tetrahedron (N–Hg–N ring angles 77.2 and 78.5°). The ethylenediamine ligands are bidentate, bonded in the usual gauche conformation. The amino-groups of one ligand form hydrogen bonds with the perchlorate oxygen (N–H · · · O 2.52 and 2.55 Å).

Crystals of dithiocyanato(ethylenediamine)mercury(II), (II), are orthorhombic, $a = 12.029(8)$, $b = 11.101(8)$, $c = 7.069(5)$ Å, space group $Pna2_1$, $Z = 4$. The structure is built up of discrete molecules in which mercury is co-ordinated by two nitrogen atoms (Hg–N 2.31 and 2.33 Å) from ethylenediamine, in the gauche conformation, and by two sulphur atoms (Hg–S 2.428 and 2.529 Å) from the thiocyanate ions in a distorted tetrahedron (N–Hg–N 80.0, S–Hg–S 111.3°). The thiocyanates are slightly bent, with S–C–N 175 and 178°.

The structures were determined from diffractometer *X*-ray intensity data and refined by full-matrix least-squares methods to R 0.062 (I) and 0.044 (II) for 941 and 635 reflections, respectively.

ALTHOUGH the crystal structures of many ethylenediamine metal complexes have been determined, little is known about the structure of the ethylenediamine complexes of mercury. It was only established [1] from *X*-ray and i.r. data that $Hg(en)Cl_2$ (en = ethylenediamine) has an open-chain structure with ethylenediamine as a bridging ligand, in contrast to most other complexes in which ethylenediamine is a chelating ligand, and forms a five-membered ring with the metal ion. It appeared to us that is should be possible to form complexes in which mercury was chelated by ethylenediamine, especially since some other bidentate ligands (based on nitrogen) are able to chelate mercury, as was shown recently by the structure analysis of *cis*-dithiocyanatobis(1,10-phenanthroline)mercury(II),[2] bis-μ-bromo-bis[bromo-(2,2′-bipyridyl)mercury(II)],[3] and tris(1,8-naphthyridine)-mercury(II) perchlorate.[4] We assumed that the nature of the co-ordination of mercury by ethylenediamine might be influenced by that of the anion present in the structure. Thus we selected two known mercury ethylenediamine complexes obtained by the action of ethylenediamine on mercury(II) perchlorate [5] and mercury(II) thiocyanate,[6] respectively. Their formulae were suggested as $[Hg(en)_2][ClO_4]_2$ and $[Hg(en)_2][Hg(SCN)]_4$, respectively. Actually, as reported here, we found the former to be correct, but that the latter should be $[Hg(en)(SCN)_2]$. In both complexes the mercury atom is chelated by ethylenediamine in essentially the same way.

EXPERIMENTAL

Crystals of the complexes, prepared as described previously,[5,6] were obtained by recrystallization from hot aqueous solution (I) and from hot aqueous ethanol (II).

Crystal Data.—(I), $Hg(C_2H_8N_2)_2(ClO_4)_2$, $M = 519.7$, Monoclinic, $a = 7.754(6)$, $b = 11.618(7)$, $c = 7.754(6)$ Å, $\beta = 100.38(3)°$, $U = 687.1$ Å^3, $D_m = 2.48$ g cm^{-3} (pycnometrically in decalin), $Z = 2$, $D_c = 2.530$ g cm^{-3}, $F(000) = 492$. Space group $P2_1$ (C_2^2, No. 4) or $P2_1/m$ (C_{2h}^2, No. 11) from systematic absences: $0k0$ when k odd; the former, non-centrosymmetric group subsequently confirmed by the structure analysis. Cu-K_α radiation, $\lambda = 1.5418$ Å; μ(Cu-K_α) = 253.1 cm^{-1}.

(II), $Hg(C_2H_8N_2)(SCN)_2$, $M = 376.8$, Orthorhombic, $a = 12.029(8)$, $b = 11.101(8)$, $c = 7.069(5)$ Å, $D_m = 2.60$ g cm^{-3} (pycnometrically in mother liquor), $Z = 4$, $D_c = 2.659$ g cm^{-3}, $F(000) = 688$. Space group $Pna2_1$ (C_{2v}^9, No. 33) or $Pnam$ (D_{2h}^{16}) from systematic absences: $0kl$ when $k + l$ odd, $h0l$ when h odd; the former, non-centrosymmetric group was established by the structure solution. Mo-K_α radiation, $\lambda = 0.7107$ Å; μ(Mo-K_α) = 167.9 cm^{-1}.

