Structural Studies of Group 5B–Halide–Dithio-ligand Complexes. Part 7.† Crystal Structures of the 1 : 1 Adducts of (*NN*-Diethyldithiocarbamato)-di-iodobismuth(III) with 2,2′-Bipyridyl and 2,2′:6′,2″-Terpyridyl

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The crystal structures of the title compounds, [Bi(S_2CNEt_2)I_2(bipy)], (1), and [Bi(S_2CNEt_2)I_2(terpy)], (2) (bipy = 2,2′-bipyridyl, terpy = 2,2′:6′,2″-terpyridyl), have been determined by single-crystal *X*-ray diffraction methods at 295(1) K and refined by least-squares procedures to conventional residuals of 0.047 and 0.045 respectively for 2 794 and 1 589 ' observed ' reflections. Crystals of (1) are triclinic, space group $P\bar{1}$, with a = 13.432(5), b = 10.122(4), c = 9.780(5) Å, α = 117.66(3), β = 98.89(4), γ = 100.42(3)°, and Z = 2. Crystals of (2) are monoclinic, space group $P2_1/c$, with a = 9.122(4), b = 11.440(6), c = 24.684(9) Å, β = 94.21(3)°, and Z = 4. The molecule of (2) is pseudopentagonal bipyramidal in its co-ordination, the two iodine atoms lying axial [Bi–I, 3.070(2), 3.031(2) Å; I–Bi–I, 169.0(1)°]. In (1), a binuclear complex is formed, [(bipy)I(Et_2NCS_2)BiI_2Bi(S_2CNEt_2)I(bipy)], with a pair of bridging iodine atoms.

THE previous paper[1] has described the isolation and structural characterization of mononuclear complexes of the form [Bi(S_2CNEt_2)X_2(py)$_3$]·py (py = pyridine), in which the bismuth atom adopts pseudo-pentagonal-bipyramidal stereochemistry with the three pyridine moieties loosely co-ordinated adjacent to each other in the equatorial plane. Given this situation it was considered to be of interest to attempt to prepare and characterize a 1 : 1 adduct of [Bi(S_2CNEt_2)X_2] and 2,2′:6′,2″-terpyridyl (terpy) in order to ascertain (*a*) the mode of co-ordination and (*b*) if tridentate, whether the planar ligand system with coplanar α-hydrogen atoms on the peripheral pyridyl rings could be successfully accommodated within the framework of a similar pentagonal bipyramid to the above. This being successful, it was also considered to be of interest to study the manner in which the molecule would resolve its plight when confronted with the bidentate 2,2′-bipyridyl (bipy) ligand and resultant pyridine deprivation.

An n-butanol solution of [Bi(S_2CNEt_2)I_2] was allowed to stand after mixing with a solution containing a five-fold excess of 2,2′-bipyridyl. After some days the inhomogeneous yellow precipitate was examined and found to contain a few small pale yellow crystals. Unit-cell determination established a volume considered to be consistent with the desired product [Bi(S_2CNEt_2)I_2(bipy)], (1), and the structure determination was proceeded with and the identity of the compound confirmed.

The same reaction carried out with 2,2′:6′,2″-terpyridyl was much cleaner and the solution slowly deposited a homogeneous orange crystalline solid. Analysis showed the compound to be the desired product [Bi(S_2CNEt_2)I_2(terpy)], (2), and a structure determination was proceeded with [Found: C, 28.6; H, 2.7; I, 29.7; N, 6.6; S, 7.7. Calc. for $C_{20}H_{21}BiI_2N_2S_4$, (2): C, 28.5; H, 2.5; I, 30.1; N, 6.6; S, 7.6%].

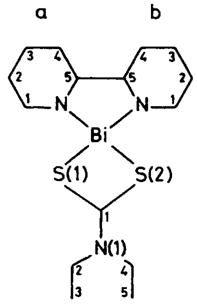
CRYSTALLOGRAPHY

Crystal Data.—(1). $C_{15}H_{18}BiI_2N_3S_2$, M = 767.1, Triclinic, space group $P\bar{1}$ (C_i^1, no. 2), a = 13.432(5), b = 10.122(4), c = 9.780(5) Å, α = 117.66(3), β = 98.89(4), γ = 100.42(3)°, U = 1 114.1(8) Å^3, D_m = 2.28(1), Z = 2, D_c = 2.29 g cm^{-3}, $F(000)$ = 700, μ(Mo) = 105 cm^{-1}. Specimen size: 0.08 × 0.15 × 0.21 mm, $2\theta_{max.}$ = 50°, n = 3 891, n_o = 2 794, R, R', S values are 0.047, 0.052, 1.62 respectively.

