Table 3. *Distances (Å) and angles (°) in the trimethylolpropane molecule*

|			
C(1)–O(1)	1·458 (1)	C(1)–H(4)	0·962 (11)
C(1)–C(4)	1·536 (1)	C(1)–H(5)	0·932 (10)
C(2)–O(2)	1·449 (1)	C(2)–H(6)	0·843 (14)
C(2)–C(4)	1·523 (1)	C(2)–H(7)	0·989 (13)
C(3)–O(3)	1·431 (1)	C(3)–H(8)	0·980 (12)
C(3)–C(4)	1·520 (1)	C(3)–H(9)	0·969 (13)
C(4)–C(5)	1·553 (1)	C(5)–H(10)	1·106 (13)
C(5)–C(6)	1·524 (2)	C(5)–H(11)	1·009 (18)
O(1)–H(1)	0·983 (27)	C(6)–H(12)	1·112 (16)
O(2)–H(2)	1·001 (17)	C(6)–H(13)	1·102 (13)
O(3)–H(3)	0·899 (12)	C(6)–H(14)	1·083 (11)
O(1)–C(1)–C(4)	110·5 (1)	C(1)–C(4)–C(5)	108·9 (1)
O(2)–C(2)–C(4)	112·3 (1)	C(2)–C(4)–C(3)	111·9 (1)
O(3)–C(3)–C(4)	111·2 (1)	C(2)–C(4)–C(5)	105·5 (1)
C(1)–C(4)–C(2)	110·1 (1)	C(3)–C(4)–C(5)	111·5 (1)
C(1)–C(4)–C(3)	108·9 (1)	C(4)–C(5)–C(6)	116·2 (1)
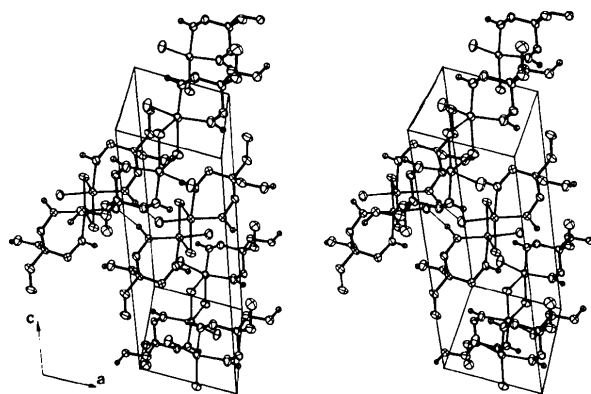
Fig. 2. A stereoscopic drawing of the molecular packing in the unit cell.

Table 4. *Distances (Å) and angles (°) associated with the possible hydrogen bonds*

X–H⋯Y	X⋯Y	X–H	H⋯Y	$\angle X$–H⋯Y
O(1)–H(1)⋯O(3^{ii})	2·679 (1)	0·98 (3)	2·21 (3)	107 (2)
O(1)–H(1)⋯Cl(2)	3·002 (1)	0·98 (3)	2·74 (3)	96 (2)
O(2)–H(2)⋯Cl(2^{iii})	3·067 (1)	1·00 (2)	2·11 (2)	160 (1)
O(3)–H(3)⋯Cl(1^{iv})	3·189 (1)	0·90 (1)	2·34 (1)	158 (2)

Symmetry code: (ii) $x - 1, y, z$; (iii) $x + 1, y, z$; (iv) $x + 1, \frac{1}{2} - y, \frac{1}{2} + z$.

Cl(2) and O(3^{ii}). On the other hand, bifurcated hydrogen bonds are a common phenomenon in molecular crystals (Ceccarelli, Jeffrey & Taylor, 1981). The observed angles around H(1) are small for a bifurcated hydrogen bond and the sum of the angles around H(1) is 300° instead of 360° as would be expected for an ideal bifurcated hydrogen bond. It is clear that O(1), H(1), Cl(2) and O(3^{ii}) are not exactly in the same plane. However, the large temperature factor of H(1) and the observed distances around H(1) indicate the existence of at least a weak hydrogen bond and possibly a bifurcated hydrogen bond.