Crystallographic Measurements and Data Collection.—Unit-cell dimensions were obtained from Weissenberg and oscillation photographs and then refined by a least-squares method from the 2θ values for 22 reflections measured on a Philips PW 1100 automatic diffractometer which was used for the three-dimensional intensity data collection. The crystals were not suitable to be ground to a spherical or cylindrical shape, so very thin needles (along the c axis in both cases) were used with the cross-section approximated to a circle giving μR 0.23 (I) and 0.24 (II); no absorption correction was therefore made. Intensities were collected by the ω—2θ scan method on a Philips PW 1100 four-circle diffractometer. The intensities of three reflections measured every 2 h dropped by 7 and 8%, respectively, during data collection, indicating slow crystal decomposition. For (I) graphite-monochromated Cu-K_α radiation was used (take-off angle 3°, scan width 1.60° θ, scan speed 0.04° θ s^{-1}) and data were collected to maximum value of sin θ/λ 0.60. The 941 reflections with a net intensity $I \geqslant 3\sigma(I)$ were used in the structure refinement [$\sigma(I)$ based on counting statistics]. For (II) graphite-monochromated Mo-K_α radiation was used (take-off angle 3°, scan width 1.20°θ, scan speed 0.03°θ s^{-1}) and data were collected to sin θ/λ 0.70. The 635 reflections with $I \geqslant 3\sigma(I)$ were used in the structure solution and refinement. Unit weights were used because all weak reflections were measured twice. Corrections for Lorentz and polarization effects were applied in the usual manner.

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TABLE 1

Atomic co-ordinates and thermal parameters, with estimated standard deviations in parentheses

(*a*) For $[Hg(en)_2][ClO_4]_2$ (I)

	x/a	y/b	z/c	B/Å^2
Hg	0.234 5(2)	0.2500	0.734 4(2)	*
Cl(1)	0.038 2(15)	0.017 7(12)	0.047 8(15)	*
Cl(2)	0.547 7(15)	0.484 3(12)	0.537 1(17)	*
N(11)	−0.065(4)	0.283(3)	0.674(4)	1.3(6)
N(12)	0.173(4)	0.226(3)	0.432(4)	1.8(7)
N(21)	0.448(5)	0.133(3)	0.883(5)	1.9(7)
N(22)	0.389(4)	0.373(3)	0.943(4)	1.0(5)
C(11)	−0.109(6)	0.300(5)	0.482(6)	2.4(9)
C(12)	−0.021(6)	0.208(4)	0.384(6)	2.2(9)
C(21)	0.584(7)	0.207(4)	0.991(7)	2.5(10)
C(22)	0.498(6)	0.303(5)	0.076(6)	2.5(9)
O(11)	0.093(5)	0.135(4)	0.064(5)	3.7(7)
O(12)	0.183(6)	−0.047(5)	0.029(6)	5.7(11)
O(13)	−0.019(6)	−0.020(4)	0.206(6)	4.9(9)
O(14)	−0.102(5)	0.002(4)	−0.106(5)	3.4(11)
O(21)	0.573(4)	0.372(3)	0.595(4)	3.1(7)
O(22)	0.709(5)	0.527(4)	0.476(5)	4.1(8)
O(23)	0.528(7)	0.555(5)	0.680(7)	6.1(11)
O(24)	0.393(6)	0.497(4)	0.410(6)	3.8(11)

* Anisotropic thermal parameters ($\times 10^4$) in the form $\exp[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + 2b_{12}hk + 2b_{13}hl + 2b_{23}kl)]$ with co-efficients:

	b_{11}	b_{12}	b_{13}
Hg	98(29)	−33(102)	−66(39)
Cl(1)	105(245)	−38(229)	81(393)
Cl(2)	94(211)	−11(220)	−18(413)

	b_{22}	b_{23}	b_{33}
Hg	45(12)	6(102)	81(28)
Cl(1)	15(79)	−4(227)	79(219)
Cl(2)	2(72)	−2(232)	152(279)

