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Journal of Organometallic Chemistry 495 (1995) 1–31

Journal of Organometallic Chemistry

Invited Review

# Mercury organometallic compounds. Classification and analysis of crystallographic and structural data

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## Abbreviations

| | |
|---|---|
| aad | 8-azaadeninate |
| ac | acetate |
| actp | N-acetyl-dl-tryptophan |
| ad | adeninate |
| ala | dl-alaninate |
| all | allopurinolate |
| 6amt | 1-methyl-6-azathyminate |
| apb | 2-amino-4-phenylbutanoate |
| app | 7-deaza-8-azaadenine |
| 6auH | 6-azauracilate |
| $5auH_2$ | 5-azauracil |
| azaH | 7-azaindole |
| ba | benzamide |
| bcb | 2-benzyl-o-carborane |
| bedo-ttf | 3,4:3′,4′-bis(ethylenedioxo)-2,2′,5,5′-tetrathiafulvalene |
| bpy | 2,2′-bipyridyl |
| $B(pz)_4$ | tetrakis(pyrazol-1-yl)borate |
| Brbsa | 2-bromobenzenesulphonanilide |
| Bu | butyl |
| $(Bu^tO)_3SiS$ | tri(tert-butyloxy)silanethiolate |
| bz | benzyl |
| bzpy | 2-benzylpyridine |
| $C_4H_6N_2S$ | 1-methylimidazoline-2-thione |
| $C_4H_7O$ | 3-oxo-2-butyl |
| $C_4H_8O_2$ | 1,4-dioxane |
| $C_5H_5N_2S$ | 2-mercapto-4-methylpyrimidinate |
| $C_5H_6N_3S$ | 4-amino-5-methyl-2-pyrimidine-thiolate |
| $C_5H_6O_2$ | 2,4-pentanedione |
| $C_5H_6N_5$ | adeninium |
| $C_5H_{10}NCl$ | (3-chloro-1-methylprop-2-enyl)-methylammonium |
| $C_5H_{12}NCl$ | (3-chloro-1-(n-propyl)prop-2-enyl)methylammonium |
| $C_6H_8O_2$ | cyclohexane-1,4-dione |
| $C_6H_{10}S_2$ | 1,2-dimercaptocyclohexane |
| $C_6H_{11}S$ | cyclohexanethiolate |
| $C_6H_{19}O_2$ | dipivaloylmethane |
| $C_7H_6NO$ | benzamide |
| $C_8H_7N_3$ | 1-(2-pyridyl)pyrazole |
| $C_8H_{12}S_2$ | 1,6-dithiacyclodeca-cis-3,cis-8-diene |
| $C_8H_{13}O_2$ | 2,3-dioxadecalinyl |
| $C_9H_9$ | 1-phenylcyclopropyl |
| $C_9H_{12}N$ | 2-{(dimethylamino)methyl}phenyl |
| $C_9H_{13}O_2$ | androsta-4,6-diene-3,17-dionate |
| $C_9H_{15}NO$ | 2,2,6,6-tetramethyl-$\Delta^4$-dehydropiperidine-1-oxyl |
| $C_9H_{18}O$ | cyclononane |
| $C_9H_{19}O_6$ | 4-acetoxy-9,10-cis-endo-dimethoxy-carbonyl-tricyclo[4.2.2.$0^{2,5}$]-dec-7-ene |
| $C_{10}H_6$ | 1,8-naphthalenediyl |
| $C_{10}H_{14}NCl_2$ | 1,1-dichloro-1-(2-methyl-5-t-butyl-2H-pyrrole) |
| $C_{10}H_{15}$ | camphenate |

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*SSDI* 0022-328X(95)05395-6

| | |
|---|---|
| $C_{10}H_{23}N_2O_2$ | 3-(morpholinomethyl)-2,2,6,6-tetramethyl-$\Delta^4$-dehydropiperidin-1-oxyl |
| $C_{11}H_8NSe$ | 2-(2-pyridyl)phenylselenium |
| $C_{11}H_9$ | 1-naphthylmethyl |
| $C_{11}H_{11}O_2$ | 1-acetoxy-1-phenyl-2-methyl-acetylenate |
| $C_{11}H_{19}OS$ | 5-mercapto-2,2,6,6-tetramethyl-4-hepten-3-onate |
| $C_{11}H_{29}NO$ | 5-amino-2,2,6,6-tetramethyl-4-hepten-3-onate |
| $C_{12}H_6NS_2$ | 2-mercaptobenzothiazolate |
| $C_{12}H_8$ | 2,2′-biphenylylene |
| $C_{12}H_8SO$ | phenoxanthrin |
| $C_{12}H_{24}O_4S_2$ | 1,4,7,10-tetraoxa-13,16-dithiacyclooctadecane |
| $C_{12}H_{24}O_6$ | 1,4,7,13,16-hexaoxacyclooctadecane (18-crown-6) |
| $C_{12}H_{26}N_2O_4$ | 1,4,10,13-tetraoxa-7,16-diazacyclooctadecane |
| $C_{13}H_{11}N_4S$ | dithizonate |
| $C_{13}H_{11}OCl_6$ | 1,2,3,4,10,10-hexachloro-1,4,4a,5,6,7,8,8a-octahydro-endo,exo-1,4 : 5,8-dimethano-exo-7-methoxy-naphthalene |
| $C_{13}H_{15}O_2$ | 1,2,3,4a,9b-hexahydro-8-methoxydibenzofuran |
| $C_{14}H_{16}N_2O$ | 2,5,5-trimethyl-2-(vinyl)-4-phenyl-3-imidazolin-1-oxyl |
| $C_{14}H_{16}N_2O_2$ | 2,5,5-trimethyl-2-vinyl-3-oxide-4-phenylimidazoline-1-oxyl |
| $C_{14}H_{24}N_4O_2$ | 3-(4-nitroso-piperazinomethyl)-2,2,6,6-tetramethyl-$\Delta^4$-dehydropiperidine-1-oxyl |
| $C_{15}H_{18}O_2FS$ | 2-fluoromethyl-6,6-dimethyl-3-[(4-methylphenyl)sulphinyl]-4,5-dihydro-6H-pyran |
| $C_{15}H_{24}N_2O$ | 1-oxyl-2,2,6,6-tetramethyl-3-piperidino-methyl-dehydropiperidinyl |
| $C_{15}H_{26}N_2O$ | 2,2,6,6-tetramethyl-3(1-piperidinylmethyl)-$\Delta^4$-dehydropiperidine-1-oxyl |
| $C_{16}H_{13}O_2$ | 1-acetoxy-1,2-diphenyl-acetylenate |
| $C_{16}H_{19}O_6$ | 4-acetoxy-tricyclo[4,2,2,0$^{2,5}$]dec-7-ene-9,10-cis-endo-dicarboxylate |
| $(C_{16}H_{18}NO_4P_2)_2$ | 7,15-bis(diethylphosphinyl)-6,7,14,15-tetrahydro-6,14-diphenoxydibenzo[e,k][1,7,3,9,2,8,4,10]-dioxadiazadiphospha-cyclododecin-6,14-dioxide |
| $C_{18}H_8$ | diphenyl |
| $C_{18}H_{12}$ | hexabenzo[1,8]cyclotetradecene |
| $C_{18}H_{17}O_3$ | 1,3-diphenyl-2-carboxymethoxy-3-methoxy-cyclopropanoate |
| $C_{18}H_{21}O_2$ | 2-tert-butylperoxy-1,2-diphenylethanyl |
| $C_{19}H_{14}F_3O_4$ | 3-fluoroacetoxy-2,3-diphenylcyclopropane-1-carboxylate |
| $C_{19}H_{40}O_2$ | androsta-4,6-diene-3,17-dionate |
| $C_{21}H_{33}O_5$ | fusicoccin desacetyl aglyone |
| $C_{28}H_{20}$ | 1,3-tetraphenylbutadiene |
| $C_{36}H_{55}O_{12}$ | fusicoccin |
| Clbsa | 2-chlorobenzenesulphonanilide |
| Cldab | 2-chlorodiazoaminobenzene |
| Clmcb | 2-chloromethyl-o-carborane |
| $(Cl_3C_6H_2)OCH_2$ | 2,4,6-trichlorophenoxymethyl |
| $C_2N_2S_3$ | 2,3-dimercapto-1,3,4-thiodiazolate |
| cp | cyclopentadienyl |
| cp* | pentamethylcyclpentadienyl |
| cre | creatinine |
| 2,2,2-cryp | 4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8,8,8]hexacosane |
| cys | cysteinato |
| dme | 1,2-dimethoxyethane |
| dmhfe | 4$\beta$,5$\beta$-dimethyl-10$\beta$-hydroxyfuranoeremophilane |
| dmpma | N-(2,6-dimethylphenyl)-N-(2-methoxyacetyl)alanine |
| dmso | dimethylsulphoxide |
| dpam | bis(diphenylarsino)methane |
| dppte | 1,2-bis(diphenylphosphinothioyl)-ethane |
| emc | 2-ethoxymethyl-o-carborane |
| Et | Ethyl |
| $Et_2$dtc | N,N′-diethyldithiocarbamate |
| $Et_3$terpy | 4,4′,4″,-triethyl-2,2′ : 6′,2″-terpyridyl |
| Fbsa | 2-fluorobenzensulphonanilide |
| glygly | glycylglycine |
| hmb | hexamethylbenzene |
| im | imidazole |
| Me | methyl |
| Meaad | methyl-8-azaadenine |
| Mead | methyladeninate |
| $Me_2$atph | dimethylaminothiophenolate |
| $Me_2$bpy | dimethyl-2,2′-bipyridyl |
| 8-MeCHqu | 8-ethynyl-quinoline |
| Megu | methylguanine |
| $Me_2$phen | dimethyl-1,10-phenanthroline |
| $Me_4$phen | tetramethyl-1,10-phenanthroline |
| Methu | 1-methyl-4-thiouracilylate |
| $Me_2$tph | dimethylthiophenolate |
| mt | methioninate |
| nbs | nitrobenzenesulphonanilidine |
| $np_3$Ph | trineopentylphenyl |
| otmim | 1-oxy-2,2,5,5-tetramethyl-4-phenyl-imidazolinate |
| pdpi | N,N-bis(phosphoric-diphenylester)imidate |

| | |
|---|---|
| pen | D,L-penicillaminate |
| Ph | phenyl |
| phen | 1,10-phenanthroline |
| pmc | 2,4-propano-6-methoxychroman |
| pp | pyranopyran |
| ppep | 2,6-bis(phosphoricdiphenylester)-imidate |
| psit | 2-phenylsulphonyl-imino-1,2-dihydrothiazole |
| py | pyridine |
| py(N-Meim)$_2$COH | bis(N-methylimidazol-2-yl)(pyridin-2-yl)methanol |
| py-2th | pyridine-2-thiolate |
| pz | pyrazole |
| qn | {(N,N′-dimethyl)ethylenediamine}-o-tolyl |
| qo | (ethylenedioxyl)-o-tolyl |
| qu-8-th | quinoline-8-thiolate |
| sami | salicylalmethyliminate |
| tf | N,N-di-para-tolylformamide |
| tfmsos | $\alpha,\beta$-bis{(trifluoromethanesulphonyl)oxy}styryl |
| thm | thymidinate |
| tht | 1,3-thiazolidine-2-thione |
| tmm | tris(N-methylimidazol-2-yl)methanol |
| top | theophyllinate |
| tp | tryptophanate |
| tpy | 2,2′ : 6′,2″-terpyridyl |
| tsh | (p-tolylsulphonyl)hydrazone |
| ttm–ttf | tetramethylthio–tetrathiofulvalene |
| tu | thiourea |
| tyr | tyrosinate |

## 1. Introduction

A vast number of organomercury compounds are known [1] and while many have useful physiological properties, for the most part they are harmful to life and the environment. There have been a number of environmental disasters attributable to mercury discharges, perhaps the best known being that of the Minimata Bay incident in Japan. The actual agent involved has been shown to be the organometallic cation $CH_3Hg^+$. This water soluble ion can enter the body and induce complex irreversible disturbances to the central nervous system. The cation is formed by biological methylation of sludge containing metallic mercury [2].

Mercury complexes have been extensively studied from a structural point of view, with over five hundred coordination compounds identified in a related review [3]. In 1975 structural data for organometallic complexes of mercury were analysed [4], however, since then many more structures have been obtained, with a total of over three hundred up to the end of 1992. This review serves to correlate all of these structures and draw comparisons and relationships with mercury coordination compounds.

The structures have been grouped by degree of nuclearity from monomers through oligomers to polymers. The compounds have been listed and referenced in order of increasing coordination number of the mercury atom, increasing complexity of the coordination sphere, and increasing atomic mass of the principle coordinated atom. In so far as the subtle difference between a useful drug and a biological poison can often depend on minor structural differences, it is hoped that this general overview of the structures may lead to a better understanding of the behaviour of organomercury derivatives.

## 2. Monomeric mercury(II) compounds

The data for these compounds is given in Table 1 where some two hundred and fifty examples can be found. The majority of these are colourless, but there are some coloured derivatives, for example yellow (8), white (5) and red-brown (2). There are no examples of mercury in the oxidation state of +1.

It is well known that mercury prefers a linear configuration [192,193] with two short bonds, but this geometry may be distorted by additional coordination interactions. Such effects have been commonly noted both for the coordination compounds [3] and the organometallic compounds. The monomeric organometallic compounds can be subdivided into three groups: ''pure'' digonal coordination; digonal with additional intramolecular coordination type interactions; digonal with additional intermolecular coordination type interactions. These longer range interactions are indicated in the chromophore column of the Table by parentheses. However, such assignments are at best somewhat arbitrary in many cases, particularly where the original paper lacks sufficient data such as interatomic distances or even the atomic coordinates.

In the first set of digonal organomercury(II) compounds, without additional interactions, the L–Hg–L bond angles range from 169 to 180° with a mean value of 176.5°.

In the series with additional intramolecular interactions the L–Hg–L bond angles range from 161 to 180°, with a mean value of 174.5°.

In the series with intermolecular interactions the range is from 164 to 180° with a mean value of 171°. These mean values are comparable to those found for the mercury(II) coordination compounds [3].