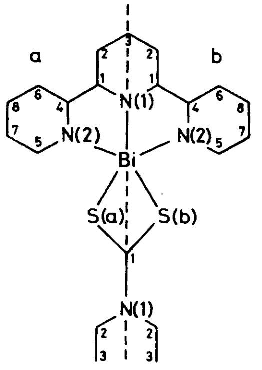
(2). $C_{20}H_{21}BiI_2N_4S_2$, M = 844.3, Monoclinic, space group $P2_1/c$ (C_{2h}^5, no. 14), a = 9.122(4), b = 11.440(6), c = 24.684(9) Å, β = 94.21(3)°, U = 2 569(2) Å^3, D_m = 2.17(1), Z = 4, D_c = 2.18 g cm^{-3}, $F(000)$ = 1 560, μ(Mo) = 94 cm^{-1}. Specimen size: 0.23 × 0.20 × 0.02 mm, $2\theta_{max.}$ = 40°, n = 2 355, n_o = 1 589, R, R', S values are 0.045, 0.052, 1.7 respectively.

Abnormal Features.—The limited data available on (2) precluded meaningful anisotropic thermal parameter refinement of the dithiocarbamate ethyl substituent carbon atoms; these were refined isotropically without associated hydrogen atoms.

Atom numbering in (1) and (2) is as shown; note that in (2) the dithiocarbamate ligand numbering is unconventional in order to take advantage of the pseudo-two-fold symmetry element for compact tabulation.



(1)



(2)

Tables 1 and 2 list the non-hydrogen atom fractional cell co-ordinates. Structure-factor amplitudes, thermal parameters, hydrogen-atom parameters, and least-squares planes are deposited in Supplementary Publication No. SUP 22982 (24 pp.).‡

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† Part 6 is ref. 1. Part 1 contains general descriptive crystallographic and definitional detail.

‡ For details see Notices to Authors No. 7, *J. Chem. Soc., Dalton Trans.*, 1979, Index issue.

TABLE 1

Non-hydrogen atom fractional cell co-ordinates for (1)

Atom	*x*	*y*	*z*
Bi	0.189 79(4)	0.181 26(5)	0.080 76(6)
I(1)	−0.046 60(8)	0.169 99(9)	0.189 74(11)
I(2)	0.280 83(11)	0.151 80(14)	0.360 21(13)
(*a*) Dithiocarbamate ligand			
S(1)	0.315 4(3)	0.056 7(4)	−0.102 3(4)
S(2)	0.378 3(3)	0.384 3(4)	0.158 5(5)
C(1)	0.411(1)	0.233(2)	0.014(2)
N(1)	0.507(1)	0.254(1)	−0.006(1)
C(2)	0.538(1)	0.129(2)	−0.131(2)
C(3)	0.522(2)	0.136(3)	−0.283(2)
C(4)	0.591(1)	0.400(2)	0.101(2)
C(5)	0.649(2)	0.399(2)	0.239(2)
(*b*) Bipyridyl ligand			
(*i*) part a			
N	0.173(1)	0.464(1)	0.222(1)
C(1)	0.195(1)	0.546(2)	0.382(2)
C(2)	0.210(1)	0.704(2)	0.468(2)
C(3)	0.200(2)	0.779(2)	0.386(2)
C(4)	0.172(1)	0.698(2)	0.220(2)
C(5)	0.159(1)	0.537(1)	0.140(2)
(*ii*) part b			
N	0.132(1)	0.291(1)	−0.098(1)
C(1)	0.110(1)	0.198(2)	−0.260(2)
C(2)	0.083(1)	0.250(2)	−0.361(2)
C(3)	0.079(1)	0.400(2)	−0.299(2)
C(4)	0.102(1)	0.496(2)	−0.134(2)
C(5)	0.130(1)	0.436(1)	−0.040(1)

TABLE 2

Non-hydrogen atom fractional cell co-ordinates for (2)