(*b*) For $[Hg(en)(SCN)_2]$ (II) †

	x/a	y/b	z/c
Hg	0.134 1(1)	0.057 9(1)	0.2500
S(1)	0.053 0(8)	0.258 0(9)	0.2344(45)
S(2)	−0.014 1(9)	−0.103 4(10)	0.235 5(54)
N(1)	−0.171(3)	0.185(4)	0.262(25)
N(2)	0.129(3)	−0.308(3)	0.254(17)
N(3)	0.279(3)	0.009(3)	0.049(5)
N(4)	0.263(3)	−0.018(3)	0.466(6)
C(1)	−0.082(3)	0.210(4)	0.258(12)
C(2)	0.071(4)	−0.225(4)	0.242(13)
C(3)	0.352(2)	−0.076(2)	0.162(5)
C(4)	0.374(3)	−0.016(3)	0.361(6)

† Anisotropic thermal parameters ($\times 10^4$) with coefficients:

	b_{11}	b_{12}	b_{13}
Hg	40(8)	25(23)	−15(165)
S(1)	55(61)	7(108)	50(376)
S(2)	53(62)	−11(112)	−6(444)
N(1)	52(265)	19(534)	−475(2 892)
N(2)	39(205)	−6(449)	112(1 696)
N(3)	36(184)	−16(336)	−28(720)
N(4)	40(196)	2(375)	12(654)
C(1)	89(295)	20(560)	167(1 956)
C(2)	112(524)	−53(762)	378(1 951)
C(3)	33(193)	1(402)	110(580)
C(4)	65(266)	25(598)	−15(990)

	b_{22}	b_{23}	b_{33}
Hg	50(10)	10(224)	125(36)
S(1)	47(64)	23(368)	33(420)
S(2)	66(74)	6(507)	58(476)
N(1)	88(350)	−681(4 649)	863(2 319)
N(2)	58(236)	−35(2 579)	154(1 006)
N(3)	29(180)	−37(698)	140(881)
N(4)	69(230)	−84(659)	6(732)
C(1)	40(336)	−71(1 608)	−60(1 025)
C(2)	72(359)	255(1 949)	284(1 886)
C(3)	68(329)	120(779)	−5(477)
C(4)	78(331)	−38(967)	78(793)

Structure Solution and Refinement.—Compound (I). The Fourier synthesis with signs determined by mercury precluded the possibility of the centrosymmetric space group $P2_1/m$ and the non-centrosymmetric space group $P2_1$ was used. The successful selection of the light-atom peaks was achieved by means of subsequent Fourier syntheses in which the light-atom positions had been included by consideration of the geometry of the ethylenediamine ligand and the perchlorate ion; R was 0.115 at this stage. Further refinement by full-matrix least-squares calculations with isotropic temperature factors reduced R to 0.102, and then with anisotropic factors for the mercury and chlorine atoms to the final value of 0.062. Because of the relatively small number of observations per parameter, refinement with anisotropic temperature factors for light atoms was not carried out. Final atomic co-ordinates and the thermal parameters are listed in Table 1.

Complex (II).—The preliminary atomic co-ordinates were obtained by the heavy-atom method for the centrosymmetric space group *Pnam* with the mercury atom located in the mirror plane (positions 4*c*). It implied C_s point-group symmetry of the molecule of (II), i.e., both thiocyanates coplanar and in the same mirror plane with the mercury atom, while the C–C bond in the ethylenediamine was perpendicular to and halved by the mirror plane. Full-matrix least-squares refinement with isotropic and then with anisotropic factors resulted in a relatively low value of R, 0.055, but the inadequate bond-length and -angle values, as well as the unusual geometry and conformation of the ethylenediamine, pointed to an incorrect choice of space group. The refinement was then repeated in the non-centrosymmetric space group $Pna2_1$, as the next sub-group of *Pnam*. After four cycles of refinement, assuming individual isotropic temperature factors, R was 0.061. The subsequent five cycles of anisotropic refinement reduced R to the final value of 0.044. The ethylenediamine appeared in the usual gauche conformation with consistent geometry, and the distances and angles within the thiocyanates were in good agreement with the known data. Final positional parameters and temperature factors are given in Table 1.

In the refinements of both structures, unit weights were assumed for all observations. Atomic scattering factors were taken from ref. 7 with corrections for anomalous scattering according to ref. 8 by refining both models: that originally chosen and the reversed one, *i.e.* with opposing signs for the y co-ordinate in structure (I) and the z co-ordinate in structure (II). The R factors did not differ, *i.e.* the values of 0.062 and 0.044 were obtained for both models of the (I) and (II) structures, respectively. Analysis of the values of bond lengths and angles as well as of the standard deviations confirmed the correctness of the originally refined structures.