Overall, the most common unidentate carbon donor ligands are methyl and phenyl moieties. The mean Hg–C(Me) bond distance of 207(12,20) pm is only 1 pm longer than that of Hg–C(Ph) at 206(13,9) pm, where the first number in parentheses is the difference

Table 1
Crystallographic and structural data for monomeric organomercury(II) compounds [a]

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| $Hg(Me)_2$ (colourless) | | | | $HgC_2$ | C [b] | 208.3(5,0) | C,C [b] | 180 | 5 |
| $Hg(CF_3)_2$ (colourless) | c Pa3 4 | 812.7(2) | | $HgC_2$ | C | 210.9(16,0) | C,C | 180 | 6 |
| $Hg(CF_3)_2$ (colourless) | | 811.8 811.5 | | $HgC_2$ | C | 213.9 | C,C | not given | 7 |
| $Hg(CF_3)_2$ at 99K | or Pbca 4 | 811.3 795.7 795.7 795.7 | | $HgC_2$ | C | 199.8 | C,C | not given | |
| $[Hg(CF_3)_2](tpy)$ | tr $P\bar{1}$ 2 | 1182.1(5) 914.1(3) 895.5(4) | 110.12(3) 95.04(3) 95.66(3) | $HgC_2$ ($N_3$) | C N | 213(3,2) 266(2,4) | C,C | 164.2(11) | 8 |
| $Hg(CF_3)_2(C_{26}H_{36}O_6)$ (white) | tr $P\bar{1}$ 2 | 1153.2(2) 1749.7(3) 824.5(2) | 98.4(2) 107.0(2) 98.1(2) | $HgC_2$ ($O_5$) | C O | 213 294(1,14) | C,C | 177.9(5) | 9 |
| $Hg\{C(COF)SF_2O\}_2$ (not given) | m $P2_1$ 2 | 358.1(4) 898.5(7) 1032.9(6) | 101.10(5) | $HgC_2$ | C | 206(3,0) | C,C | 171(3) | 10 |
| $Hg\{CH(COOMe)_2\}_2$ (colourless) | tr $P\bar{1}$ 2 | 1077.2(2) 850.2(4) 858.5(3) | 71.28(3) 64.70(4) 78.26(2) | $HgC_2$ ($O_2$) | C O | 212.9(8,2) 274.5(7,79) | C,C | 173.8(4) | 11 |
| $Hg\{CH(COOEt)\}_2$ (colourless) | tr $P\bar{1}$ 2 | 930.5(3) 1057.9(3) 1065.9(3) | 112.51(4) 65.45(3) 98.04(4) | $HgC_2$ ($O_2$) | C O | 214.4(6,9) 270.3(7,21) | C,C | 173.7(3) | 11 |
| $Hg(ClCH_2CC)_2(phen)$ [c] (colourless) | tr $P\bar{1}$ 4 | 2166(1) 984.6(5) 881.4(4) | 91.13(4) 101.14(5) 103.90(7) | $HgC_2$ ($N_2$) $HgC_2$ ($N_2$) | C N C N | 207(4,2) 271(4,1) 203(4,1) 270(4,5) | C,C C,C | 165 168 | 12a |
| $Hg(Cl_2CCCl)_2(Me_4phen)$ (colourless) | m C2/c 8 | 1897.6(6) 1387.6(4) 1840.1(5) | 107.32(6) | $HgC_2$ ($N_2$) | C N | 208.7(10,5) 265.8(8,29) | C,C | 164.8(3) | 12b |
| $Hg(Et_2NCO)_2$ (colourless) | m $P2_1/a$ 2 | 1501.4(8) 1193.0(9) 408.2(2) | 115.13(3) | $HgC_2$ | C | 213(2,0) | C,C | 180 | 13 |
| $Hg\{C(SiMe_3)_3\}_2$ | tr $P\bar{1}$ | 900.0 1191.41 917.92 | 97.109 118.184 104.973 | $HgC_2$ | C | 214.2(4,0) | C,C | 180 | 14 |
| $Hg\{C(SiMe_3)_2(SiMe_2OMe)\}$ | m C2/c 4 | 1679.7(11) 935.4(8) 2294.8(8) | 108.71(4) | $HgC_2$ | C | 207(2,0) | not given | | 15 |
| $Hg\{2\text{-}(Me_3Si)_2C(py)\}_2$ | m $P2_1/c$ 4 | 944.5(4) 1924.9(7) 1751.3(7) | 97.02(3) | $HgC_2$ ($N_2$) | C N | 216 278 | C,C | 179.5(3) | 16 |
| $Hg(cp)_2$ (colourless) at 100K | tg $I4_1$ 8 | 1734.7(5) – 581.0(3) | | $HgC_2$ | C | 212(1) 215(1) | C,C | 177.9(6) | 17 |
| $Hg(Ph)_2$ (colourless) | m $P2_1/a$ 2 | 1156(1) 830(1) 559(1) | 112.20 | $HgC_2$ | C | 210 | C,C | 180 | 18 |
| $Hg(Ph)_2$ (colourless) | m $P2_1/c$ 2 | 551.9(2) 834.1(3) 1166.3(5) | 112.78(4) | $HgC_2$ | C | 208.5(7,0) | C,C | 180 | 19 |
| $Hg(Ph)_2(Me_4phen)$ [c] (colourless) | m Cm 4 | 2109 1454 1465 | 120.34 | $HgC_2$ ($N_2$) $HgC_2$ ($N_2$) | C N C N | 210(–,0) 287(–,4) 213(–,0) 292(–,4) | C,C C,C | 180 180 | 20 |
| $Hg(Ph)_2(Me_2phen)$ [d] | or | 1542 | | $HgC_2$ | C | 210(–,0) | C,C | 180 | 20 |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | *a* [pm] *b* [pm] *c* [pm] | $\alpha$ [°] $\beta$ [°] $\gamma$ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| (colourless) | Pbca | 1428 | | $(N_2)$ | N | 290(−,8) | | | |
| | 4 | 1425 | | | | | | | |
| $Hg(Ph)_2 \cdot (dppte)$ | tr | 953.2(3) | 118.07(4) | $HgC_2$ | C | 206.9(7,0) | C,C | 180 | 21 |
| | $P\bar{1}$ | 1006.5(2) | 96.29(3) | | | | | | |
| | 1 | 1011.3(3) | 94.41(2) | | | | | | |
| $\{Hg(Ph)_2 \cdot 2[Hg(PPh_3)_2(SCN)_2]$ | tr | 1042.6(1) | 94.26(3) | $HgC_2$ | C | 207.8(7,0) | C,C | 180 | 22 |
| (colourless) | $P\bar{1}$ | 1957.6(3) | 97.00(4) | | | | | | |
| | 1 | 982.1(2) | 87.08(2) | $HgS_2P_2$ | S | 256.9(1,3) | S,S | 104.73(5) | |
| | | | | | P | 251.0(1,12) | P,P | 114.11(3) | |
| | | | | | | | S,P | 109.4(1,11.6) | |
| $Hg(PhCH_2)_2$ | tg | 1288.1(5) | | $HgC_2$ | C | 206.5(17,0) | C,C | 177.7(16) | 23 |
| (colourless) | $P4_2/n$ | – | | | | | | | |
| | 4 | 707.6(3) | | | | | | | |
| $Hg\{2,4,6\text{-}(MeO)_3C_6H_2\}_2$ | m | 1462.4(4) | | $HgC_2$ | C | 207(1,0) | C,C | 180 | 24 |
| (colourless) | $P2_1/c$ | 1773.1(5) | 93.98(3) | | | | | | |
| | 4 | 722.1(3) | | | | | | | |
| $Hg(2,3,4,5\text{-}F_4C_6H)_2$ | m | 1178.6(4) | | $HgC_2$ | C | 209.6(16,0) | C,C | 180 | 25 |
| | $P2_1/c$ | 487.1(6) | 127.4(1) | | | | | | |
| | 2 | 1311.4(5) | | | | | | | |
| $Hg(C_6F_5)_2$ | or | 2052(2) | | $HgC_2$ | C | 210(−,1) | C,C | 176.2(1.2) | 26 |
| (colourless) | $P2_12_12_1$ | 1079(1) | | | | | | | |
| | 4 | 589(1) | | | | | | | |
| $Hg(C_6F_5)_2$ | or | 576.2(1) | | $HgC_2$ | C | 205.0(6,3) | C,C | 178.8(3) | 27 |
| (colourless) | $P2_12_12_1$ | 1064.5(1) | | | | | | | |
| | 4 | 2029.6(2) | | | | | | | |
| $[Hg(C_6F_5)_2]_2(dpam)$ | m | 1407(2) | | $HgC_2$ | C | 211(4,4) | C,C | 173(1.4) | 28 |
| | C2/c | 1734(2) | 91.3(6) | (As) | As | 340(2) | | | |
| | 4 | 1933(2) | | | | | | | |
| Hg(p-tolyl)$_2$ | m | 1012(1) | | $HgC_2$ | C | 208(2,0) | C,C | 180 | 29 |
| (colourless) | $P2_1/c$ | 507(1) | 91.8(3) | | | | | | |
| | 2 | 1165(2) | | | | | | | |
| Hg($\sigma$-tolyl)$_2$ | m | 1097(2) | | $HgC_2$ | C | 209(1,0) | C,C | 178.0(4) | 30 |
| (colourless) | C2/c | 1044.8(3) | 115.48(2) | | | | | | |
| | 4 | 1140.9(3) | | | | | | | |
| $Hg(PhCH{=}CH)_2$ | or | 1541.3(6) | | $HgC_2$ | C | 207(4,0) | C,C | 178(2) | 31 |
| (colourless) | Pbcn | 1116.1(9) | | | | | | | |
| | 4 | 766.8(5) | | | | | | | |
| $Hg(PhCC)_2(phen)$ | m | 2256.4(3) | | $HgC_2(N_2)$ | C | 204(1,1) | C,C | 165.6(4) | 32 |
| | $P2_1/n$ | 957.7(5) | 96.20(1) | $(N_2)$ | N | 265(1,1) | | | |
| | 4 | 1033.9(5) | | | | | | | |
| $Hg(C_9H_9)_2$ | m | 1069.3(2) | | $HgC_2$ | C | 211.4(8,10) | C,C | 178.0 | 33 |
| (colourless) | $P2_1/a$ | 1111.8(4) | 95.51(2) | | | | | | |
| | 4 | 1256.2(4) | | | | | | | |
| $Hg(C_{11}H_9)_2$ | m | 1118.5(1) | | $HgC_2$ | C | 209(1,0) | C,C | 180 | 34 |
| (white) | $P2_1/n$ | 1133.5(1) | 111.84(1) | | | | | | |
| | 4 | 1438.7(2) | | | | | | | |
| $Hg(C_6H_{19}O_2)_2$ | tr | 1062(1) | 90.8(1) | $HgC_2$ | C | 216(3,3) | C,C | 180 | 35 |
| (colourless) | $P\bar{1}$ | 1237(1) | 111.5(1) | $(O_2)$ | O | 270(2) | | | |
| | 2 | 1028(1) | 97.8(1) | | | | | | |
| $Hg(Ph_2pz)_2(ClO_4)_2$ | tr | 1026.8(9) | 106.38(5) | $HgC_2$ | C | 206(1,0) | C,C | 180 | 36 |
| (colourless) | $P\bar{1}$ | 1019.7(7) | 97.19(5) | | | | | | |
| | 1 | 788.3(5) | 74.28(5) | | | | | | |
| $Hg(2,4,6\text{-}Bu^tC_6H_2)_2$ | m | 1983.0(15) | | $HgC_2$ | C | 208.0(6,3) | C,C | 173.4(2) | 37 |
| (colourless) at 118K | $P2_1/c$ | 1030.9(7) | 120.69(6) | | | | | | |
| | 4 | 1891.9(13) | | | | | | | |
| $Hg\{(2,4,6\text{-}Cl_3C_6H_2)OCH_2\}_2$ | tr | 1564.8(12) | 94.13(7) | $HgC_2$ | C | 211(1,0) | C,C | 180 | 38 |
| (colourless) | $P\bar{1}$ | 746.2(10) | 95.60(5) | | | | | | |
| | 1 | 396.0(5) | 106.23(14) | | | | | | |
| $Hg(qn)_2$ | m | 1544(2) | | $HgC_2$ | C | 210(2,3) | C,C | 172 | 39 |
| (colourless) | $P2_1/a$ | 1010(1) | 109.3(1) | $(N_2)$ | N | 295(2,3) | | | |
| | 4 | 1168(1) | | | | | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| $Hg(qo)_2$ (colourless) | or $Pbn2_1$ 4 | 2321(2) 1168(1) 525(1) | | $HgC_2$ | C | 210(6,3) | C,C | 174 | 39 |
| $Hg(otmim)_2$ | or Pcab 8 | 2108.7(6) 1440.4(6) 1744.1(6) | | $HgC_2$ ($N_2$) | C N | 209(−,1) 263(−,1) | C,C | 178.6 | 40 |
| $Hg(2\text{-thienyl})_2$ (colourless) | m C2/c 4 | 2172.0(3) 536.8(3) 774.6(1) | 103.63(1) | $HgC_2$ | C | 206.1(18,0) | C,C | 180 | 41 |
| $Hg(2\text{-furyl})_2$ (colourless) | m $P2_1/n$ 2 | 544.4(2) 755.6(3) 951.5(15) | 91.90(2) | $HgC_2$ | C | 205.9(5) | C,C | 180 | 42 |
| $Hg(C_9H_{12}N)_2$ (colourless) | m $P2_1/n$ 2 | 618.6(3) 1214.6(5) 1209.5(5) | 101.46(4) | $HgC_2$ ($N_2$) | C N | 210(1,0) 298(1) | C,C | 180 | 43 |
| $Hg(MesPCH_2)_2$ [c] (colourless) | m $P2_1/c$ 4 | 1389.00(7) 1449.38(6) 1985.04(5) | 104.494(3) | $HgC_2$ $HgC_2$ | C C | 204.2(11,0) 207.9(10,0) | C,C C,C | 180 180 | 44 |
| $Hg\{Ph(S)PCH_2\}_2$ (white) | m C2/c 4 | 2509.0(8) 1088.6(5) 918.9(4) | 91.83(3) | $HgC_2$ | C | 212.4(16,0) | C,C | 179.3(2) | 45 |
| $Hg(tfmsos)_2$ | or Pbca 8 | 1231.2(4) 2036.4(6) 2619.2(4) | | $HgC_2$ | C | 204.3(15,12) | C,C | 177.9(6) | 46 |
| Hg(Me)(CN) (colourless) | or Pnma 4 | 912(2) 614(2) 701(2) | | $HgC_2$ | NC $C_{Me}$ | 201(5) 215(5) | C,C | 180(6) | 47 |
| Hg(Me)(CN) by neutron diffraction | | 911(2) 614(2) 701(2) | | $HgC_2$ | NC $C_{Me}$ | 205(1) 208(2) | C,C | 180(2) | 47 |
| Hg(Me)(emc) (colourless) at 153K | m $P2_1/n$ 4 | 739.4(1) 1284.4(3) 1508.7(4) | 96.30(2) | $HgC_2$ (O) | $C_{Me}$ $C_{emc}$ | 207.3(8) 211.3(6) | C,C | 175.8(3) | 48 |
| Hg(Me)(bcb) [c] (colourless) | m $P2_1/n$ 8 | 2044(1) 758.0(5) 2207(1) | 108.79(4) | $HgC_2$ $HgC_2$ | $C_{Me}$ $C_{bcb}$ $C_{Me}$ $C_{bcb}$ | 207(2) 211(2) 209(2) 211(1) | C,C C,C | 174.4(6) 173.0(6) | 49 |
| Hg(Ph)(CN) (colourless) | tg $P4_2/n$ 8 | 1516.1(3) – 614.6(1) | | $HgC_2$ | NC $C_{Ph}$ | 205.1(15) 209.4(16) | C,C | 177.5(7) | 50 |
| Hg(Ph)(CN)(phen) (colourless) | m $P2_1/a$ 4 | 1015.2(1) 1850.2(2) 886.1(1) | 99.59(1) | $HgC_2$ ($N_2$) | NC $C_{Ph}$ N | 206.3(14) 206.7(12) 267.0(9,10) | C,C | 167.5(4) | 51 |
| Hg(Ph)($C_6Cl_5$) | or $P2_12_12_1$ 4 | 684.9(1) 1057.0(2) 1922.0(2) | | $HgC_2$ | $C_{Ph}$ $Cl_5C_6$ | 205.2(20) 213.5(16) | C,C | 178.3(7) | 52 |
| Hg(Ph)($C_{10}H_{14}NCl_2$) (colourless) | m $P2_1/c$ 4 | 626.1(2) 1540.0(4) 1759.4(6) | 96.08(2) | $HgC_2$ | $C_{Ph}$ C | 206(2) 208(1) | C,C | 173.3(6) | 53 |
| [Hg(Me)(dmso)]$BF_4$ (white) at 223K | m $P2_1/c$ 4 | 719.4(1) 1256.6(2) 1044.5(2) | 97.44(1) | HgOC | O $C_{Me}$ | 206.6(8) 205(1) | O,C | 178.7(5) | 54 |
| Hg(Me)(actp) | m $P2_1/c$ 4 | 833.0(2) 1932.4(3) 938.0(3) | 96.76(2) | HgOC | O $C_{Me}$ | 208.5(9) 207(1) | O,C | 178.1(5) | 55 |
| $Hg(CH_2COOH)(NO_3)$ (colourless) | m $P2_1/n$ 4 | 2026.7(4) 542.4(2) 522.6(1) | 90.34(2) | HgOC | O C | 210(2) 208(2) | O,C | 176.2(6) | 56 |
| $Hg(Ph)(MeCO_2)$ (colourless) | m $P2_1/c$ 4 | 518.5(3) 2410.4(10) 746.2(1) | 113.80(1) | HgOC ($O_3$) | O $C_{Ph}$ (O) | 208.1(13) 203.8(19) 290.7(14,88) | O,C | 176.6(6) | 57 |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| Hg(Ph)($CF_3CO_2$) | m | 1024.0(6) | | HgOC | O | 212.1(13) | O,C | 176.6(7) | 57 |
| (colourless) | $P2_1/c$ | 515.9(1) | 104.24(4) | ($O_2$) | $C_{Ph}$ | 205.1(17) | | | 58 |
| | 4 | 1796.0(12) | | | (O) | 289.0(15,62) | | | |
| Hg(Ph)(2-Cl-4-Br-$C_6H_3O$) | tr | 766(1) | 94.0(8) | HgOC | O | 210 | O,C | 174 | 59 |
| (colourless) | $P\bar{1}$ | 630(2) | 71.8(1) | | $C_{Ph}$ | 207 | | | |
| | 2 | 1355(6) | 93.3(0) | | | | | | |
| Hg{Et($MeCO_2$)CCEt}- | m | 1008.2(2) | | HgOC | O | 208(1) | O,C | 178(1) | 60 |
| ($MeCO_2$) | $P2_1/c$ | 1331.5(2) | 97.12(2) | | C | 205(1) | | | |
| (colourless) | 4 | 956.9(2) | | | | | | | |
| Hg($C_{11}H_{19}O_2$)($MeCO_2$) | m | 2380(2) | | HgOC | O | 210(1) | O,C | 175(1) | 61 |
| (colourless) | $P2_1/n$ | 1142(1) | 102.84(5) | | C | 211(2) | | | |
| | 8 | 1244(1) | | | | | | | |
| Hg($CF_3$)(NCO) | m | 944.9(2) | | HgNC | N | 203(2) | N,C | 178.3(10) | 62 |
| | $P2_1/c$ | 611.5(1) | 116.43(1) | | $F_3C$ | 202(2) | | | |
| | 4 | 977.2(2) | | | | | | | |
| α-Hg($CF_3$)($N_3$) | m | 972.0(3) | | HgNC | N | 202(2) | N,C | 177.3(9) | 62 |