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Structure of Bis(trifluoromethyl)mercury(II)–2,2′:6′,2″-Terpyridyl

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Abstract. $[Hg(CF_3)_2].C_{15}H_{11}N_3$, triclinic, $P\bar{1}$, $a = 11·821$ (5), $b = 9·141$ (3), $c = 8·955$ (4) Å, $\alpha = 110·12$ (3), $\beta = 95·04$ (3), $\gamma = 95·66$ (3)°, $V = 896·5$ (7) Å³, μ(Mo $K\alpha$) = 8·83 mm⁻¹, $Z = 2$, $D_m = 2·22$, $D_x = 2·118$ Mg m⁻³. The structure was refined by least-squares procedure to $R = 0·069$ for 2561 reflexions with $I > 3\sigma(I)$. The crystal structure is built up of F_3C–Hg–CF_3 and 2,2′:6′,2″-terpyridyl (tpy)

units. The Hg–C distances are 2·14 (3) and 2·11 (3) Å and the C–Hg–C angle is 164 (1)°. Three Hg···N contacts of 2·62 (3), 2·65 (2) and 2·70 (2) Å complete the five coordination around Hg.

Introduction. The only known structure of Hg^{II} with tpy is [MeHg(Et₃tpy)]NO₃ (Canty, Hayhurst, Chaichit & Gatehouse, 1980). In this structure, as well as in the structure reported here, tpy acts as a tridentate ligand, giving effectively a five-coordinate Hg atom. Other examples of the type $HgX_2 \cdot tpy$ ($X = Cl^-$, Br^-, I^-, ClO_4^-, NO_3^-) were identified only by means of chemical analysis and IR spectroscopy (Douglas & Wilkins, 1969). The title adduct was prepared for the first time by dissolving equimolar quantities of bis(trifluoro-methyl)mercury and tpy in a mixture of ethanol and water (1:1). Beautiful transparent prismatic crystals were obtained from the same solution. A crystal of dimensions 0·21 × 0·35 × 0·06 mm was used for unit-cell determination and data collection. The intensities of 2698 independent reflexions within the range $6° < 2\theta < 60°$ were measured on a Philips PW 1100 four-circle automatic computer-controlled diffractometer (graphite-monochromatized Mo $K\alpha$ radiation) with an ω–2θ scanning technique, a scan range of 1·20° and a scan speed of 0·04° s⁻¹. The usual corrections were made for Lorentz and polarization effects. No absorption correction was applied. The 2561 reflexions with $I > 3\sigma(I)$ were used for the structure determination. Several weighting schemes were applied but no improvement in the accuracy of the results was achieved so that unit weights were allotted to all observations. The Patterson synthesis enabled location of the Hg atom and one cycle of full-matrix least-squares refinement of the positional parameters and an isotropic thermal parameter gave $R = 0·183$. All non-hydrogen atoms were located in the subsequent Fourier maps. Several cycles of block-diagonal refinement with anisotropic thermal parameters led to a final R of 0·069.* No improvement was found on inclusion of the H atoms at their expected positions.

The atomic scattering factors were those from *International Tables for X-ray Crystallography* (1968) with corrections for anomalous scattering for the Hg atom according to Cromer & Liberman (1970).

Discussion. The final atomic coordinates are given in Table 1, and interatomic distances and angles in Table 2. Fig. 1 illustrates the structure and the atom-numbering scheme. The crystal structure consists of two moieties: bis(trifluoromethyl)mercury and tpy, showing again that the Hg atom in organomercury

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36628 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($\times 10$) *with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