Calculations were carried out on the UNIVAC 1110 of the S.R.C.E., University Computing Centre, Zagreb, with the system of programmes of ref. 9. Observed and calculated structure factors are listed in Supplementary Publication No. SUP 21639 (18 pp., 1 microfiche).*

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* See Notice to Authors No. 7, in *J.C.S. Dalton*, 1975, Index issue.

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[8] D. T. Cromer and D. Liberman, *J. Chem. Phys.*, 1970, **53**, 1891.

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DESCRIPTION OF THE STRUCTURE AND DISCUSSION

Structure (I).—The crystal structure of the ethylenediamine complex with mercury(II) perchlorate is built up of bis(ethylenediamine)mercury(II) cations and perchlorate anions (Figure 1) and the correct formulation of the complex is $[Hg(en)_2][ClO_4]_2$. The mercury ion is chelated by both ethylenediamine ligands, the four nitrogen atoms of the amino-group forming an orthorhombic disphenoid ('elongated and twisted tetrahedron') about the mercury ion. There is no other atom in the structure which could be considered to belong to the mercury co-ordination sphere, since the closest perchlorate oxygen atom is 3.12 Å from the mercury atom, *i.e.*, more than the sum of the accepted van der Waals radii. Consequently, the effective co-ordination about the mercury atom is based upon the characteristic tetrahedral co-ordination, according to the classification suggested previously.[10] The distortion may be considered to be composed of (*a*) the elongation of the tetrahedron along the bisector of the N–Hg–N angle in the rings, and (*b*) of a twist around it of 27°. The first component is due to the small 'bite' of the bidentate ligand and a comparatively large Hg–N bond length, which both stretch the five-membered ring. The twisting component of the deformation is due to N–H · · · O hydrogen bonding between the amino-group and the perchlorate ion. It is not symmetric, *i.e.*, only one of two ethylenediamine ligands in the complex [that labelled (1)] is in a favourable position for the formation of strong hydrogen bonds: N(11) · · · O(13) 2.52 and N(12) · · · O(22) 2.55 Å. The other half of the complex [labelled (2)] is fixed only by weak intermolecular contacts between the perchlorate oxygens and the methylene groups. Thus the angle between the planes, defined by the positions of Hg, N(11), N(12) and Hg, N(21), N(22), is 63° instead of 90° as expected for the only 'elongated' tetrahedron.

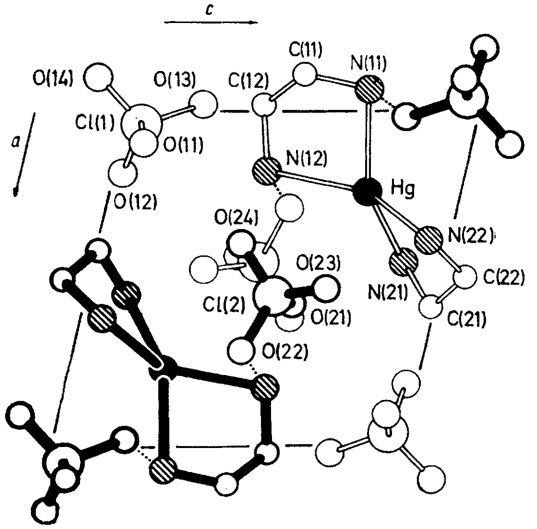

FIGURE 1 The crystal structure of $[Hg(en)_2][ClO_4]_2$ seen in the projection on the *ac* plane. Hydrogen bonds N–H · · · O are shown by dotted lines

The ethylenediamine ligands are in the gauche conformation, as expected.[11] Its geometry is given by the dihedral angle (ω) between the planes which are defined by the C–C–N(1) and C–C–N(2) bonds, respectively. Again, owing to the different surrounding, the ω-value is not equal for both ligands, being 64.7 and 58.6° for ligands (1) and (2), respectively. The parameters z, giving the distances of the carbon atoms from the plane defined by the metal atom and both nitrogen atoms in the same ligand,[10,12] have the values z(11) −0.36, z(12) 0.43 Å and z(21) 0.35, z(22) −0.35 Å, which are

TABLE 2

Interatomic distances (Å) and bond angles (°), with standard deviations in parentheses

(*a*) For $[Hg(en)_2][ClO_4]_2$ (I)