| | $P2_1/c$ | 572.1(1) | 116.05(3) | | $F_3C$ | 196(2) | | | |
| | 4 | 993.8(2) | | | | | | | |
| β-Hg($CF_3$)($N_3$) | or | 1368(5) | | HgNC | | | | | 62 |
| | Pbca | 681(3) | | | | | | | |
| | 8 | 1050(4) | | | | | | | |
| Hg(Me)($N_3$) | m | 906(1) | | HgNC | N | 222(14) | N,C | 173(4) | 63 |
| at 100K | $P2_1/c$ | 687(1) | 107.4(2) | | C | 227(11) | | | |
| | 4 | 689(2) | | | | | | | |
| [Hg(Me)(py)]$NO_3$ | or | 1323.0(3) | | HgNC | N | 212(2) | N,C | 179.7(6) | 64 |
| (colourless) | Pnma | 653.8(1) | | | $C_{Me}$ | 204(3) | | | |
| | 4 | 980.8(5) | | | | | | | |
| [Hg(Me)(2-bzpy)]$NO_3$ | m | 1488.7(4) | | HgNC | N | 210(2) | N,C | 180 | 65 |
| | $P2_1/n$ | 1115.9(3) | 90.60(3) | | $C_{Me}$ | 207(3) | | | |
| | 4 | 874.5(3) | | | | | | | |
| [Hg(Me){($py)_2CH_2$}]($NO_3$) | m | 1687.5(2) | | HgNC | N | 216(1) | N,C | 172(1) | 66 |
| | $P2_1/n$ | 854.0(1) | 96.544(8) | (ON) | $C_{Me}$ | 210(2) | | | |
| | 4 | 935.3(1) | | | (O) | 276(2) | | | |
| | | | | | (N) | 275(2) | | | |
| [Hg(Me)($Et_3$terpy)]($NO_3$) | m | 911.5(2) | | HgNC | N | 226(2) | N,C | 171(1) | 66 |
| | $P2_1/n$ | 1572.5(3) | 94.46(1) | ($N_2O$) | C | 206(3) | | | |
| | 4 | 1556.6(3) | | | (N) | 256(2,5) | | | |
| | | | | | (O) | 278(2) | | | |
| [Hg(Me)(ppep)]$NO_3 \cdot H_2O$ | m | 2094.6(9) | | HgNC | N | 228.3(9) | N,C | 166.3(5) | 67 |
| | $P2_1/n$ | 1476.7(4) | 91.12(2) | ($N_2$) | $C_{Me}$ | 204.8(15) | | | |
| | 4 | 981.7(3) | | | (N) | 257.1(11,25) | | | |
| [Hg(Me){py(N-Meim)$_2$- | m | 1578.6(4) | | HgNC | N | 212(1) | N,C | 170.5(7) | 68 |
| COH}] · ($NO_3$) | $P2_1/n$ | 1506.5(3) | 91.24(2) | | $C_{Me}$ | 207(2) | | | |
| | 4 | 771.5(2) | | | (N) | 274(1,16) | | | |
| [Hg(Me){($py)_2$(N-Meim) · | tr | 1173.9(6) | 94.70(4) | HgNC | N | 213(1) | N,C | 112(0,2) | 69 |
| COH}]($NO_3$) | $P\bar{1}$ | 968.9(2) | 95.58(2) | ($N_2$) | $C_{Me}$ | 205(1) | | 170(0) | |
| | 2 | 818.2(2) | 97.00(2) | | (N) | 269(1,3) | | | |
| [Hg(Me){3,3'-$Me_2$bpy]- | m | 1052(5)4 | | HgNC | N | 211(1) | N,C | 172.7(5) | 70 |
| ($NO_3$) | $P2_1/c$ | 931.0(5) | 106.6(1) | ($O_3$) | $C_{Me}$ | 201(1) | | | |
| | 4 | 1657.0(8) | | | O | 287(1,3) | | | |
| Hg(Me)(4-$NO_2$im) | rh | 1143.4(9) | 111.40(9) | HgNC | N | 207(3) | N,C | 175.3(15) | 71 |
| (colourless) | R3c | | | | $C_{Me}$ | 201(4) | | | |
| | 6 | | | | | | | | |
| [Hg(Me)(tmm)]$NO_3$ | m | 1442.1(4) | | HgNC | N | 212.5(7) | N,C | 176.1(5) | 72 |
| | $P2_1/n$ | 1181.9(2) | 107.41(2) | (O) | $C_{Me}$ | 205(1) | | | |
| | 4 | 1098.5(3) | | | O | 268.0(6) | | | |
| [Hg(Me)($C_8H_7N_3$)]($NO_3$) | tr | 1020.1(9) | 91.16(2) | HgNC | N | 221(3) | N,C | 168.4(16) | 73 |
| | $P\bar{1}$ | 1034.7(9) | 106.89(3) | (N) | $C_{Me}$ | 195(4) | | | |
| | 2 | 765.0(7) | 127.07(2) | | (N) | 261(5) | | | |
| [Hg(Me)($pz_2CH_2$)]($NO_3$) | tr | 845.7(9) | 100.68(1) | HgNC | N | 216(1) | N,C | 178.5(7) | 73 |
| | $P\bar{1}$ | 1046.1(7) | 107.73(2) | (N) | $C_{Me}$ | 202(2) | | | |
| | 2 | 845.5(5) | 114.39(2) | | (N) | 296(2) | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | *a* [pm] *b* [pm] *c* [pm] | *α* [°] *β* [°] *γ* [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| Hg(Me){B(pz)$_4$} | tr | 1273(2) | 109.80(8) | HgNC | N | 207(2) | N,C | 169(2) | 74 |
| (colourless) | $P\bar{1}$ | 888(1) | 99.16(9) | (N) | $C_{Me}$ | 205(4) | | | |
| | 2 | 810(1) | 103.05(10) | | (N) | 265(4) | | | |
| Hg(Me)(tsh) | m | 1069.5(1) | | HgNC | N | 205(2) | N,C | 175(5) | 75 |
| (colourless) | $P2_1/a$ | 1416.6(2) | 104.06(3) | | $C_{Me}$ | 204(2) | | | |
| | 4 | 1503.2(3) | | | | | | | |
| Hg(Me)(glygly) | or | 792.0(6) | | HgNC | N | 210(3) | N,C | 176(1) | 76 |
| (colourless) | $Pna2_1$ | 1347.3(5) | | | $C_{Me}$ | 213(4) | | | |
| | 4 | 805.9(3) | | | | | | | |
| Hg(Me)(DL-ala) | m | 946.0(2) | | HgNC | N | 214(2) | N,C | 175.6(9) | 77 |
| (colourless) | $P2_1/c$ | 879.4(2) | 97.49(2) | (O) | $C_{Me}$ | 204(3) | | | |
| | 4 | 872.3(2) | | | O | 263(1) | | | |
| Hg(Me)(L-ala) | or | 576.3(3) | | HgNC | N | 210(3) | N,C | 173(1) | 78 |
| (colourless) | $P2_12_12_1$ | 685.1(6) | | | $C_{Me}$ | 208(3) | | | |
| | 4 | 1875(2) | | | | | | | |
| Hg(Me)(serine) | or | 582.1(2) | | HgNC | N | 212.8(7) | N,C | 174.0(4) | 79 |
| (colourless) | $P2_12_12_1$ | 805.2(1) | | ($O_2$) | $C_{Me}$ | 208(1) | | | |
| | 4 | 1430.7(3) | | | O | 280.8(7,82) | | | |
| [Hg(Me)(L-tyr)]$H_2O$ | m | 908.4(1) | | HgNC | N | 217(2) | N,C | 169(1) | 80 |
| (white) | $P2_1$ | 615.0(1) | 110.52(2) | (O) | $C_{Me}$ | 212(2) | | | |
| | 2 | 1156.5(1) | | | O | 262(2) | | | |
| Hg(Me)(apb) | or | 1485.3(4) | | HgNC | N | 215(3) | N,C | 177(2) | 80 |
| (white) | $Pca2_1$ | 943.8(3) | | ($O_2$) | $C_{Me}$ | 212(3) | | | |
| | 4 | 875.5(2) | | | O | 275(3,3) | | | |
| Hg(Me)(mt) | m | 704.8(9) | | HgNC | N | 206(4) | N,C | 173(2) | 81 |
| (colourless) | $P2_1/c$ | 582.6(4) | 93.2(2) | ($O_2$) | $C_{Me}$ | 211(5) | | | |
| | 4 | 2532.3(53) | | | O | 270(3,3) | | | |
| Hg(Me)(ad) | or | 1465.8(8) | | HgNC | N | 207.0(7) | N,C | 176.5(3) | 82 |
| (colourless) | Pbcn | 840.7(5) | | | $C_{Me}$ | 207.6(9) | | | |
| | 88 | 1300.6(9) | | | | | | | |
| [Hg(Me)(ad)]$H_2O$ | m | 1979.6(6) | | HgNC | N | 207(1) | N,C | 176.8(7) | 83 |
| (colourless) | C2/c | 711.9(3) | 128.83(2) | ($O_2$) | C | 206 | | | |
| | 8 | 1647.1(4) | | | O | 299(1,2) | | | |
| Hg(Me)(3-Mead) | m | 1421.8(4) | | HgNC | N | 212.5(7) | N,C | 177.5(3) | 84 |
| | C2/C | 2347.5(1) | 105.13(4) | ($O_3$) | $C_{Me}$ | 205.7(10) | | | |
| | 8 | 695.1(2) | | | O | 285.7(9,79) | | | |
| [Hg(Me)(9-Mead)]$NO_3$ | tr | 701.0(3) | 82.62(3) | HgNC | N | 213(1) | N,C | 175.6(4) | 85 |
| (colourless) | $P\bar{1}$ | 743.2(3) | 86.76(3) | | $C_{Me}$ | 207(1) | | | |
| | 2 | 1076.3(2) | 87.39(4) | | | | | | |
| [Hg(Me)(aadH)]($NO_3$) | m | 645.6(1) | | HgNC | N | 211(1) | N,C | 173.2(8) | 86 |
| (colourless) | $P2_1/m$ | 967.9(2) | 110.76(2) | (N) | $C_{Me}$ | 207(2) | | | |
| | 2 | 858.5(1) | | | (N) | 274(1) | | | |
| [Hg(Me)(aad)] · $4H_2O$ | tr | 720.4(1) | 90.76(2) | HgNC | N | 206.4(9) | N,C | 171.4(5) | 86 |
| (colourless) | $P\bar{1}$ | 1263.5(2) | 96.13(1) | (N) | $C_{Me}$ | 206(1) | | | |
| | 2 | 687.5(1) | 106.04(2) | | (N) | 282.4(8) | | | |
| [Hg(Me)(Meaad)]$NO_3$ | m | 1089.4(1) | | HgNC | N | 211(1) | N,C | 178.4(9) | 87 |
| | Pc | 746.0(1) | 90.57(1) | ($O_2$) | $C_{Me}$ | 209(3) | | | |
| | 2 | 687.6(1) | | | O | 287(2,4) | | | |
| Hg(Me)(app) | m | 676.0(1) | | HgNC | N | 209.6(4) | | not given | 88 |
| (colourless) | $P2_1/n$ | 1315.3(2) | 96.37(2) | | $C_{Me}$ | not given | | | |
| | 4 | 958.0(2) | | | | | | | |
| [Hg(Me)(2-Megu)]$NO_3$ | m | 419.6(1) | | HgNC | N | 209(2) | N,C | 175(1) | 89 |
| (white) | $P2_1/c$ | 1506.0(4) | 90.17(2) | ($O_2$) | $C_{Me}$ | 206(2) | | | |
| | 4 | 1828.8(5) | | | O | 287(2,12) | | | |
| [Hg(Me)(7-Megu)]2$H_2O$ | m | 1137.5(3) | | HgNC | N | 210.1(5) | N,C | 177.6(3) | 90 |
| (colourless) | $P2_1/c$ | 1373.2(3) | 105.54(2) | ($O_2$) | C | 205.1(8) | | | |
| | 4 | 747.1(2) | | | O | 290.2(7,10) | | | |
| [Hg(Me)(7-MeguH)]- | tr | 866.7(3) | 90.38(3) | HgNC | N | 211.1(4) | N,C | 176.4(2) | 90 |
| ($NO_3$)$H_2O$ | $P\bar{1}$ | 1023.2(3) | 100.35(3) | (O) | $C_{Me}$ | 206.2(7) | | | |
| (colourless) | 2 | 711.2(3) | 91.93(3) | | O | 284.1(5) | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| Hg(Me)(bzahx) | or | 1082.6(1) | | HgNC | N | 213(2) | N,C | 173(1) | 91 |
| (colourless) | Aba2 | 2703.0(2) | | (ON) | $C_{Me}$ | 204(3) | | | |
| | 8 | 881.1(2) | | | O | 295(2) | | | |
| | | | | | (N) | 299(2) | | | |
| Hg(Me)(tap) · $H_2O$ | m | 1088.4(5) | | HgNC | N | 206(2) | N,C | 171.5(8) | 92 |
| (colourless) | $P2_1/c$ | 918.7(7) | 131.02(3) | (ON) | $C_{Me}$ | 204(3) | | | |
| | 4 | 1445.8(4) | | | $H_2O$ | 294(1) | | | |
| | | | | | (N) | 298.1(1) | | | |
| [Hg(Me)(azaH)]$NO_3$ | tr | 781.8(3) | 97.89(3) | HgNC | N | 213(1) | N,C | 174.8(5) | 93 |
| (colourless) | $P\bar{1}$ | 788.4(3) | 109.13(3) | ($O_2$) | $C_{Me}$ | 203(1) | | | |
| | 2 | 913.5(4) | 103.28(3) | | O | 297(1,2) | | | |
| Hg(Me)(aza) [c] | tr | 1092.6(10) | 92.13(8) | HgNC | N | 211(2) | N,C | 173.8(11) | 93 |
| (colourless) | $P\bar{1}$ | 1133.3(8) | 104.83(9) | | $C_{Me}$ | 211(3) | | | |
| | 6 | 1164.7(10) | 111.86(7) | HgNC | N | 196(2) | N,C | 177.0(9) | |
| | | | | (N) | $C_{Me}$ | 207(3) | | | |
| | | | | | (N) | 288(2) | | | |
| | | | | HgNC | N | 205(2) | N,C | 176.0(10) | |
| | | | | (N) | $C_{Me}$ | 208(3) | | | |
| | | | | | (N) | 282(2) | | | |
| Hg(Me)(6auH) | m | 1722.8(2) | | HgNC | N | 208(1) | N,C | 176.3(7) | 94 |
| (colourless) | $P2_1/n$ | 408.2(1) | 92.71(2) | (O) | $C_{Me}$ | 206(2) | | | |
| | 4 | 941.5(1) | | | O | 289(1) | | | |
| [Hg(Me)(6amt)](5au$H_2$) | or | 1643.9(2) | | HgNC | N | 208(2) | N,C | 178(1) | 94 |
| (colourless) | Pbcm | 847.5(1) | | | $C_{Me}$ | 213(4) | | | |
| | 4 | 652.1(1) | | | | | | | |
| Hg(Me)(tuSM) | m | 828.4(1) | | HgNC | N | 212(1) | N,C | 176.3(5) | 95 |
| | $P2_1/n$ | 950.1(2) | 96.88(2) | (O) | $C_{Me}$ | 209(2) | | | |
| | ? | 1097.6(2) | | | O | 291(2) | | | |
| Hg(Me)(thm) | m | 479.8(6) | | HgNC | N | 207(1) | N,C | 178.3(6) | 96 |
| (colourless) | $P2_1$ | 1427.0(8) | 102.74(9) | (O) | $C_{Me}$ | 201(2) | | | |
| | 2 | 1039.0(4) | | | O | 296(1) | | | |
| [Hg(Me)(thm)] · 0 · 69$H_2O$ [c] | or | 1048.4(3) | | HgNC | N | 210(1) | N,C | 178.5(7) | 96 |
| (colourless) | $P2_12_12_1$ | 1463.3(3) | | ($O_3$) | $C_{Me}$ | 207(2) | | | |
| | 8 | 1853.8(5) | | | O | 296(2) | | | |
| | | | | HgNC | N | 210(1) | N,C | 176.8(7) | |
| | | | | ($O_3$) | $C_{Me}$ | 203(2) | | | |
| | | | | | O | 293(1,6) | | | |
| [Hg(Me)(Meth)] · $\frac{1}{2}H_2O$ | tg | 811.8(1) | | HgNC | N | 205.0(8) | N,C | 176.0(3) | 97 |
| (colourless) | $P4_122$ | – | | (O) | $C_{Me}$ | 198(1) | | | |
| | 8 | 3008.4(5) | | | O | 288(3) | | | |
| [Hg(Me)(Meth)] · $\frac{1}{2}NaNO_3$ [c] | or | 1108.8(3) | | HgNC | N | 209.2(8) | N,C | 175.9(3) | 97 |
| (colourless) | Pnma | 678.5(2) | | | $C_{Me}$ | 205.8(10) | | | |
| | 8 | 2731(2) | | HgNC | N | 210.0(8) | N,C | 174.4(3) | |
| | | | | | $C_{Me}$ | 207.2(10) | | | |
| Hg(Me)(all) | m | 1130.3(2) | | HgNC | N | 208(1) | N,C | 171.8(6) | 98 |
| (white) | $P2_1/c$ | 1055.0(1) | 96.56(2) | | $C_{Me}$ | 208(3) | | | |
| | 4 | 727.1(1) | | | | | | | |
| [Hg(Me)(all)] · 2$H_2O$ | m | 1983.8(3) | | HgNC | N | 213(1) | N,C | 175.1(6) | 98 |
| (white) | C2/c | 705.8(2) | 119.32(1) | ($O_2$) | $C_{Me}$ | 212(2) | | | |
| | 8 | 1786.9(3) | | | O | 290(1,2) | | | |
| [Hg(Me)(Mall)] · | or | 3185.4(2) | | HgNC | N | 212(2) | N,C | 165(2) | 98 |
| [$Hg_2(Me)_2$(Mall)]$NO_3$ | $Pna2_1$ | 1037.1(1) | | (O) | $C_{Me}$ | 207(4) | | | |
| | 4 | 652.5(1) | | | O | 293(4) | | | |
| | | | | HgNC dimer | see Table 2 | | | | |
| Hg(Ph)(tf) [c] | m | 2358.6(4) | | HgNC | N | 213(3) | N,C | 176(1) | 99 |
| (colourless) | $P2_1/c$ | 2132.4(3) | 91.29(2) | (N) | $C_{Ph}$ | 208(4) | | | |
| | 8 | 724.0(1) | | | (N) | 268(2) | | | |
| | | | | HgNC | N | 202(3) | N,C | 174(1) | |
| | | | | | $C_{Ph}$ | 196(4) | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| Hg(Ph)(nbs) | or | 819.1(2) | | HgNC | N | 212(1) | N,C | 178.0(4) | 100 |
| (colourless) at 153K | $Pn2_1a$ | 1092.7(3) | | (O) | $C_{Ph}$ | 199(1) | | | |
| | 4 | 2006.9(3) | | | O | 287.1(7) | | | |
| Hg(Ph)(psit) [c] | m | 1551.6(2) | | HgNC | N | 207(1) | N,C | 170.3(4) | 101 |
| (colourless) at 153K | $P2_1/c$ | 1053.4(1) | 105.294(2) | | C | 203(1) | | | |