	Part a			Part b		
Atom	*x*	*y*	*z*	*x*	*y*	*z*
Bi	0.285 92(9)	0.217 13(8)	0.123 29(4)			
I	0.481 19(21)	0.024 29(17)	0.176 59(8)	0.124 32(17)	0.397 64(16)	0.051 57(9)
(*a*) Dithiocarbamate ligand						
S	0.023 3(7)	0.147 3(6)	0.164 6(3)	0.223 1(9)	0.317 6(8)	0.220 1(4)
C(1)	0.066(2)	0.241(2)	0.218(1)			
N(1)	−0.031(2)	0.255(2)	0.255(1)			
C(2)	−0.177(3)	0.186(3)	0.251(1)	−0.001(3)	0.342(3)	0.298(1)
C(3)	−0.230(5)	0.163(4)	0.301(2)	0.092(3)	0.302(3)	0.347(1)
(*b*) Terpyridyl ligand						
N	0.444(2)	0.225(2)	0.038 5(7)			
C(3)	0.527(3)	0.288(2)	−0.062 5(9)			
C(1)	0.396(2)	0.162(2)	−0.007 1(9)	0.538(2)	0.315(2)	0.035 2(9)
C(2)	0.436(3)	0.192(2)	−0.058 6(11)	0.580(2)	0.346(2)	−0.014 3(10)
N(2)	0.234(2)	0.057(1)	0.048 7(7)	0.511(2)	0.357(2)	0.128 4(7)
C(4)	0.296(2)	0.062(2)	0.001 2(8)	0.591(2)	0.372(2)	0.084 6(8)
C(5)	0.150(2)	−0.036(2)	0.058 3(9)	0.558(2)	0.408(2)	0.175 7(11)
C(6)	0.271(2)	−0.024(2)	−0.039 0(8)	0.725(2)	0.429(2)	0.088 2(10)
C(7)	0.122(2)	−0.123(2)	0.021 5(10)	0.689(3)	0.476(3)	0.181 8(12)
C(8)	0.181(2)	−0.116(2)	−0.027 1(9)	0.768(3)	0.482(2)	0.135 1(12)

DISCUSSION

Complex (1).—The structure determination establishes the stoicheiometry of the compound to be [Bi(S_2CNEt$_2$)I$_2$(bipy)]. In [Bi(S_2CNEt$_2$)I$_2$(py)$_3$] [1] and [Bi(S_2CNEt$_2$)I$_2$(terpy)], (2) (see below), we find the complex to be mononuclear with pseudo-pentagonal-bipyramidal seven-co-ordinate co-ordination geometry, the axial positions being filled by ***trans*** iodide ligands; this disposition persists, in fact, in all [Bi(S_2CNEt$_2$)X$_2$(py)$_3$] (X = halide) derivatives. In (1) (Figure 1), the ligand systems have one less nitrogen available for co-ordination; we find that in maintaining a seven-co-ordinate bismuth environment (Table 3), the two iodines now lie *cis* to each other in the co-ordination polyhedron, one adopting a bridging role, so that three of the co-ordination sites are filled by iodine, and the complex is binuclear, [(bipy)I(Et$_2$NCS$_2$)BiI$_2$Bi(S_2CNEt$_2$)I(bipy)], one half of the dimer comprising the asymmetric unit of the structure and related to the other half by a crystallographic centre of symmetry. The separation of the two bismuth atoms in the dimer is 5.227(3) Å; the bonds to the bridging iodine are both quite long [3.501(2), 3.250(2) Å] and the angle they subtend at the iodine is 101.41(4)°. The dithiocarbamate and bipyridyl ligands are both substantially symmetrically co-ordinated and planar {σ[defining atoms (non-hydrogen)], 0.04, 0.08 Å}; the methyl groups in the former are disposed on opposite sides of the plane. The dihedral angle between the two planes is 85.4° and the deviation of the bismuth atom 0.24, 0.31 Å respectively. The 2,2′-bipyridyl ligand geometry (Table 4) does not deviate substantially from that recorded for the monoprotonated bipyridylium ion [2] (which, unlike 2,2′-bipyridyl itself, is *cis* about the ring junction as in the co-ordinated form [3]). The most reasonable description of the metal-atom stereochemistry appears to be that presented by considering I(2)–Bi–N(b) as the axis of a pentagonal bipyramid; given this, the deviations of the remaining five atoms from their 'plane' S(1,2),N(a),I[1,1($\bar{x},\bar{y},\bar{z}$)] respectively are 0.35, 0.82, −1.82, 0.72, −0.07 Å (σ 1.08 Å); the bismuth deviation is 0.66 Å. The angle sum in the 'plane' about the bismuth is 362.5°. The position of any sterically active lone pair in such a disposition is not at all obvious.