|	x	y	z	B_{eq} (Å²)
Hg	2074 (1)	1977 (1)	1577 (1)	42·0 (2)
C(1)	501 (19)	2955 (30)	1723 (31)	56 (9)
C(2)	3465 (24)	779 (38)	750 (38)	73 (11)
N(1)	1696 (18)	329 (21)	3406 (26)	55 (7)
C(3)	1813 (18)	995 (34)	4983 (36)	59 (10)
C(4)	1612 (24)	52 (53)	6018 (47)	94 (18)
C(5)	1284 (30)	–1587 (52)	5186 (75)	108 (23)
C(6)	1189 (32)	–2200 (51)	3554 (64)	100 (19)
C(7)	1386 (26)	–1267 (26)	2650 (44)	80 (13)
N(3)	3387 (16)	4821 (22)	2741 (26)	56 (8)
C(11)	3843 (27)	5376 (37)	1661 (45)	82 (14)
C(12)	4574 (34)	6796 (45)	2134 (70)	108 (22)
C(13)	4806 (29)	7630 (40)	3804 (76)	109 (23)
C(14)	4337 (25)	7064 (34)	4936 (50)	90 (14)
C(15)	3601 (17)	5617 (25)	4299 (29)	47 (7)
N(2)	2657 (13)	3317 (23)	4716 (22)	47 (6)
C(16)	3048 (18)	4960 (28)	5374 (26)	50 (8)
C(17)	2941 (25)	5972 (38)	6880 (35)	75 (12)
C(18)	2381 (28)	5276 (49)	7860 (34)	92 (14)
C(19)	1977 (25)	3674 (44)	7331 (33)	76 (13)
C(20)	2168 (20)	2736 (23)	5684 (26)	48 (6)
F(1)	342 (14)	3775 (22)	767 (21)	88 (8)
F(2)	382 (12)	3917 (19)	3219 (18)	72 (6)
F(3)	–475 (15)	1864 (20)	1241 (28)	107 (9)
F(4)	4029 (24)	288 (42)	1680 (36)	170 (17)
F(5)	4258 (33)	1553 (31)	369 (59)	264 (29)
F(6)	3229 (20)	–504 (40)	–377 (41)	239 (17)
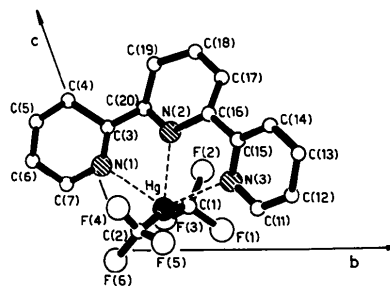
Fig. 1. The structure of the adduct of bis(trifluoromethyl)mer-cury(II) with tpy viewed along the a axis.

compounds is a weak acceptor. The Hg···N distances of 2·62 (3), 2·65 (2) and 2·70 (2) Å are significantly smaller than the sum of the van der Waals radii for Hg and N, 1·54 and 1·60 Å respectively (Grdenić, 1977, 1981; Gilli, Cano & Garcia-Blanco, 1976). Although all three N atoms from tpy enter into the effective coordination sphere of Hg (Grdenić, 1965) they have little effect on the Hg–C bond lengths but a more obvious effect on the geometry of the $(CF_3)_2Hg$ molecule. The characteristic coordination of Hg is digonal with Hg–C(1) and Hg–C(2) bond lengths of 2·14 (3) and 2·11 (3) Å, respectively. Both values are very close to the value of 2·109 (16) Å found for such a

Table 2. *Interatomic distances (Å) and angles (°) with e.s.d.'s in parentheses*

Hg–C(1)	2·14 (3)	C(13)–C(14)	1·42 (8)
Hg–C(2)	2·11 (3)	C(14)–C(15)	1·41 (3)
Hg···N(1)	2·62 (3)	C(15)–C(16)	1·47 (4)
Hg···N(2)	2·65 (2)	N(2)–C(16)	1·42 (3)
Hg···N(3)	2·70 (2)	N(2)–C(20)	1·31 (3)
N(1)–C(3)	1·32 (4)	C(16)–C(17)	1·37 (4)
N(1)–C(7)	1·38 (3)	C(17)–C(18)	1·42 (5)
C(5)–C(4)	1·42 (6)	C(18)–C(19)	1·39 (6)
C(5)–C(6)	1·36 (8)	C(19)–C(20)	1·48 (3)
C(4)–C(3)	1·49 (6)	C(1)–F(1)	1·33 (4)
C(6)–C(7)	1·38 (7)	C(1)–F(2)	1·36 (3)
C(3)–C(20)	1·50 (3)	C(1)–F(3)	1·38 (3)
N(3)–C(11)	1·36 (5)	C(2)–F(4)	1·25 (5)
N(3)–C(15)	1·32 (3)	C(2)–F(5)	1·26 (5)
C(11)–C(12)	1·40 (5)	C(2)–F(6)	1·24 (4)
C(12)–C(13)	1·41 (8)		