| | 8 | 2287.7(3) | | HgNC | N | 208(1) | N,C | 176.6(4) | |
| | | | | | C | 205(1) | | | |
| Hg(Ph)(Fbsa) | or | 1695.7(2) | | HgNC | N | 218(4) | N,C | 176(2) | 102 |
| | $P2_1ca$ | 552.46(6) | | ($O_2$) | $C_{Ph}$ | 207(4) | | | |
| | 4 | 1788.8(3) | | | O | 295(3,3) | | | |
| Hg(Ph)(Clbsa) | m | 1260.7(2) | | HgNC | N | 208.4(28) | N,C | 177(1) | 103 |
| | $P2_1/c$ | 1451.1(2) | 96.90(5) | ($O_2$) | C | 203.9(32) | | | |
| | 4 | 990.6(3) | | | O | 284.6(23,91) | | | |
| Hg(Ph)(Brbsa) | m | 1260.5(2) | | HgNC | N | 209.0(10) | N,C | 171.5(2) | 103 |
| | $P2_1/c$ | 1481.0(2) | 96.95(5) | ($O_2$) | $C_{Ph}$ | 203.2(14) | | | |
| | 4 | 991.7(1) | | | O | 283.9(9,62) | | | |
| Hg(Ph)(pdpi) | m | 970.1(2) | | HgNC | N | 212.5(8) | N,C | 175.0(3) | 104 |
| (colourless) | $P2_1/c$ | 2473.1(3) | 96.85(1) | | $C_{Ph}$ | 203.8(9) | | | |
| | 4 | 1184.7(1) | | | | | | | |
| Hg(Ph)(ba) | m | 1444(1) | | HgNC | N | 204(2) | N,C | 179(1) | 105 |
| (colourless) | $P2_1/c$ | 969(1) | 105.9(1) | | $C_{Ph}$ | 202(2) | | | |
| | 4 | 860(1) | | | | | | | |
| $[Hg(Ph)(cre)]NO_3 \cdot H_2O$ | m | 1025.5(5) | | HgNC | N | 203(2) | N,C | 174(1) | 106a |
| | $P2_1/n$ | 1983.8(9) | 97.81(10) | (O) | $C_{Ph}$ | 204(2) | | | |
| | 4 | 685.9(3) | | | O | 294(2) | | | |
| Hg(Ph)(Cldab) | or | 776.5(5) | | HgNC | N | 214 | N,C | 173 | 106b |
| (orange-yellow) | Pbca | 1920.1(1) | | (N) | $C_{Ph}$ | 215 | | | |
| | 8 | 2248.4(9) | | | (N) | 246 | | | |
| Hg(Ph)(py)($F_3CCO_2$) [c] | or | 3443(3) | | HgNC | $N_{py}$ | 219(4) | N,C | 178(2) | 107 |
| (colourless) | $Pca2_1$ | 740.4(7) | | ($O_3$) | $C_{Ph}$ | 209(4) | | | |
| | 8 | 1064(1) | | | O | 286(4,8) | | | |
| | | | | HgNC | N | 211(4) | N,C | 167(2) | |
| | | | | ($O_4$) | C | 201(4) | | | |
| | | | | | O | 285(4,12) | | | |
| Hg($C_4H_7O$)(py)($CF_3CO_2$) | tr | 981(1) | 117.7(1) | HgNC | N | 216(1) | N,C | 174.4(6) | 108 |
| | $P\bar{1}$ | 920(1) | 61.72(6) | ($O_4$) | C | 212(2) | | | |
| | 2 | 1004(1) | 110.7(1) | | O | 283(2,6) | | | |
| Hg($MeOCH_2CH_2$)(top) | m | 830.5(2) | | HgNC | N | 208(1) | N,C | 173.3(6) | 109 |
| (white) | $P2_1/c$ | 934.9(3) | 97.36(1) | (ON) | C | 213(2) | | | |
| | 4 | 1637.0(4) | | | O | 289(1) | | | |
| | | | | | (N) | 291(1) | | | |
| Hg(4-Mep)(2-NO-4Mep) [c] | tr | 1026(2) | 97.2(2) | HgNC | N | 208(3) | N,C | 174 | 110 |
| (dark red) | $P\bar{1}$ | 2271(3) | 93.1(2) | ($O_2$) | C | 207(4) | | | |
| | 4 | 561(1) | 91.1(2) | | O | 281(3,24) | | | |
| | | | | HgNC | N | 220(4) | N,C | 176 | |
| | | | | ($O_2$) | C | 201(5) | | | |
| | | | | | O | 276(3,21) | | | |
| Hg(Me)(Clmcb) | m | 1249.7(3) | | HgCCl | C | 210 | C,Cl | 174 | 111 |
| (colourless) | $P2_1$ | 739.6(1) | | | Cl | 210 | | | |
| | 2 | 735.0(1) | 99.58(2) | | | | | | |
| Hg(MeOCO)Cl | or | 830 | | HgCCl | C | 196(5) | C,Cl | 180 | 112 |
| (colourless) | Pccn | 1720 | | | Cl | 235(4) | | | |
| | 8 | 752 | | | | | | | |
| Hg(ClCH=CH)Cl [e] | tr | 1860 | 92 | HgCCl | C | 211 | C,Cl | 175 | 113 |
| (colourless) | $P\bar{1}$ | 1060 | 80 | | Cl | 228 | C,Cl | 163 | |
| | 6 | 410 | 100 | HgCCl | C | 194 | C,Cl | 164 | |
| | | | | | Cl | 234 | | | |
| | | | | HgCCl | C | 227 | | | |
| | | | | | Cl | 229 | | | |
| Hg(ClCH=CH)Cl (gaseous) | | | | HgCCl | C | 214(2) | C,Cl | 168.5(1.5) | 114 |
| by electron diffraction | | | | | Cl | 227(1) | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | *a* [pm] *b* [pm] *c* [pm] | *α* [°] *β* [°] *γ* [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| $Hg(CH_2CHO)Cl$ | tr | 814.7(8) | 92.0(1) | HgCCl | C | 211(2) | C,Cl | 172.2(5) | 115 |
| | $P\bar{1}$ | 637.7(6) | 81.3(1) | ($O_2$) | Cl | 232.6(6) | | | |
| | 2 | 451.1(4) | 101.6(1) | | O | 286(2,2) | | | |
| $Hg(Et_2NCH_2CH_2)Cl$ | m | 850.9(4) | | HgCCl | C | 213(3) | C,Cl | 167.1(8) | 116 |
| (white) | $P2_1/n$ | 1705.2(7) | 95.82(15) | (N) | Cl | 236(1) | | | |
| | 4 | 630.6(2) | | | N | 277(2) | | | |
| $Hg(C_{16}H_{19}O_6)Cl$ | m | 1027.3(6) | | HgCCl | C | 211.7(18) | C,Cl | 180 | 117 |
| | $P2_1/n$ | 1531.6(8) | 112.86 | | Cl | 232.1(6) | | | |
| | 2 | 1222.6(6) | | | | | | | |
| $\alpha$-$Hg(2\text{-}MeOC_6H_{10})Cl$ | tr | 820(1) | 83.58(10) | HgCCl | C | 234 | C,Cl | 178 | 118 |
| | $P\bar{1}$ | 1058(2) | 116.2(1) | | Cl | 253 | | | |
| | 2 | 607(1) | 102.48(10) | | | | | | |
| $\beta$-$Hg(2\text{-}MeOC_6H_{10})Cl$ | tr | 788(1) | 88.29(10) | HgCCl | C | 215 | C,Cl | 180 | 118 |
| | $P\bar{1}$ | 929(1) | 102.18(10) | | Cl | 250 | | | |
| | 2 | 637(1) | 92.57(10) | | | | | | |
| $Hg(C_{14}H_{16}N_2O)Cl$ | tg | 2334.1(9) | | HgCCl | C | 205.8(7) | C,Cl | 178.7(3) | 119 |
| at 153K | I43/a | – | | (O) | Cl | 232.5(2) | | | |
| | 16 | 1063.5(4) | | | O | 298.1(7) | | | |
| $Hg(C_{19}H_{14}F_3O_4)Cl$ [c] | m | 1759.5(2) | | HgCCl | C | 212(4) | C,Cl | 178.4(7) | 120 |
| | $P2_1/c$ | 1104.54(9) | 97.281(8) | (O) | Cl | 230(1) | | | |
| | 8 | 2093.3(1) | | | O | 274(2) | | | |
| | | | | HgCCl | C | 212(3) | C,Cl | 178.7(7) | |
| | | | | (O) | Cl | 232(1) | | | |
| | | | | | O | 277(2) | | | |
| Hg(2-pyPh))Cl | m | 1033.4(2) | | HgCCl | C | 207(1) | C,Cl | 178.1(4) | 121 |
| (colourless) | $P2_1/n$ | 748.4(1) | 97.60(2) | (N) | Cl | 231(4) | | | |
| | 8 | 2705.2(6) | | | N | 263(1) | | | |
| $[PPh_3(CH_2Ph)][HgCl\{2,3,4\text{-}(MeO)_3C_6HCO_2\}]$ at 178K | tr | 1136.5(4) | 68.63(2) | HgCCl | C | 206.0(5) | C,Cl | 178.0(2) | 122 |
| | $P\bar{1}$ | 1265.9(4) | 76.57(2) | (O) | Cl | 231.5(2) | | | |
| | 2 | 1292.9(4) | 65.33(2) | | O | 257.3(4) | | | |
| $Hg(C_9H_{15}NO)Cl$ [f] | m | 1634.9(1) | | HgCCl | C | 205(2) | C,Cl | 177.1(7) | 123 |
| (colourless) | $P2_1/n$ | 1893.1(3) | 106.70(4) | | Cl | 232.4(6) | | | |
| | 20 | 2010.5(4) | | HgCCl | C | 207(2) | C,Cl | 178.2(6) | |
| | | | | | Cl | 232.4(6) | | | |
| | | | | HgCCl | C | 202(2) | C,Cl | 178.1(7) | |
| | | | | | Cl | 231.5(6) | | | |
| | | | | HgCCl | C | 204(3) | C,Cl | 177.2(8) | |
| | | | | | Cl | 232.4(6) | | | |
| | | | | HgCCl | C | 204(3) | C,Cl | 178.8(8) | |
| | | | | | Cl | 232.2(6) | | | |
| $Hg\{(py)_2Ph\}(Cl)$ [c] | m | 1033.4(2) | | HgCCl | C | 206.9(13) | C,Cl | 178.1(4) | 124 |
| (pale yellow) | $P2_1/n$ | 748.4(1) | 97.60(2) | (N) | Cl | 231.4(4) | | | |
| | 8 | 2705.2(6) | | | N | 262.7(12) | | | |
| | | | | HgCCl | C | 207.0(13) | C,Cl | 176.9(4) | |
| | | | | (N) | Cl | 233.5(4) | | | |
| | | | | | N | 267.3(12) | | | |
| $Hg(C_{15}H_{18}O_2FS)Cl$ | or | 744.9(2) | | HgCCl | C | 207(2) | C,Cl | 178.1(6) | 125 |
| | $P2_12_12_1$ | 996.8(7) | | (O) | Cl | 232.7(5) | | | |
| | 4 | 2337.8(9) | | | O | 281(2) | | | |
| $Hg(C_{10}H_{15})Cl$ | or | 1492.8(1) | | HgCCl | C | 209(2) | C,Cl | 177.7(3) | 126 |
| | $P2_12_12_1$ | 1178.4(1) | | | Cl | 235.2(2) | | | |
| | 4 | 615.14(7) | | | | | | | |
| $Hg(C_{10}H_{15})Cl$ | m | 694.3(2) | | HgCCl | C | 208 | C,Cl | 175 | 127 |
| at 153K | $P2_1$ | 1191.5(4) | | | Cl | 235(2) | | | |
| | 2 | 683.1(2) | 106.89(2) | | | | | | |
| $Hg(C_{18}H_{17}O_3)Cl$ | m | 964.3(9) | | HgCCl | C | 212(2) | C,Cl | 177.5(5) | 128 |
| | $P2_1$ | 1193.9(15) | | | Cl | 231.4(5) | | | |
| | 2 | 798.1(1) | 103.00(9) | | | | | | |
| $Hg(C_{13}H_{11}OCl_6)Cl$ | m | 815.3(4) | | HgCCl | C | 208(2) | C,Cl | 177.3(5) | 129 |
| (white) | $P2_1/c$ | 1953.0(5) | 107.20(3) | | Cl | 231.7(5) | | | |
| | 4 | 1213.2(5) | | | | | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | *a* [pm] *b* [pm] *c* [pm] | *α* [°] *β* [°] *γ* [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| $Hg(C_{16}H_{19}O_6)Cl$ | m | 1027.3(6) | | HgCCl | C | 211.7(18) | C,Cl | 177.1(5) | 130 |
| (colourless) | $P2_1/c$ | 1531.6(8) | 112.86(4) | | Cl | 232.1(6) | | | |
| | 4 | 1222(6) | | | | | | | |
| $2Hg(C_{19}H_{40}O_2)Cl,(Me_2CO)$ [c] | m | 729.5(8) | | HgCCl | C | 200(3) | C,Cl | 177.0(10) | 131 |
| (pale yellow) | $P2_1$ | 2412(1) | 108.0(1) | | Cl | 237.2(7) | | | |
| | 2 | 1221.5(12) | | HgCCl | C | 211(3) | C,Cl | 174.5(10) | |
| | | | | | Cl | 237.9(12) | | | |
| $Hg(C_{14}H_{24}N_4O_2)Cl$ | m | 1207.4(3) | | HgCCl | C | 206.1(8) | C,Cl | 176.9(3) | 132 |
| (light yellow) at 153K | $P2_1/a$ | 945.3(3) | 105.09(3) | (N) | Cl | 232.4(2) | | | |
| | 4 | 1581.2(7) | | | N | 269.0(8) | | | |
| Hg(cp*)Cl | tr | 831.5(2) | 91.80(2) | HgCCl | C | 208(2) | C,Cl | 176.8(7) | 133 |
| (yellow) | $P\bar{1}$ | 1185.9(2) | 101.24(2) | | Cl | 235.0(6) | | | |
| | 4 | 1245.8(5) | 109.34(2) | HgCCl | C | 210(2) | C,Cl | 173.9(5) | |
| | | | | | Cl | 236.1(5) | | | |
| $Hg(C_{10}H_{23}N_2O_2)Cl$ | m | 1570.5(11) | | HgCCl | C | 206.8(4) | C,Cl | 176.0(1) | 134 |
| (colourless) | $P2_1/c$ | 941.3(3) | 111.24(6) | (N) | Cl | 232.3(1) | | | |
| | 4 | 1210.6(9) | | | N | 270.2(3) | | | |
| $Hg(C_{18}H_{17}O_3)Cl$ | m | 950.1(3) | | HgCCl | C | 210(2) | C,Cl | 176.1(4) | 135 |
| at 153K | $P2_1/n$ | 1059.1(4) | 98.70(3) | (O) | Cl | 229.6(4) | | | |
| | 4 | 1771.6(6) | | | O | 278(1) | | | |
| $Hg(C_{16}H_{13}O_2)Cl$ | m | 1064.8(4) | | HgCCl | C | 205.4(9) | C,Cl | 176 | 136 |
| | $P2_1$ | 1037.8(5) | 114.95 | | Cl | 232.0(3) | | | |
| | 2 | 771.5(7) | | | | | | | |
| Hg{PhC(OEt)CPh}Cl | m | 864.1(2) | | HgCCl | C | 203(2) | C,Cl | 173.6(4) | 137 |
| (yellow) | $P2_1/c$ | 1910.7(3) | 99.41(4) | | Cl | 232(1) | | | |
| | 4 | 971.8(3) | | | | | | | |
| $Hg\{PhC(OCHMe_2)CPh\}Cl$ | m | 837.9(2) | | HgCCl | C | 205.5(10) | C,Cl | 176.3(2) | 137 |
| (yellow) | $P2_1/c$ | 2251.4(2) | 101.74(3) | | Cl | 232.0(3) | | | |
| | 4 | 915.2(3) | | | | | | | |
| $Hg\{2\text{-}MeC(O)C_6H_4\}Cl$ | or | 534.6(1) | | HgCCl | C | 207(1) | C,Cl | 176 | 138 |
| (white) at 123K | $P2_12_12_1$ | 1054.3(3) | | | Cl | 232.3(2) | | | |
| | 4 | 1474.3(2) | | | | | | | |
| $Hg(C_{11}H_{11}O_2)Cl$ [e] | m | 1781.5 | | HgCCl | not given | | C,Cl | 175.9 | 139 |
| | $P2_1/n$ | 1567.2 | | | | | | | |
| | 8 | 929.9 | 111.25 | HgCCl | not given | | C,Cl | 176.4 | |
| $[ClHg(C_6H_{12}NCl)][HgCl_3]$ [c] | m | 1053.2(6) | | HgCCl | C | 203(3) | C,Cl | 175.3(9) | 140 |
| | Pc | 986.6(2) | 99.23(6) | | Cl | 237(1) | | | |
| | 4 | 1409.3(7) | | HgCCl | C | 209(4) | C,Cl | 173.6(9) | |
| | | | | | Cl | 228(1) | | | |
| | | | | $HgCl_3$ | Cl | 241(1,6) | Cl,Cl | 90.1(4,7.1) | |
| | | | | | | | | 129.0(4,8.8) | |
| | | | | $HgCl_3$ | Cl | 241(1,13) | Cl,Cl | 90.4(4,14.7) | |
| | | | | | | | | 128.1(4,14.1) | |
| $[ClHg(C_5H_{12}NCl]_2 \cdot$ | m | 2767.9(4) | | HgCCl | C | 206(2) | C,Cl | 174.6(5) | 140 |
| $[HgCl_4] \cdot (C_6H_6) \cdot H_2O$ | C2/c | 814.0(1) | 97.17(2) | | Cl | 232.2(5) | | | |
| | 4 | 1416.4(2) | | $HgCl_4$ | Cl | 238.7(5) | Cl,Cl | 100.7(2,4.5) | |
| | | | | | | 264.3(4) | | 141.1(2) | |
| $[ClHg(C_5H_{10}NCl)] \cdot$ | or | 1318.6(2) | | HgCCl | C | 205(4) | C,Cl | 166.4(11) | 140 |
| $[Hg_2Cl_6]$ | $Pn2_1a$ | 1850.1(2) | | | Cl | 232(1) | | | |
| | 4 | 1118.9(1) | | HgCCl | C | 209(3) | C,Cl | 176.9(9) | |
| | | | | | Cl | 231(1) | | | |
| | | | | $HgCl_4$ | Cl | 232(2,2) | Cl,Cl | 94.0(4,8.0) | |
| | | | | | $\mu$Cl | 288(1,14) | | 163.0(6,4.2) | |
| Hg(dmhfe)Cl | | | | HgCCl | C | 203(2) | C,Cl | 174(1) | 141 |
| | | | | | Cl | 230(1) | | | |
| Hg(PhCOCHCH)Cl | m | 761(1) | | HgCCl | C | 223(12) | C,Cl | 173(2) | 142 |
| | $P2_1/b$ | 2228(2) | | (O) | Cl | 237.0(19) | | | |
| | 4 | 577(1) | 106.0(3) | | O | 288 | | | |
| $Hg(C_9H_{13}O_2)Cl$ | m | 1410(1) | | HgCCl | C | 210(6) | C,Cl | 173(2) | 143 |
| | $P2_1/c$ | 1048(1) | 96.33(7) | | Cl | 232(2) | | | |