Hg–N(11)	2.32(3)	Cl(1)–O(11)	1.42(4)
Hg–N(12)	2.33(3)	Cl(1)–O(12)	1.38(5)
Hg–N(21)	2.30(4)	Cl(1)–O(13)	1.44(5)
Hg–N(22)	2.32(3)	Cl(1)–O(14)	1.47(4)
N(11)–C(11)	1.48(5)	Cl(2)–O(21)	1.38(4)
N(12)–C(12)	1.50(6)	Cl(2)–O(22)	1.50(4)
N(21)–C(21)	1.50(6)	Cl(2)–O(23)	1.41(6)
N(22)–C(22)	1.46(6)	Cl(2)–O(24)	1.42(4)
C(11)–C(12)	1.54(7)	O(24) · · · N(12)	2.55(6)
C(21)–C(22)	1.51(7)	O(13I) · · · N(11)	2.52(6)
N(11)–Hg–N(12)	78.5(11)	Hg–N(12)–C(12)	106.4(25)
N(11)–Hg–N(21)	143.8(13)	Hg–N(21)–C(21)	108.1(28)
N(11)–Hg–N(22)	114.3(11)	Hg–N(22)–C(22)	108.4(27)
N(12)–Hg–N(21)	115.8(13)	N(11)–C(11)–C(12)	111.2(37)
N(12)–Hg–N(22)	139.8(12)	N(12)–C(12)–C(11)	107.3(35)
N(21)–Hg–N(22)	77.2(12)	N(21)–C(21)–C(22)	110.4(39)
Hg–N(11)–C(11)	105.4(24)	N(22)–C(22)–C(21)	110.2(38)
O(11)–Cl(1)–O(12)	107.3(28)	O(21)–Cl(2)–O(22)	109.3(24)
O(11)–Cl(1)–O(13)	110.2(26)	O(21)–Cl(2)–O(23)	108.9(27)
O(11)–Cl(1)–O(14)	110.7(23)	O(21)–Cl(2)–O(24)	112.3(25)
O(12)–Cl(1)–O(13)	107.8(29)	O(22)–Cl(2)–O(23)	105.8(28)
O(12)–Cl(1)–O(14)	110.1(27)	O(22)–Cl(2)–O(24)	113.3(25)
O(13)–Cl(1)–O(14)	110.7(25)	O(23)–Cl(2)–O(24)	106.9(29)

Transformation of the asymmetric unit (x,y,z): I $-x$, $\frac{1}{2}+y$, $1-z$.

(*b*) For $[Hg(en)(SCN)_2]$ (II)

Hg–S(1)	2.428(10)	Hg · · · C(3)	3.08(4)
Hg–S(2)	2.529(11)	Hg · · · C(4)	3.10(5)
Hg–N(3)	2.31(4)	N(1) · · · N(4)	3.01(6)
Hg–N(4)	2.33(4)	N(2) · · · N(3)	3.11(6)
S(1)–C(1)	1.71(4)	N(3) · · · N(4)	2.97(6)
S(2)–C(2)	1.69(5)	N(3) · · · C(4)	2.50(6)
C(1)–N(1)	1.11(5)	N(4) · · · C(3)	2.48(5)
C(2)–N(2)	1.17(6)	N(1) · · · N(3^{I})	3.23(6)
N(3)–C(3)	1.52(4)	N(4) · · · N(1^{I})	3.00(6)
N(4)–C(4)	1.52(5)	N(2^{II}) · · · N(3^{III})	3.11(6)
C(3)–C(4)	1.58(5)	N(2^{II}) · · · N(4^{III})	3.43(6)
Hg · · · C(1)	3.10(3)	S(1) · · · N(1^{IV})	3.38(4)
Hg · · · C(2)	3.23(4)		
S(1)–Hg–S(2)	111.3(3)	Hg–S(1)–C(1)	95.3(14)
N(3)–Hg–N(4)	80.0(13)	Hg–S(2)–C(2)	97.8(18)
S(1)–Hg–N(3)	119.2(8)	Hg–S(1)–N(1)	96.8(9)
S(1)–Hg–N(4)	128.9(9)	Hg–S(2)–N(2)	97.8(7)
S(2)–Hg–N(3)	109.9(8)	S(1)–C(1)–N(1)	175(10)
S(2)–Hg–N(4)	103.9(8)	S(2)–C(2)–N(2)	178(10)
Hg–N(3)–C(3)	105.1(22)	N(3)–C(3)–C(4)	107(3)
Hg–N(4)–C(4)	105.0(26)	N(4)–C(4)–C(3)	107(3)

Transformation of the asymmetric unit (x,y,z): I $-x$, $-y$, $\frac{1}{2}+z$ II x, $1+y$, z III $\frac{1}{2}-x$, $\frac{1}{2}+y$, $\frac{1}{2}+z$ IV $\frac{1}{2}+x$, $\frac{1}{2}-y$, z

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[10] D. Grdenić, *Quart. Rev.*, 1965, **19**, 303. See also: D. Grdenić, Crystal Chemistry of Mercury, in 'Handbook of Geochemistry,' vol. II/1, ed. K. H. Wedepohl, Springer–Verlag, Berlin, 1969, p. 80 A 1.