C(1)–Hg–C(2)	164·2 (11)	C(16)–N(2)–C(20)	115 (2)
N(1)···Hg···N(3)	121·2 (6)	C(15)–C(16)–C(17)	118 (2)
N(1)···Hg···N(2)	60·7 (6)	C(15)–C(16)–N(2)	115 (2)
N(2)···Hg···N(3)	61·4 (7)	C(17)–C(16)–N(2)	127 (3)
N(1)···Hg–C(1)	97·2 (9)	C(16)–C(17)–C(18)	115 (3)
N(1)···Hg–C(2)	91·4 (11)	C(17)–C(18)–C(19)	122 (3)
N(2)···Hg–C(1)	91·3 (7)	C(18)–C(19)–C(20)	116 (3)
N(2)···Hg–C(2)	104·5 (8)	N(2)–C(20)–C(19)	125 (2)
N(3)···Hg–C(2)	93·2 (8)	C(3)–C(20)–C(19)	122 (3)
N(3)···Hg–C(1)	93·7 (6)	C(3)–C(20)–N(2)	114 (2)
C(3)–N(1)–C(7)	122 (3)	C(11)–N(3)–C(15)	122 (2)
C(6)–C(5)–C(4)	120 (6)	N(3)–C(11)–C(12)	122 (4)
C(5)–C(4)–C(3)	115 (4)	C(11)–C(12)–C(13)	116 (5)
N(1)–C(3)–C(4)	121 (3)	C(12)–C(13)–C(14)	123 (3)
N(1)–C(3)–C(20)	117 (3)	C(13)–C(14)–C(15)	116 (3)
C(6)–C(7)–N(1)	120 (3)	N(3)–C(15)–C(14)	122 (3)
C(5)–C(6)–C(7)	122 (4)	N(3)–C(15)–C(16)	118 (2)
C(4)–C(3)–C(20)	122 (3)	C(14)–C(15)–C(16)	120 (3)
F(2)–C(1)–Hg	114 (2)	Hg–C(2)–F(4)	118 (3)
F(3)–C(1)–Hg	115 (2)	Hg–C(2)–F(5)	116 (3)
F(1)–C(1)–Hg	114 (2)	Hg–C(2)–F(6)	117 (2)
F(1)–C(1)–F(2)	106 (2)	F(4)–C(2)–F(5)	101 (3)
F(1)–C(1)–F(3)	102 (2)	F(4)–C(2)–F(6)	97 (3)
F(2)–C(1)–F(3)	105 (2)	F(5)–C(2)–F(6)	106 (3)

bond in the crystal structure of $(CF_3)_2Hg$ itself (Brauer, Bürger & Eujen, 1977). Similar values for Hg–C bond lengths are also found in other organomercury compounds with characteristic digonal coordination of the Hg atom (Grdenić, 1977). The $(CF_3)_2Hg$ molecule is bent, the C(1)–Hg–C(2) angle being 164 (1)°, obviously indicating a weak but clear donor–acceptor interaction between $(CF_3)_2Hg$ and tpy. Similar arrangements are encountered in the crystal structure of the adducts of bis(phenylethynyl)mercury(II)–1,10-phenanthroline (Gutiérrez-Puebla, Vegas & García-Blanco, 1978) and phenylmercury(II) cyanide–1,10-phenanthroline (Ruiz-Amil, Martínez-Carrera & García-Blanco, 1978) where these C–Hg–C angles are 165·6 (4) and 167·5 (4)°, respectively.

The tpy molecule is almost perpendicular to the C–Hg–C fragment. The least-squares best planes

through $Hg,C(1),C(2)$ and $N(1),N(2),N(3)$ intersect at an angle of 87·7 (8)°. The pyridine rings in the tpy ligand are not in the same plane. The angles between the least-squares best planes through the atoms in the N(1) and N(2), and N(2) and N(3) pyridine rings are 20·5 (9) and 21·5 (9)°, respectively. The N–C and C–C bond lengths and angles in the tpy ligand are comparable with those found in similar complexes (Goldschmied & Stephenson, 1970).

Some F atoms, in particular those linked to C(2), show relatively large thermal vibrations. There was no indication that this trifluoromethyl group is disordered. The large thermal vibrations are most probably due to the high degree of libration of the trifluoromethyl group about the Hg–C bond. This can be supported by the fact that the C(2)–F bond lengths (mean value 1·25 Å) are significantly shorter than the C(1)–F bond lengths (mean value 1·36 Å).

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