| | 4 | 721.8(1) | | | | | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | *a* [pm] *b* [pm] *c* [pm] | $\alpha$ [°] $\beta$ [°] $\gamma$ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| $Hg(C_{10}H_{14}NCl_2)C$ [c] | m | 1654.9(4) | | HgCCl | C | 205 | C,Cl | 166 | 53 |
| (colourless) | $P2_1/c$ | 1148.4(4) | 113.9(2) | | Cl | 234 | | | |
| | 8 | 1624.2(3) | | HgCCl | C | 209 | C,Cl | 173 | |
| | | | | | Cl | 230 | | | |
| $Hg(C_{12}H_9N_2)Cl$ | m | 1064.8(3) | | HgCCl | C | 201(2) | C,Cl | not given | 144 |
| | $P2_1/c$ | 458.2(4) | 94.05(2) | (N) | Cl | 230.9(2) | | | |
| | 4 | 2390.0(7) | | | N | 270(2) | | | |
| $Hg(C_7H_{13}O_5)Cl$ | or | 668(1) | | HgCCl | C | not given | | | 145 |
| (colourless) | $P2_12_12_1$ | 1360(10) | | | Cl | 238(10) | | | |
| | 4 | 1190(10) | | | | | | | |
| Hg(o-EtOCOph)Cl | m | 1061.1(2) | | HgCCl | C | 216 | C,Cl | 178.3(4) | 146 |
| (colourless) | $P2_1/c$ | 498.7(1) | 95.74(2) | (O) | Cl | 248 | | | |
| | 4 | 1941.6(5) | | | O | 273.4 | | | |
| $Hg(PhCH_2)Cl$ [c] | m | 888.6(3) | | HgCCl | C | 210(2) | C,Cl | 178.9(6) | 147 |
| (colourless) | $P2_1/n$ | 601.0(2) | 98.47(3) | | Cl | 236.1(5) | | | |
| | 4 | 2846.7(9) | | HgCCl | C | 210(2) | C,Cl | 176.8(6) | |
| | | | | | Cl | 237.0(6) | | | |
| $Hg(C_{13}H_{15}O_2)Cl$ | m | 821.9(5) | | HgCCl | not given | | | | 148 |
| | $P2_1/c$ | 1195.2(2) | 95.68(5) | | | | | | |
| | 8 | 2685.5(3) | | | | | | | |
| Hg(pmc)Cl | m | 907.5(3) | | HgCCl | not given | | | | 148 |
| | $P2_1/c$ | 672.6(3) | 98.59(5) | | | | | | |
| | 4 | 2114.4(4) | | | | | | | |
| Hg( $\beta$-lactam)Cl | m | 1392.6(2) | | HgCCl | not given | | | | 149 |
| | $P2_1/c$ | 1400.2(3) | 109.23(1) | | | | | | |
| | 4 | 929.7(2) | | | | | | | |
| Hg(o-tolyl)Cl | or | 2749.8(4) | | HgCCl | C | 209(2) | C,Cl | 178.5(5) | 190 |
| | Pnma | 660.5(2) | | | Cl | 233.1(9) | | | |
| | 4 | 437(2) | | | | | | | |
| $Hg(Me)(C_5H_6N_3S)$ | m | 1193.2(6) | | HgCS | $C_{Me}$ | 209(1) | C,S | 178.6(4) | 150 |
| | $P2_1/c$ | 582.4(3) | 99.75(6) | (N) | S | 239.3(4) | | | |
| | 4 | 1289.5(6) | | | N | 280(2) | | | |
| $Hg(Me)(C_4H_4N_3OS)$ | m | 731.2(4) | | HgCS | $C_{Me}$ | 209(2) | C,S | 178.6(9) | 150 |
| | $P2_1/c$ | 870.2(4) | 94.43(5) | (N) | S | 239.0(6) | | | |
| | 4 | 1491.1(7) | | | N | 295(2) | | | |
| $Hg(Me)(C_{12}H_6NS_2)$ [c] | tr | 800.9(4) | 101.25(2) | HgCS | C | 206(2) | C,S | 177.7(7) | 151 |
| (white) | $P\bar{1}$ | 1004.2(4) | 102.61(3) | | S | 236.9(6) | | | |
| | 4 | 1307.4(3) | 101.42(3) | HgCS | C | 210(3) | C,S | 178.8(6) | |
| | | | | | S | 237.5(6) | | | |
| $[Hg(Me)(thtH)]NO_3$ | m | 715.8(14) | | HgCS | $C_{Me}$ | 206.9(15) | C,S | 178.4(5) | 152 |
| | $P2_1/c$ | 1015.6(7) | 108.21(4) | (O) | S | 239.1(4) | | | |
| | 4 | 1347.2(12) | | | O | 285.4(11) | | | |
| Hg(Me)(tht) | hx | 1350.2(8) | | HgCS | $C_{Me}$ | 211.0(19) | C,S | 175.7(10) | 152 |
| | $P6_3$ | 1350.2(8) | | | S | 235.8(4) | | | |
| | 6 | 698.4(7) | | | | | | | |
| $[Hg(Me)(cys)] \cdot H_2O$ | or | 638.6(6) | | HgCS | $C_{Me}$ | 210(4) | C,S | 177.6(9) | 153 |
| | $P2_12_12_1$ | 2602.6(13) | | (O) | S | 235.2(12) | | | |
| | 4 | 528.2(4) | | | O | 285(2) | | | |
| $[Hg(Me)(C_4H_6N_2S)]NO_3$ | tr | 714.6(2) | 72.95(3) | HgCS | $C_{Me}$ | 209(1) | C,S | 176.1(4) | 154 |
| | $P\bar{1}$ | 778.3(3) | 71.09(3) | (O) | S | 238.2(2) | | | |
| | 2 | 1018.4(5) | 81.83(2) | | O | 283.3(8) | | | |
| $Hg(Me)(C_4H_5N_2S)$ | m | 773.4(1) | | HgCS | $C_{Me}$ | 205(10) | C,S | 176(2) | 154 |
| | Cc | 1712.5(3) | 99.66(3) | | S | 233.8(7) | | | |
| | 4 | 606.1(3) | | | | | | | |
| Hg(Me)(py-2-th) | m | 1083.4(5) | | HgCS | $C_{Me}$ | 208.9(7) | C,S | 176.4(2) | 155 |
| (white) | $P2_1/n$ | 420.6(3) | 101.91(1) | (N) | S | 237.4(2) | | | |
| | 4 | 1714.4(2) | | | N | 298.0(5) | | | |
| $Hg(Me)(C_5H_5N_2S)$ | m | 1828.1(4) | | HgCS | C | 215 | C,S | 176(1) | 156 |
| (yellow) | C2/c | 1217.0(4) | 154.20(7) | | S | 243.7(8) | | | |
| | 8 | 1735.0(5) | | | | | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| Hg(Me)(2,4,6-$Pr^i_3C_6H_2S$) | tr | 596.2(1) | 79.60(1) | HgCS | $C_{Me}$ | 207.0(27) | C,S | 175.7(7) | 15 |
| (colourless) | $P\bar{1}$ | 964.9(1) | 79.58(1) | | S | 234.4(4) | | | |
| | 2 | 1595.1(2) | 84.68(1) | | | | | | |
| [HgMe(pen)] · $H_2O$ [c] | m | 2315.4(33) | | HgCS | $C_{Me}$ | 207(6) | C,S | 175(2) | 157 |
| (colourless) | C2/c | 981.9(14) | 106.4(1) | | S | 238(1) | | | |
| | 16 | 1932.1(27) | | HgCS | $C_{Me}$ | 209(5) | C,S | 175(2) | |
| | | | | | S | 236(1) | | | |
| Hg(Me)($C_4H_3N_2S$) | or | 406.3(2) | | HgCS | $C_{Me}$ | 213(6) | C,S | 174 | 158 |
| (white) | $P2_12_12_1$ | 990.1(4) | | (N) | S | 239(2) | | | |
| | 4 | 1880.8(5) | | | N | 283(3) | | | |
| Hg(Me)($Et_2$dtc) | m | 715.5(5) | | HgCS | C | 204(3) | C,S | 171.2(8) | 159 |
| (colourless) | $P2_1/c$ | 775.7(4) | 96.1(1) | (S) | S | 241.8(7) | | | |
| | 4 | 1824.8(7) | | | (S) | 296.4(7) | | | |
| Hg(Me)($Ph_2$tc) | tr | 1486.6(7) | 89.30(5) | HgCS | $C_{Me}$ | 206(2) | C,S | 165.9(5) | 160 |
| (red brown) | $P\bar{1}$ | 1119.4(6) | 95.85(5) | (N) | S | 238.9(4) | | | |
| | 2 | 455.7(3) | 97.62(5) | | N | 258(1) | | | |
| Hg(Ph)($Ph_2$tc) | m | 599.1(3) | | HgCS | $C_{Ph}$ | 212(2) | C,S | 167.9(7) | 160 |
| (red brown) | $P2_1/c$ | 2068(1) | 99.40(5) | (N) | S | 237.2(7) | | | |
| | 4 | 1712.9(9) | | | N | 265(2) | | | |
| Hg(Ph)(2-$Me_2$atph) | m | 774.9(2) | | HgCS | $C_{Ph}$ | 207.6(6) | C,S | 178.0(2) | 161 |
| (colourless) at 153K | $P2_1/c$ | 1150.4(3) | 100.34(2) | (N) | S | 236.5(2) | | | |
| | 4 | 1569.7(3) | | | N | 265.7(6) | | | |
| Hg(Ph)($Ph_2PS_2$) | tr | 918.9(1) | 105.79(1) | HgCS | $C_{Ph}$ | 208(1) | C,S | 175.0(3) | 162 |
| (colourless) | $P\bar{1}$ | 1194.5(3) | 96.03(1) | | S | 237.9(3) | | | |
| | 2 | 699.3(1) | 78.92(2) | | | | | | |
| Hg(Ph)($Et_2$dtc) [c] | tr | 995.9(2) | 65.53(2) | HgCS | $C_{Ph}$ | 204.7(9) | C,S | 171.8(3) | 163 |
| (not given) | $P\bar{1}$ | 1235.9(4) | 65.81(2) | (S) | S | 238.7(2) | | | |
| | 4 | 1309.8(2) | 81.26(2) | | (S) | 297.8(2) | | | |
| | | | | HgCS | $C_{Ph}$ | 206(1) | C,S | 172.3(3) | |
| | | | | (S) | S | 238.8(2) | | | |
| | | | | | (S) | 292.3(3) | | | |
| Hg(Ph)($MeOCS_2$) | m | 3773(2) | | HgCS | $C_{Ph}$ | 205(3) | C,S | 174.1(7) | 163 |
| | C2/c | 482.5(1) | 101.21(2) | | S | 238.8(10) | | | |
| | 8 | 1268.6(1) | | | | | | | |
| Hg(Ph)($Pr^iOCS_2$) [e] | m | 1367.8(5) | | HgCS | $C_{Ph}$ | 203(1) | C,S | 176.6(4) | 163 |
| | $P2_1/a$ | 2134.7(7) | 114.99(2) | | S | 237.4(4) | | | |
| | 12 | 1457.0(6) | | HgCS | $C_{Ph}$ | 203(1) | C,S | 175.6(3) | |
| | | | | | S | 238.4(3) | | | |
| | | | | HgCS | $C_{Ph}$ | 210(1) | C,S | 174.3(3) | |
| | | | | | S | 239.4(4) | | | |
| Hg(Ph)(2,6-$Me_2$tph) | m | 982.9(5) | | HgCS | $C_{Ph}$ | 197(6) | C,S | 172(1) | 164 |
| (colourless) | $P2_1/b$ | 2509.0(2) | 92.95(7) | | S | 233(1) | | | |
| | 4 | 540.0(6) | | | | | | | |
| Hg(Ph)($C_{13}H_{11}N_4S$) | m | 599.1(3) | | HgCS | $C_{Ph}$ | 210(3) | C,S | 168.0(7) | 165 |
| (yellow) | $P2_1/c$ | 2068(1) | 99.40(5) | (N) | S | 237(3) | | | |
| | 4 | 1712.9(9) | | | N | 266(3) | | | |
| Hg(Ph)(qu-8-th) [c] | m | 673.2(3) | | HgCS | C | 207(3) | C,S | 160.9(8) | 166 |
| (colourless) at 153K | $P2_1/c$ | 2743(2) | 95.68(4) | (N) | S | 240.2(7) | | | |
| | 8 | 1681.1(8) | | | N | 246(2) | | | |
| | | | | HgCS | C | 210(3) | C,S | 162.3(7) | |
| | | | | (N) | S | 240.1(7) | | | |
| | | | | | N | 246(2) | | | |
| Hg($PhCH_2$)($Ph_3CS$) | m | 1186.2(7) | | HgCS | C | 210 | C,S | 179 | 167 |
| (white) | $P2_1/a$ | 1813.7(15) | 128.93(3) | | S | 236.3 | | | |
| | | 1293.2(8) | | | | | | | |
| Hg(methu)($C_6H_4CO_2H$) | or | 1602.0(2) | | HgCS | C | 207.2(9) | C,S | 177.3(5) | 168 |
| (colourless) | Pbca | 1361.6(1) | | | S | 234.2(3) | | | |
| | 8 | 1179.6(1) | | | | | | | |
| [Hg(Ph)($Ph_3P$)]$NO_3$ | m | 1311.9(5) | | HgCP | $C_{Ph}$ | 209.0(5) | C,P | 167.5(2) | 169 |
| (colourless) | $P2_1/n$ | 1052.9(2) | 102.79(1) | ($O_3$) | P | 243.1(2) | | | |
| | 4 | 1623.3(4) | | | O | 287.9(2,102) | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| $Hg(Cl_3CH)Br$ [c] | or | 1828 | | HgCBr | C | not given | not given | | 170 |
| | Pbnm | 1066 | | | Br | 236(2) | | | |
| | 8 | 656 | | HgCBr | C | not given | | | |
| | | | | | Br | 243(2) | | | |
| Hg(Ph)Br | tg | 490 | | HgCBr | C | 206 | C,Br | 180 | 171 |
| by electron diffraction | P4/nmm | – | | | Br | 243 | | | |
| | 2 | 1420 | | | | | | | |
| $Hg(C_{18}H_{21}O_2)Br$ | m | 1148(1) | | HgCBr | C | 213(3) | C,Br | 177(1) | 172 |
| | $P2_1/c$ | 1053(1) | 120.5(1) | (O) | Br | 244.0(4) | | | |
| | 4 | 1766(2) | | | O | 268(4) | | | |
| $Hg(C_{14}H_{16}N_2O_2)Br$ | or | 1081.4(8) | | HgCBr | C | 206(2) | C,Br | 176.6(6) | 173 |
| at 153K | Pbca | 1573(1) | | (O) | Br | 243.3(3) | | | |
| | 8 | 1851(1) | | | O | 284(2) | | | |
| $Hg(C_3H_5OH)Br$ | tr | 675.2(1) | 83.14(1) | HgCBr | C | 208(4) | C,Br | 176(1) | 174 |
| (white) | $P\bar{1}$ | 573.3(1) | 95.53(1) | ($O_2$) | Br | 244.1(5) | | | |
| | 2 | 797.9(1) | 101.47(1) | | O | 282(2,1) | | | |
| $Hg(C_{15}H_{26}N_2O)Br$ | m | 1206(2) | | HgCBr | C | 207(2) | C,Br | 175.5(7) | 175 |
| (colourless) | $P2_1/a$ | 950(1) | 110.3(1) | (N) | Br | 243.5(3) | | | |
| | 4 | 1588(2) | | | N | 266(2) | | | |
| $Hg(C_{15}H_{24}N_2O)Br$ | | | | HgCBr | C | 207(2) | C,Br | not given | 176 |
| | | | | (N) | Br | 243.5(3) | | | |
| | | | | | N | 266 | | | |
| Hg(8-MeCHqu)Br | m | 408.4(1) | | HgCBr | C | 211(1) | C,Br | 174.6(3) | 177 |
| at 153K | $P2_1/c$ | 1982.8(11) | 92.80(3) | (N) | Br | 245.3(1) | | | |
| | 2 | 1321.3(8) | | | N | 291.6(9) | | | |
| $Hb(C_8H_{13}O_2)Br$ | m | 1179(1) | | HgCBr | C | 212(3) | C,Br | not given | 178 |
| | $P2_1/c$ | 1144(1) | 95.36(10) | | Br | 244.0(4) | | | |
| | 4 | 831(1) | | | | | | | |
| $Hg\{PhC(H)CO_2C_{10}H_{19}\}Br$ | | | | HgCBr | C | 205 | | not given | 179 |
| (colourless) | | | | | Br | 246 | | | |
| $Hg(C_8H_{15}B_{10})Br$ | m | 775.3(2) | | HgCBr | C | 208(1) | C,Br | 174.9(4) | 180 |
| | $P2_1/n$ | 1080.0(4) | | | Br | 239.8(1) | | | |
| | 4 | 1802.9(9) | 90.73(3) | | | | | | |
| α-$Hg(2\text{-}MeOC_6H_{10})Br$ | tr | 833(2) | 83.4(2) | HgCBr | not given | | | | 118 |
| | $P\bar{1}$ | 1073(3) | 115.28(20) | | | | | | |
| | 2 | 609(2) | 104.1(2) | | | | | | |
| β-$Hg(2\text{-}MeOC_6H_{10})Br$ | tr | 796(2) | 86.22(20) | HgCBr | not given | | | | 118 |
| | $P\bar{1}$ | 941(2) | 102.0(2) | | | | | | |
| | 2 | 646(2) | 93.4(2) | | | | | | |
| $Hg(C_{36}H_{35}O_{12})Br$ | m | 1137 | | HgCBr | not given | | | | 181 |
| | C2 | 942 | 97.37 | | | | | | |
| | 4 | 4262 | | | | | | | |
| $Hg(C_{21}H_{33}O_5)Br$ | tg | 1955.0 | | HgCBr | not given | | | | 181 |
| | I4 | – | | | | | | | |
| | 8 | 1337.5 | | | | | | | |
| $[Hg(Me)(Se\text{-}urea)]NO_3$ | or | 752.4(1) | | HgCSe | $C_{Me}$ | 213(3) | C,Se | 177.0(8) | 182 |
| (colourless) | Pn21c | 1120.4(2) | | | Se | 247.7(3) | | | |
| | 4 | 973.8(2) | | | | | | | |
| $Hg(C_{12}H_{21}OSi)I$ [c] | m | 1071.5(3) | | HgCI | C | 210(2) | C,I | 173.5(7) | 183 |
| (yellow) | $P2_1/n$ | 953.9(2) | 95.43(2) | | I | 260.4(2) | | | |
| | 8 | 3323.5(7) | | HgCI | C | 208(2) | C,I | 172.8(7) | |
| | | | | | I | 259.4(2) | | | |
| Hg(α-naphthyl)I | m | 872 | | HgCI | C | not given | | | 184 |
| | $P2_1/m$ | 508 | 97.13 | | I | 261 | | | |
| | 2 | 1019 | | | | | | | |
| $Hg(C_8H_{15}B_{10})I$ | m | 778.2(2) | | HgCI | C | 209.6(7) | C,I | 171.6(2) | 180 |
| | $P2_1/n$ | 1094.5(2) | | | I | 256.7(1) | | | |
| | 4 | 1814.1(6) | 90.08(2) | | | | | | |