Complex (2).—The structure determination establishes the stoicheiometry of the compound to be [Bi(S_2CNEt$_2$)I$_2$(terpy)], as expected, the complex being mononuclear with one molecule comprising the asymmetric unit of the cell (Figure 2). The structure of the molecule is of

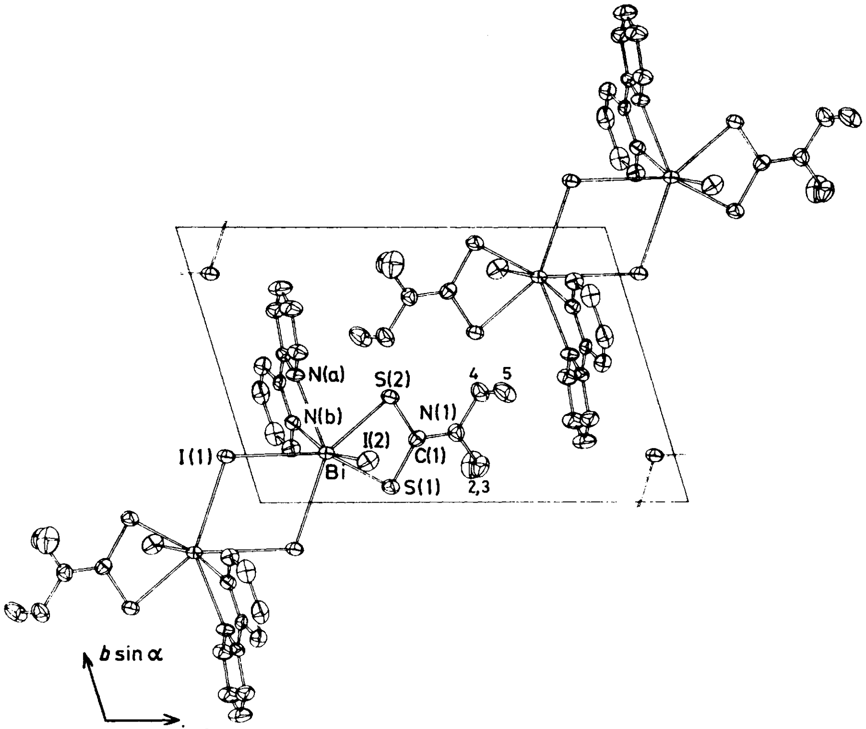


FIGURE 1 Unit-cell contacts of (1) projected down *c*

interest, closely resembling that of $[Bi(S_2CNEt_2)I_2(py)_3]$ with the two iodine atoms lying axial in a pentagonal-bipyramidal co-ordination sphere (Figure 3). The symmetry of the molecule approximates to *mm*, the only serious (minor) perturbation being the disposition of the dithiocarbamate terminal methyl groups. The equatorial plane contains a bidentate dithiocarbamate ligand and the three pyridyl nitrogen atoms; again, the departure from linearity in the I–Bi–I string takes the form of a deviation of the iodine atoms away from the dithiocarbamates and towards the central nitrogen atom. The Bi–I distances [3.070(2), 3.031(2) Å] resemble those of $[Bi(S_2CNEt_2)I_2(py)_3]$ closely [3.101(2), 3.021(2) Å], as does the I–Bi–I angle [169.0(1), 174.2(1)°], suggesting that any contacts from the I atoms to the pyridine *ortho*-hydrogen atoms in the pyridine complex must be at the van der Waals distance or greater, and have no influence on the Bi–I distance (Table 5).

Whereas the BiI_2 geometry is similar in the two pyridine complexes and (2), the geometries in the equatorial plane (Table 6) differ rather radically. For the S_2N_3Bi plane in the di-iodo–pyridine adduct, σ is 0.07 Å; in the present complex we find it is much higher, being 0.17 Å. Individual atom deviations are shown in Figure 4, and show that the terpyridyl ring system is extensively buckled, primarily by movement of the central ring out of the plane of the other two, although ring a is also considerably twisted relative to the median BiS_2N_3 plane. The dihedral angles of the individual pyridine rings with the latter plane are 27.2 (central), 19.5, 15.4° (a, b), the estimated standard deviation of the defining C_5N skeleton in each case is 0.02, 0.01, 0.03 Å. Such drastic distortion is unusual in 2,2′:6′,2″-terpyridyl complexes, and appears to originate in the relatively weak interaction and consequent long bonds to the metal atom; we therefore hypothesize that the distortion is due to the diminished strain in the two BiN_2 chelate rings allowing the hydrogen atoms at C(2) and C(6) in each section to come into contact with each other.