[11] S. Jamet-Delcroix, *Bull. Soc. chim. France*, 1974, 45.

[12] J. R. Gollogly and C. J. Hawkins, *Inorg. Chem.*, 1969, **8**, 1168.

common for the ethylenediamine ligand in six-co-ordinated (octahedral) and four-co-ordinated (planar) metal complexes. As far as we know, no previous analysis of a tetrahedral ethylenediamine metal complex has been reported, thus no comparisons can be made.

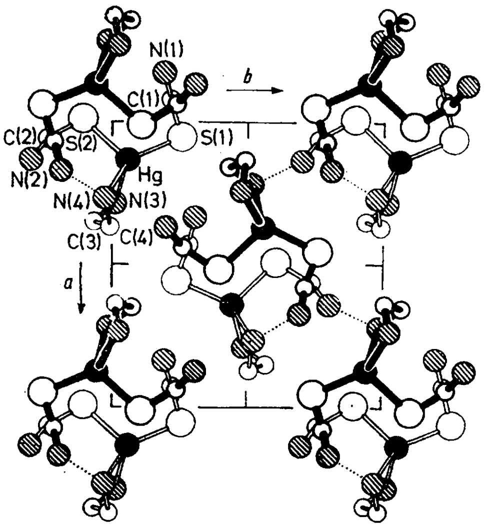

FIGURE 2 The crystal structure of $[Hg(en)(SCN)_2]$ seen in projection on the *ab* plane. Hydrogen bonds N–H ··· N are shown by dotted lines

Interatomic distances and bond angles in the complex (Table 2) are as expected. The Hg–N bond lengths are almost equal, mean 2.32 Å. This is longer than in many structures [13] containing mercury in characteristic digonal co-ordination with nitrogen, but approximately the same as in mercury(II) complexes with 1,10-phenanthroline,[2] 2,2′-bipyridyl,[3] and 1,8-naphthyridine.[4] It is greater by 0.12 Å than the sum of the tetrahedral covalent radii (1.48 for mercury and 0.70 Å for nitrogen),[10,14] which may be explained by the departure from the ideal tetrahedral co-ordination.

The geometry of the perchlorate ions is as expected.[15]

Structure of (II).—The crystal structure of the ethylenediamine complex with mercury(II) thiocyanate (Figure 2) is composed of discrete molecules and the compound is accordingly formulated as $[Hg(en)(SCN)_2]$. The mercury atom is chelated by the ethylenediamine ligand and covalently bonded with two sulphur atoms of the thiocyanate ions in an effectively tetrahedral co-ordination. The planes defined by Hg, S(1), Hg(2) and Hg, N(3), N(4) are almost normal to each other (89.8°), so that the departure from the ideal tetrahedron is essentially due to the different kinds of ligands. The difference in length between the Hg–S bonds (2.428 and 2.529 Å) is interesting and may be due to the influence of hydrogen bonds (see later). However, different Hg–S bond lengths within the same molecule have already been observed.[2,16] Interatomic distances and bond angles within the ligands are as expected.[11,17]

The ethylenediamine ligand is in the usual gauche comformation defined by the parameters z of 0.443, −0.434 Å, for the carbon atoms C(4) and C(3) respectively, and ω of 68.9°, in agreement with the values in other metal ethylenediamine complexes.[11]

There are no intermolecular distances shorter than the sum of the van der Waals radii except those between the thiocyanate nitrogen and the amino-group of two molecules related by the screw axis and the diagonal glide plane, *i.e.* $N(1^{I}) \cdots N(4)$ 3.00 and $N(2^{II}) \cdots N(3^{II})$ 3.11 Å, which could be attributed to N ··· H–N hydrogen bonds.[18] These bonds certainly contribute to the geometry of the complex as a whole, as described earlier.

We had intended to study the structures of the compounds described as ethylenediammonium tri- and tetra-thiocyanatomercurate(II).[19] However, we found that the former is identical with dithiocyanato(ethylenediamine)mercury(II) (II), while we were not able to prepare the latter.

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