Table 1 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|
| α-Hg(2-$MeOC_6H_{10}$)I | tr | 858(2) | 84.0(2) | HgCI | not given | | | | 118 |
| | $P\bar{1}$ | 1987(3) | 115.4(2) | | | | | | |
| | 2 | 612(2) | 102.5(2) | | | | | | |
| β-Hg(2-$MeOC_6H_{10}$)I | tr | 818(2) | 84.36(20) | HgCl | not given | | | | 118 |
| | $P\bar{1}$ | 963(2) | 102.52(20) | | | | | | |
| | 2 | 657(2) | 94.49(20) | | | | | | |
| [Hg(Me)(bpy)]$NO_3$ | tr | 1029.9(5) | 88.98(4) | $HgN_2C$ | N | 234(3,10) | N,N | 69(1) | 185 |
| | $P\bar{1}$ | 928.9(5) | 105.57(5) | ($O_2$) | $C_{Me}$ | 207(5) | N,C | 126(1) | |
| | 2 | 684.1(4) | 84.81(4) | | O | 299(3,0) | | 164(1) | |
| Hg(Ph)(sami) [c] | tr | 1014.8(2) | 99.08(5) | HgNC | $C_{Ph}$ | 202(4) | N,C | 167(1) | 186 |
| (colourless) | $P\bar{1}$ | 1119.5(2) | 109.56(5) | (O) | N | 215(3) | | | |
| | 4 | 1438.6(2) | 104.16(5) | | O | 244(3) | | | |
| | | | | HgNC | $C_{Ph}$ | 193(4) | N,C | 166(1) | |
| | | | | (O) | N | 209(3) | | | |
| | | | | | O | 241(3) | | | |
| α-Hg(Ph)(quo) [c] | or | 2312(3) | | HgONC | O | 219(4) | O,N | 74(1) | 187 |
| | Pnam | 1659(2) | | | N | 229(4) | O,C | 142(2) | |
| | 8 | 662(1) | | | $C_{Ph}$ | 218(6) | N,C | 144(2) | |
| | | | | HgONC | O | 215(4) | O,N | 75(1) | |
| | | | | | N | 240(4) | O,C | 154(2) | |
| | | | | | $C_{Ph}$ | 214(5) | N,C | 131(2) | |
| β-Hg(Ph)(quo) | or | 558.4(2) | | HgOC | O | 206(2) | O,N | 72.1(5) | 187 |
| | $P2_12_12_1$ | 990.2(3) | | (N) | C | 205(2) | O,C | 175.0(7) | |
| | 4 | 2207.3(9) | | | N | 257(2) | N,C | 112.8(7) | |
| Hg(Ph)(mquo) | m | 2296.1(8) | | HgONC | $C_{Ph}$ | 205(2) | O,C | 151.86(6) | 187 |
| | C2/c | 914.2(2) | 127.75(2) | (O) | O | 216(1) | O,N | 73.0(5) | |
| | 8 | 1641.2(6) | | | N | 236(1) | N,C | 134.8(7) | |
| | | | | | (O) | 279(1) | | | |
| [Hg(Me){$py_3COH$}]$NO_3$ | tr | 1021.6(4) | 103.71(2) | HgNC | $C_{Me}$ | 203(2) | N,C | 150(1) | 69 |
| | $P\bar{1}$ | 1262.8(5) | 129.67(2) | ($N_2$) | N | 228(1) | | | |
| | 2 | 961.4(3) | 91.86(3) | | (N) | 249(1,4) | | | |
| [Hg(Me)(np)$_3$]$CF_3 \cdot C_7H_8$ | or | 3449.1(12) | | $HgP_3C$ | $C_{Me}$ | 218(3) | P,P | 99.5(3,2.4) | 188 |
| (colourless) | $Pb2_1a$ | 1269.4(5) | | | P | 260.8(9,8) | P,C | 118.0(9,7.0) | |
| | 4 | 1118.4(5) | | | | 280.8(7) | | | |
| Hg(P-tolyl)($MeCO_2$) | tr | 713 | 86.23 | | | | | | 189 |
| | P1 | 1353 | 106.56 | | | | | | |
| | 2 | 513 | 81.25 | | | | | | |
| Hg(pp)ce | | | | | | | | | 191 |