TABLE 3

The bismuth environment in (1): r_{Bi-X} is in Å; the other entries in the matrix are the angles (°) subtended by the relevant atoms. I(1′) is generated from I(1) by the symmetry operation $(\bar{x}, \bar{y}, \bar{z})$

Atom	r_{Bi-X}	I(2)	S(1)	S(2)	N(a)	N(b)	I(1′)
I(1)	3.501(2)	88.08(5)	153.53(7)	140.12(9)	71.6(3)	91.9(3)	78.59(4)
I(2)	2.985(2)		97.9(1)	86.2(1)	101.9(3)	163.4(2)	104.22(5)
S(1)	2.692(5)			66.3(1)	131.2(3)	89.5(3)	74.94(8)
S(2)	2.699(4)				71.1(3)	83.2(3)	140.9(1)
N(a)	2.61(1)					62.5(3)	92.1(2)
N(b)	2.56(1)						139.3(2)
I(1′)	3.250(2)						

TABLE 4

Ligand non-hydrogen geometries in (1)

(*a*) Dithiocarbamate ligand

(*i*) Distances/Å

S(1)–C(1)	1.72(1)	N(1)–C(2)	1.48(2)
S(2)–C(1)	1.72(1)	N(1)–C(4)	1.47(2)
S(1) · · · S(2)	2.946(5)	C(2)–C(3)	1.50(3)
C(1)–N(1)	1.32(2)	C(4)–C(5)	1.46(3)

(*ii*) Angles/°

Bi–S(1)–C(1)	88.1(5)	C(1)–N(1)–C(2)	123(1)
Bi–S(2)–C(1)	87.8(5)	C(1)–N(1)–C(4)	122(1)
S(1)–C(1)–S(2)	117.5(9)	C(2)–N(1)–C(4)	115(1)
S(1)–C(1)–N(1)	122.1(10)	N(1)–C(2)–C(3)	111(2)
S(2)–C(1)–N(1)	120.3(9)	N(1)–C(4)–C(5)	111(2)

(*b*) Bipyridyl ligand; entries for parts a, b

(*i*) Distances/Å

N–C(1)	1.34(2), 1.36(2)
N–C(5)	1.33(2), 1.32(2)
C(5)–C(5)	1.50(2)
C(1)–C(2)	1.38(2), 1.36(3)
C(2)–C(3)	1.34(3), 1.36(3)
C(3)–C(4)	1.39(2), 1.39(2)
C(4)–C(5)	1.41(2), 1.36(3)

(*ii*) Angles/°

Bi–N–C(1)	120(1), 119(1)
Bi–N–C(5)	120.7(7), 122.7(9)
C(1)–N–C(5)	119(1), 119(1)
N–C(5)–C(5)	116(1), 117(1)
C(4)–C(5)–C(5)	124(2), 120(1)
N–C(5)–C(4)	121(1), 123(1)
N–C(1)–C(2)	123(2), 121(1)
C(1)–C(2)–C(3)	118(1), 119(1)
C(2)–C(3)–C(4)	121(1), 120(2)
C(3)–C(4)–C(5)	118(2), 118(2)

There also appears to be a significant contact between the C(5) hydrogen atoms and the dithiocarbamate sulphur atoms. These contacts are shown in Figure 4 and should be compared with the axial van der Waals estimates of 3.05 and 2.4 Å for S · · · H and H · · · H contacts. A number of terpyridyl structures have been determined; many are imprecise and/or disordered. Table 7 gives comparative angular geometries about the chelate rings for (i) [Co(terpy)(OH)(CO_3)],[4] the compound with the shortest metal–nitrogen distances, (ii) [Cd(terpy){Mn(CO)$_5$}],[5] the compound with the hitherto longest metal–nitrogen distances, and (iii) the present compound. Values of σ for the defining atoms of the terpyridyl skeletal plane are also given. Both compounds (i) and (ii) have substantially coplanar terpyridyl skeletons, in contrast with (2). As the metal–ligand distance increases, the disparity between the central and distant metal–nitrogen distances diminishes and is reversed. Angles within the chelate rings are generally found to increase substantially in parallel with this trend, with the exception of those about the central nitrogen atom, and at the metal itself, the latter diminishing very greatly. No significant trend is observed in any angle within any of the pyridyl rings at the present rather low level of precision. The distance between C(2) and C(6) diminishes appreciably, and presumably it is only for the bismuth complex that the compressive strain in this region of the ligand is large enough to cause distortion.