[a] Where more than one chemically equivalent distance or angle is present, the mean value is tabulated. The first number in parenthesis is the e.s.d., and the second is the maximum deviation from the mean.
[b] The chemical identity of the coordinated atom or ligand is specified in these columns.
[c] There are two crystallographically independent molecules.
[d] There are four crystallographically independent molecules.
[e] There are three crystallographically independent molecules.
[f] There are five crystallographically independent molecules.

between the shortest value and the mean and the second number is the difference between the longest and the mean. These mean values indicate no significant change in bond length despite the change from $sp^3$ hybridization to $sp^2$. The overall mean Hg–C bond length found in these complexes is 207(15,25) pm.

The mean Hg–L bond length for other unidentate ligands increases with the covalent radius of the coordinating atom in the sequence: 209 pm (OL, 73 pm) < 211 pm (NL, 75 pm) < 233.3 pm (Cl, 99 pm) < 243.0 pm (Br, 114 pm) < 259.4 pm (I, 133 pm). The mean Hg-L bond lengths found in the mercury(II) coordination complexes are: 205 pm (NL) < 231.1 pm (Cl) < 242.0 pm (Br) < 261.7 pm (I), which are all shorter except for the iodide.

There are several examples in which two different isomeric forms are found [6,7,26,27,62,118,126,127, 167], differing mostly by degree of distortion. In another set of examples [12,20,44,49,53,96,97,99,101, 107,110,118,120,124,131,139,140,151,163,166,170, 183,186,187] two crystallographically independent molecules are observed. Three such independent molecules are found in three cases [93,113,163], with one example containing four independent molecules

Table 2
Crystallographic and structural data for dimeric organomercury compounds [a]

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | Hg–Hg [pm] Hg–L–Hg [°] | L–Hg–Hg [°] L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|---|
| $[Hg^1(Me_6C_6)]_2[AlCl_4]_2 \cdot$ PhMe (colourless) | m $P2_1/c$ 4 | 2116(1) 1095.1(7) 1880(1) | 104.9(1) | $HgC_3$ | c [b] | 259(2,25) | 251.5(2) | C,Hg [b] | 69.7(2,5.7) 93.3(2) | 195 |
| $(HgCl)_2\{PhCC(Ph)(OMe)_2\}$ (white) | tr $P\bar{1}$ 2 | 1483.6(2) 923.9(3) 723.2(2) | 110.41(3) 102.03(2) 73.47(2) | HgCCl | μC Cl | 211.6(12,6) 231.7(5,4) | 321.3(7) 98.9(5) | C,Cl | 176.4(3,2) | 196 |
| $Hg_2Cl_2(CH_3CH_2COOH)$-(dmso) | m $P2_1/c$ 4 | 1024.9(9) 1118.4(2) 1137.7(7) | 110.68(2) | HgCCl | μC Cl | 212(2,2) 232.2(7,12) | 101(1) | C,Cl | 177.8(5,2) | 197 |
| $Hg_2Cl_2\{CH_3(CH_2)_2COOH\} \cdot$ (dmso) | or Pbcn 8 | 1223.3(3) 1136.2(1) 1889.5(1) | | HgCCl | μC Cl | 209.3(32,4) 232.9(9,0) | 103(1) | C,Cl | 178(1,0) | 198 |
| $Hg_2(C_5H_6O_2)Cl_2$ (colourless) | m C2/c ? | 1504.8(2) 1092.1(6) 1608.0(4) | 134.74(1) | HgCCl | μC Cl | 213(4,2) 230.2(9,0) | 103(1) | C,Cl | 173(2 1) | 199 |
| $(HgCl)_2(EtCCHO)$ (white) | or $Pna2_1$ 4 | 1114.6(6) 1121.3(5) 657.3(3) | | HgCCl | C Cl | 213(2,4) 233(1) | 103(1) | C,Cl | 173(1 1) | 200 |
| $(HgCl)_2(CH_2)$ | or Pnma 4 | 713.7(4) 643.6(4) 1221.7(8) | | HgCCl | μC Cl | 208.1(18,42) 233.3(5,1) | 344.1(1) 111.6(3) | C,Cl | 177.9(5 1) | 201 |
| $Hg_2(Me)_2$(Mead-2H) (colourless) | tr | 870.1(6) 912.7(2) 1504.3(2) | 82.08(2) 88.86(4) 78.15(4) | HgNC | μN $C_{Me}$ | 205(2,2) not given | 123(1) | N,C | 177(1) | 202 |
| $[Hg_2(Ph)_2(OH)](BF_4) \cdot H_2O$ (white) | or Pnma 4 | 1109.6(4) 1704.8(2) 809.9(1) | | HgOC | μHO $C_{Ph}$ | 204 198 | 363.9 126 | O,C | not given | 203 |
| $Hg_2(Me)_2(C_6H_{10}S_2)$ (white) | m $P2_1/c$ 4 | 960.9(3) 1342.8(3) 1026.8(3) | 112.87(2) | HgCS $HgS_2C$ | C μS C S μS | 208(2) 236.3(4) 212(2) 236.7(4) 285.7(3) | 385.9(1) 100.6(1) | C,S S,S S,C μS,C | 177.1(5) 84.0(1) 167.8(5) 107.8(5) | 204 |
| Hg(2-Mepy)(Me)$(CF_3CO_2)$ (white) | tr $P\bar{1}$ 2 | 869.7(1) 1021.8(1) 747.1(1) | 104.60(1) 111.65(1) 90.04(1) | $HgO_2NC$ | N $C_{Me}$ μO | 214.8(9) 208.1(15) 273.7(9,69) | not given 112.5(3) 67.5(3) | N,C N,μO C,μO | 169.6(5) 87.1(3,1.5) 100.9(6 3.6) | 205 |
| $(PPh_4)[Hg(CF_3)_2Cl]$ (white) | m $P2_1/c$ 4 | 1078.3(2) 1402.3(6) 1871.9(5) | 111.42(3) | $HgC_2Cl_2$ | C μCl | 205.5(23,13) 283.0(4,7) | not given 92.3 87.7(2) | C,C | 160.5(8) | 206 |
| $[Hg(Me_2SC_5H_4)I_2]_2$ | tr $P\bar{1}$ 1 | 918.8(5) 727.2(2) 949.3(3) | 96.87(5) 101.66(4) 77.38(4) | $HgI_3C$ | I μI C | 270.6(1) 296.4(1,68) 219.6(14) | 389.1(1) 82.0 97.93(3) | I,μI I,C μI,C | 103.6(4,8) 133.6(4) 106.1(4,5.0) | 207 |
| $[Hg(Ph_3PC_5H_4)I_2]_2$ (yellow) | tr $P\bar{1}$ 1 | 1078.6(2) 1141.2(2) 1101.6(2) | 116.01(2) 104.93(2) 93.60(2) | $HgI_3C$ | I μI C | 268.1(1) 296.0(1,23) 229.2(8) | not given 86.23(2) 93.76(2) | I,μI I,C μI,C | 110.2(1,8) 131.5(2) 102.1(2,5.1) | 208 |
| $Hg_2(C_6H_4)(CF_3CO_2)_2$ (colourless) at 175K | m $P2_1/n$ 2 | 507.1(4) 1117.4(9) 1275.0(5) | 94.10(5) | HgOC | O C | 205.3(12) 208.1(16) | | O,C | 177.7(6) | 209 |
| $[Hg_2(MeOCS_2)_2(C_6H_4)] \cdot$ $CH_2Cl_2$ | tr $P\bar{1}$ 2 | 1063.7(2) 1202.2(2) 769.2(1) | 101.60(1) 98.75(1) 89.96(1) | HgCS | C S | 206(2,1) 239.0(5,11) | | C,S | 177.5(5,2.0) | 210 |
| $Hg_2(C_6H_4)Cl_2$(dmf) (colourless) | m $P2_1/c$ 4 | 927.5(6) 1608.6(6) 863.4(9) | 91.02(6) | HgOCCl | C Cl μO | 204.5(16,2) 234.0(5,6) 272.9(13,48) | 84.0(4) | C,Cl C,O Cl,O | 174.1(5 2.6) 100.3(5 7) 85.4(3 1.5) | 211 |
| $[Hg_2Me_2(MecyH)]NO_3$ (colourless) | or Pbca 8 | 1201.4(3) 1357.3(4) 1635.3(2) | | HgNC | N $C_{Me}$ | 213(2,2) 206(3,1) | 315.0 | N,C | 176(1,0) | 212 |
| $[Hg_2Ph_2(creatH)](NO_3)$ (colourless) | m $P2_1/c$ 4 | 1338.9(6) 760.5(3) 1792.4(8) | 93.32 | HgNC | N $C_{Ph}$ | 203(3,3) 203(2,1) | | N,C | 172(1 2) | 213 |