The bismuth–nitrogen distances in the present complex are appreciably shorter than their counterparts in [Bi(S_2CNEt_2)I_2(py)$_3$] {2.63(2), 2.61(2), 2.61(2) for (2); 2.86(1), 2.71(1), 2.72(1) Å for [Bi(S_2CNEt_2)I_2(py)$_3$]; the central distance is given first in each case}; *i.e.* in spite

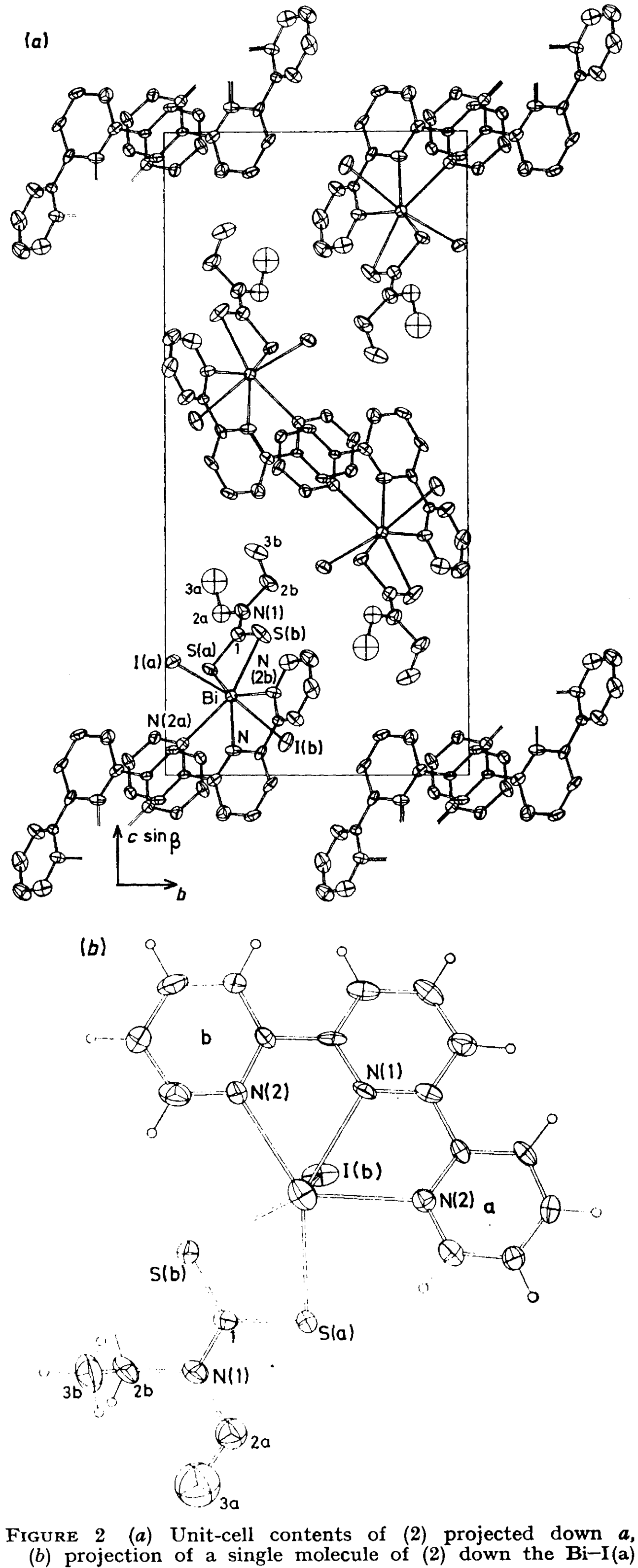


FIGURE 2 (*a*) Unit-cell contents of (2) projected down *a*, (*b*) projection of a single molecule of (2) down the Bi–I(a) bond

TABLE 5

The bismuth environment in (2). Presentation is as for Table 3

Atom	r_{Bi-X}	I(b)	S(a)	S(b)	N(1)	N(2a)	N(2b)
I(a)	3.070(2)	169.0(1)	97.2(1)	94.5(2)	91.7(4)	82.5(4)	89.5(4)
I(b)	3.031(2)		90.8(1)	95.7(2)	77.5(4)	90.5(4)	87.5(4)
S(a)	2.788(7)			64.1(2)	146.7(4)	86.6(4)	148.8(4)
S(b)	2.750(9)				147.2(4)	150.0(4)	85.1(4)
N(1)	2.63(2)					62.8(5)	62.7(5)
N(2a)	2.61(2)						124.5(5)
N(2b)	2.61(2)						

TABLE 6

Ligand non-hydrogen atom geometries in (2). The two entries are for parts a and b respectively where relevant

(*a*) Dithiocarbamate ligand	
(*i*) Distances/Å	
S–C(1)	1.73(2), 1.68(2)
S · · · S	2.94(1)
C(1)–N(1)	1.31(3)
N(1)–C(2)	1.54(3), 1.48(4)
C(2)–C(3)	1.39(6), 1.49(4)
(*ii*) Angles/°	
Bi–S–C(1)	87.4(8), 89.6(9)
S–C(1)–S	119(1)
S–C(1)–N(1)	119(2), 122(2)
C(1)–N(1)–C(2)	121(2), 119(2)
C(2)–N(1)–C(2)	120(2)
N(1)–C(2)–C(3)	114(3), 116(2)
(*b*) Terpyridyl ligand	
(*i*) Distances/Å	
N–C(1)	1.38(3), 1.35(3)
C(1)–C(2)	1.39(3), 1.36(3)
C(2)–C(3)	1.39(3), 1.42(3)
C(1)–C(4)	1.48(3), 1.44(3)
N(2)–C(4)	1.34(3), 1.36(3)
N(2)–C(5)	1.35(3), 1.34(3)
C(4)–C(6)	1.41(3), 1.38(3)
C(5)–C(7)	1.36(3), 1.42(3)
C(6)–C(8)	1.38(3), 1.35(4)
C(7)–C(8)	1.35(3), 1.41(4)
(*ii*) Angles/°	
Bi–N–C(1)	118(1), 117(1)
C(1)–N–C(1)	121(2)
N–C(1)–C(2)	122(2), 119(2)
N–C(1)–C(4)	117(2), 118(2)
C(4)–C(1)–C(2)	121(2), 123(2)
C(1)–C(2)–C(3)	117(2), 122(2)
C(2)–C(3)–C(2)	119(2)
C(1)–C(4)–N(2)	117(2), 117(2)
C(1)–C(4)–C(6)	121(2), 121(2)
N(2)–C(4)–C(6)	122(2), 122(2)
Bi–N(2)–C(4)	121(1), 120(1)
Bi–N(2)–C(5)	120(1), 120(1)
C(4)–N(2)–C(5)	118(2), 119(2)
C(4)–C(6)–C(8)	117(2), 118(2)
N(2)–C(5)–C(7)	123(2), 122(2)
C(5)–C(7)–C(8)	119(2), 115(2)
C(6)–C(8)–C(7)	121(2), 123(2)

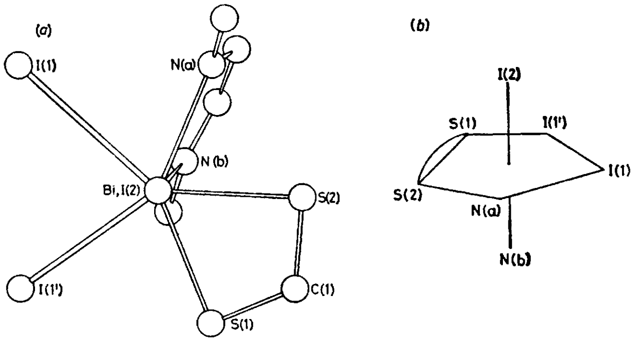


FIGURE 3 (*a*) Projection of the bismuth environment of (1) down the Bi–I(2) bond, (*b*) idealized stereochemistry about the bismuth atom of (1)

of their closer proximity to each other {N–Bi–N, 62.8(5), 62.7(5)° in (2); 71.5(3), 75.4(4)° in [Bi(S$_2$CNEt$_2$)I$_2$(py)$_3$]} the metal–nitrogen bonds are stronger. One contributing factor here could be that the equatorial plane of the

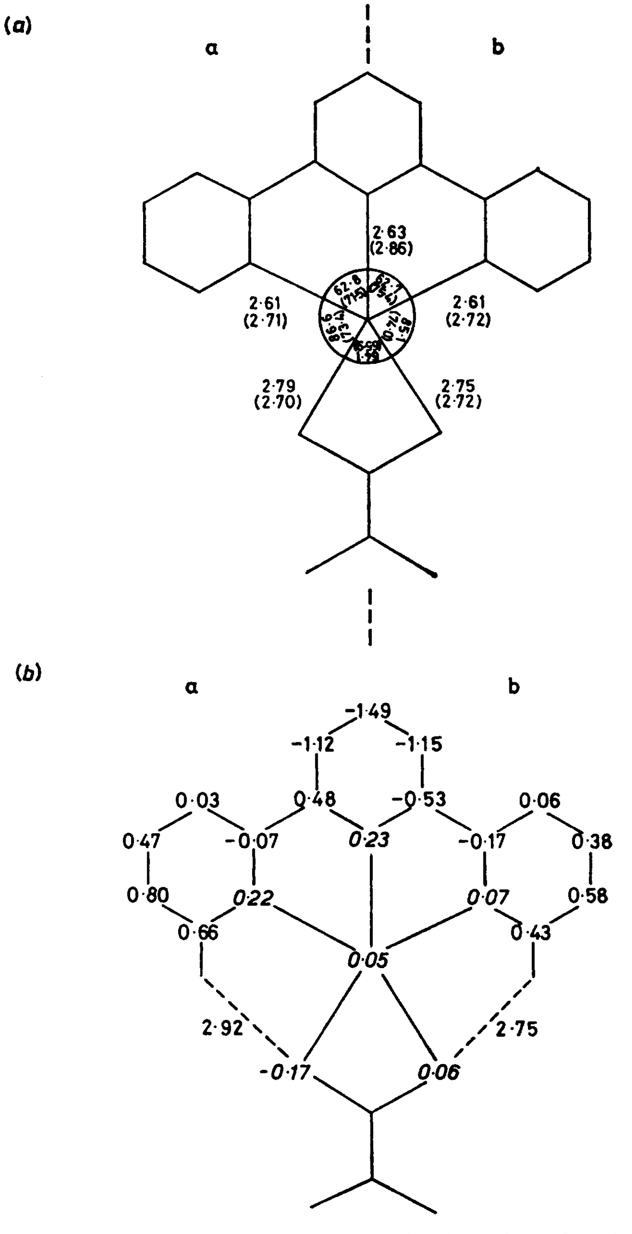
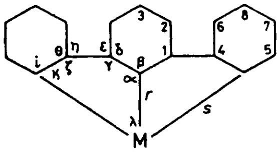


FIGURE 4 (*a*) Median plane geometry for (2); the values in parentheses are those for [Bi(S$_2$CNEt$_2$)I$_2$(py)$_3$]. Distances are in Å and angles in degrees. (*b*) Ligand atom deviations from the median plane in (2). Values for the defining atoms are italicised

TABLE 7

Comparative terpyridyl geometries for (i) [Co(terpy)(OH)(CO_3)], (ii) [Cd(terpy){Mn$(CO)_5$}], and (iii) [Bi(S_2CNEt_2)I_2(terpy)]. Distances are rounded to the nearest 0.01 Å; angles are rounded to the nearest degree; σ/Å is given for the skeletal atoms of the terpyridyl ' plane ' in each case



Parameter	(i)	(ii)	(iii)
σ	0.01	0.06	0.17
r	1.85	2.40	2.63
s	1.95	2.48	2.61
α	119	121	118
β	123	119	121
γ	112	116	118
δ	120	122	121
ε	128	121	122
ζ	114	118	117
η	126	122	121
θ	120	120	122
i	120	120	119
κ	113	119	121
λ	83	66	63

molecule is now filled with a mutually coplanar array of strong π-bonding ligands. The Bi–S distances, however, are longer than in [Bi(S_2CNEt_2)$I_2$$(py)_3$] [2.788(7), 2.750(9); *cf.* 2.695(4), 2.715(4) Å]; this may in part be a consequence of repulsive interaction with the H(5) hydrogen atoms of the terpy ligands. The change, however, is relatively small. The dithiocarbamate ligand geometry is otherwise symmetrical and normal, except that one of the terminal methyl groups has high thermal motion and a seemingly unusual disposition, both methyl groups lying to the one side of the ligand plane.

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