Table 2 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | *a* [pm] *b* [pm] *c* [pm] | $\alpha$ [°] $\beta$ [°] $\gamma$ [°] | Chromo-phore | Hg–L [pm] | | Hg–Hg [pm] Hg–L–Hg [°] | L–Hg–Hg [°] L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|---|
| $[Hg_2Me_2(tht)](NO_3)$ | m | 2520.0(10) | | HgNC | N | 205(2) | | N,C | 174.3(12) | 152 |
| (colourless) | C2/c | 702.9(6) | 128.99(3) | | $C_{Me}$ | 200(4) | | | | |
| | 8 | 1794.6(8) | | HgCS | $C_{Me}$ | 200(3) | | C,S | 176.0(10) | |
| | | | | | S | 236.8(7) | | | | |
| $[Hg_2Me_2(app)](NO_3) \cdot H_2O$ [c] | m | 1341.9(3) | | HgNC | | not given | 309.2(1) | not given | | 88 |
| (colourless) | $P2_1/c$ | 1367.6(6) | 90.68(2) | | | | | | | |
| | 8 | 1457.1(2) | | HgNC | | not given | 338.8(1) | not given | | |
| $[Hg_2Me_2(appH)](NO_3)_2$ | m | 376.1(1) | | HgNC | | not given | | | | 88 |
| (colourless) | $P2_1$ | 1793.3(3) | 90.07(2) | | | | | | | |
| | 2 | 1139.3(3) | | | | | | | | |
| $[Hg_2Me_2(6\text{-}Me_2adH)] \cdot$ | m | 1101.2(3) | | HgNC | N | 213(2,1) | 325.3(1) | N,C | 177.9(8 1.6) | 214 |
| $(NO_3)_2 \cdot H_2O$ | $P2_1/c$ | 2366.9(7) | 95.25(4) | | $C_{Me}$ | 206(2,1) | | | | |
| (white) | 4 | 674.8(4) | | | | | | | | |
| $[Hg_2Me_2(6\text{-}Me_2adH)](ClO_4)$ | m | 931.9(3) | | HgNC | N | 210(2,1) | 331.5(1) | N,C | 178.5(7 1.2) | 214 |
| (colourless) | $P2_1/c$ | 958.1(8) | 118.23(3) | | $C_{Me}$ | 206(2,2) | | | | |
| | 4 | 1962.4(8) | | | | | | | | |
| $[Hg_2Me_2(aad)](NO_3) \cdot H_2O$ | tr | 716.7(1) | 91.96(3) | HgNC | N | 211.3(6,20) | 347.6(1) | N,C | 176.0(4,8) | 86 |
| (colourless) | $P\bar{1}$ | 1385.4(3) | 102.01(3) | | $C_{Me}$ | 205(1,1) | | | | |
| | 2 | 674.8(3) | 90.02(2) | | | | | | | |
| $[Hg_2Me_2(Meaad)]ClO_4$ | m | 1136.3(3) | | HgNC | N | 211(2,2) | | N,C | 177.6(1) | 87 |
| | $P2_1/c$ | 1619.0(4) | 99.45(3) | | $C_{Me}$ | 213(3,2) | | | | |
| | 4 | 786.0(2) | | | | | | | | |
| $[Hg_2Me_2(9\text{-}Mead)]ClO_4$ | m | 1090.3(5) | | HgNC | N | 208(2,1) | | N,C | 175.5(7,1.7) | 215 |
| (colourless) | $P2_1/c$ | 1269(1) | 115.32(6) | | $C_{Me}$ | 207(1,0) | | | | 216 |
| | 4 | 1147.9(7) | | | | | | | | |
| $[Hg_2Me_2(ad)](NO_3) \cdot 2H_2O$ | m | 936.5(2) | | HgNC | N | 208(2,0) | | N,C | 177.0(8 6) | 215 |
| (colourless) | $P2_1/c$ | 2077.4(5) | 94.79(2) | | $C_{Me}$ | 205(2,2) | | | | 217 |
| | 4 | 766.1(2) | | | | | | | | |
| $[Hg_2Me_2(ad)](ClO_4) \cdot H_2O$ | tr | 818.9(3) | 69.93(1) | HgNC | N | 213(2,1) | | N,C | 176.8(9,1.1) | 218 |
| (colourless) | $P\bar{1}$ | 986.3(2) | 68.62(3) | | $C_{Me}$ | 209(2,2) | | | | |
| | 2 | 1072.6(2) | 73.66(3) | | | | | | | |
| $[Hg_2Me_2(ad)]EtOH$ [c] | m | 799.9(3) | | HgNC | N | 206.0(19,3) | | NC | 174.7(8,1.7) | 219 |
| (colourless) | $P2_1/c$ | 2405.6(8) | 90.56(2) | | $C_{Me}$ | 204.6(22,59) | | | | |
| | 8 | 1462.5(2) | | | | | | | | |
| $[Hg_2Me_2(ad)][Hg_3Me_3(ad)] \cdot$ | m | 1071.7(7) | | HgNC | N | 211(4,4) | | N,C | 178(1,1) | 220 |
| $(NO_3) \cdot 3H_2O$ | $P2_1/c$ | 2668.0(8) | 102.59(4) | | $C_{Me}$ | 208(3,1) | | | | |
| (colourless) | 4 | 1177.8(2) | | HgNC trimer | | see Table 3 | | | | |
| $[Hg_2Me_2(3\text{-}Mead)](NO_3)_2$ | m | 1182.9(3) | | HgNC | N | not given | | | | 84 |
| | $P2_1/c$ | 1184.6(4) | 99.96(4) | | $C_{Me}$ | not given | | | | |
| | 4 | 1211.6(4) | | | | | | | | |
| $[Hg_2Me_2(in)](ClO_4)$ | or | 880.6(8) | | HgNC | N | 208(2,3) | | N,C | 175(1,2) | 221 |
| | $P2_12_12_1$ | 1067(1) | | | $C_{Me}$ | 209(3,0) | | | | |
| | 4 | 2149(2) | | | | | | | | |
| $[Hg_2Me_2(7\text{-}Megu)]NO_3)$ | tr | 955.6(1) | 108.58(2) | HgNC | N | 205(3,1) | | N,C | 177(1,2) | 90 |
| (colourless) | $P\bar{1}$ | 1068.4(2) | 94.83(2) | | $C_{Me}$ | 200(4,3) | | | | |
| | 2 | 718.1(2) | 82.86(1) | | | | | | | |
| $Hg_2Me_2(ahx)$ | m | 1066.4(2) | | HgNC | N | 209.9(10,17) | | N,C | 174.6(5,4.0) | 91 |
| (colourless) | C2/c | 1493.5(3) | 105.08(2) | | $C_{Me}$ | 207.3(13,11) | | | | |
| | 8 | 1259.3(2) | | | | | | | | |
| $[Hg_2Me_2(all)] \cdot 2H_2O$ | m | 702.5(2) | | HgNC | N | 209(1,1) | | N,C | 172.9(6,2.6) | 98 |
| (colourless) | $P2_1/n$ | 1122.0(2) | 92.86(3) | | $C_{Me}$ | 211(2,1) | | | | |
| | 4 | 1511.9(3) | | | | | | | | |
| $[Hg_2Me_2(all)\} \cdot$ | or | 3185.4(2) | | HgNC | N | 212(3,2) | | N,C | 169(1,2) | 98 |
| $\{HgMe(Mall)] \cdot NO_3$ | $Pna2_1$ | 1037.1(1) | | | $C_{Me}$ | 212(4,1) | | | | |
| (colourless) | 4 | 652.5(1) | | HgNC monomer | N | 212(1) | | N,C | 165(2) | |
| | | | | | C | 207(4) | | | | |
| $Hg_2\{Me_3C_6H_2N(CH_2)_2\}_2Cl_2$ | tr | 1116.8(7) | 70.46(5) | HgCCl | C | 207(4,3) | | C,Cl | 177(1,2) | 222 |
| (colourless) | $P\bar{1}$ | 1028.4(7) | 68.36(2) | | Cl | 235(1,1) | | | | |
| | 2 | 853.3(4) | 67.18(6) | | | | | | | |

Table 2 (continued)

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | Hg–Hg [pm] Hg–L–Hg [°] | L–Hg–Hg [°] L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|---|
| $Hg_2Me_2(tp)$ | tr | 550.8(4) | 77.70(4) | HgNC | N | 210(3,3) | | N,C | 176(1,3) | 55 |
| | $P\bar{1}$ | 949.7(5) | 87.62(6) | | $C_{Me}$ | 204(3,1) | | | | |
| | 2 | 1406.4(8) | 80.83(5) | | | | | | | |
| $Hg_2Me_2(pen)]$ | or | 1969.5(23) | | HgNC | $C_{Me}$ | 207(4) | | N,C | 170(1) | 157 |
| (colourless) | Pbcn | 1047.8(13) | | | N | 213(3) | | | | |
| | 8 | 1197.1(26) | | HgSC | $C_{Me}$ | 204 | | C,S | 176(1) | |
| | | | | | S | 235(1) | | | | |
| $Hg_2Me_2(C_2N_2S_3)$ | tg | 2160.0(6) | | HgCS | $C_{Me}$ | 204(6,4) | | C,S | 178(1,1) | 223 |
| (colourless) | $I4_1/a$ | – | | | S | 239(1,2) | | | | |
| | 16 | 947.0(4) | | | | | | | | |
| $[Hg_2(Me)_2(glygly)]ClO_4$ | m | 640.7(4) | | HgOC | O | 207(2) | | O,C | 177(1) | 76 |
| (colourless) | $P2_1/c$ | 2443.9(6) | 93.82(4) | | $C_{Me}$ | 209(3) | | | | |
| | 4 | 846.1(2) | | HgNC | N | 214(3) | | N,C | 176(1) | |
| | | | | | $C_{Me}$ | 209(3) | | | | |
| Hg(Me)(bta) | m | 961.8(2) | | $HgN_2C$ | N | 207.4(4) | | N,N | 95.1(1) | 224 |
| (colourless) | $P2_1/n$ | 1813.4(1) | 90.00(2) | | N | 270.7(4) | | N,C | 93.6(2) | |
| | 4 | 456.3(2) | | | $C_{Me}$ | 207.2(7) | | | 171.2(2) | |
| $[Hg(C_{10}H_6)]_2$ | m | 1011.6(1) | | $HgC_2$ | C | 209.6(5,4) | 279.1(1) | C,C | 173.3(6) | 225 |
| (colourless) | $P2_1/n$ | 554.1(1) | 94.12(1) | | | | | | | |
| | 2 | 1311.2(1) | | | | | | | | |
| $[Hg(C_{10}H_6)Cl]_2 \cdot (dmso)$ | m | 718.0(1) | | HgCCl | C | 206.4(8,8) | 310.2(1) | C,Cl | 174.3(2,2.1) | 225 |
| (colourless) | $P2_1/n$ | 935.4(1) | 92.88(1) | | Cl | 233.7(2,3) | | | | |
| | 4 | 2251.3(4) | | | | | | | | |
| $Hg_2\{(CH_2)_2O(CH_2)_2\}_2$ | m | 1927.3(8) | | $HgC_2$ | C | 213(6,1) | 355.0(3) | C,C | 176.0(1.9) | 226 |
| (colourless) | C2/c | 446.1(2) | 120.4(4) | | | | | | | |
| | 4 | 1466.7(8) | | | | | | | | |
| [Hg(pei)]$_2$ | tr | 903.6(2) | 87.73(2) | HgNC | N | 215.1(11) | | N,C | 174.9(6) | 227 |
| (colourless) | $P\bar{1}$ | 1081.0(3) | 73.06(2) | | C | 206.1(14) | | | | |
| | 1 | 1448.0(3) | 88.30(2) | | | | | | | |
| $Hg(C_{10}H_{21}NO_2P)(NO_3)$ | tr | 963.1(3) | 67.31(3) | $HgO_3C$ | C | 211.0(10) | 410.9(1) | O,O | 49.8(3) | 228 |
| (colourless) at 233K | $P\bar{1}$ | 965.6(3) | 77.22(3) | | O | 249.4(6,11) | | O,C | 109.2(3,2.2) | |
| | 2 | 986.6(3) | 77.24(3) | | $O_2NO$ | 213.4(11) | | | 164.4(3) | |
| $[Hg(C_{18}H_{12})]_2$ | m | 1731.5(3) | | $HgC_2$ | C | 208.9(13,6) | | C,C | 184.5(4,1) | 229 |
| (colourless) | $P2_1/n$ | 1657.6(2) | 114.60(4) | | | | | | | |
| | 4 | 1054.5(6) | | | | | | | | |
| $Hg(hmb)(CF_3CO_2)_2$ | tr | 1233.8(0) | 79.86(6) | $HgO_4C_2$ | O | not given | | | 230 | |
| (pale yellow) at 108K | $P\bar{1}$ | 998.4(0) | 107.10(5) | | C | 257(–,1) | | | | |
| | 1 | 890.0(0) | 116.29(6) | | | | | | | |

[a] Where more than one chemically equivalent distance or angle is present, the mean value is tabulated. The first number in parenthesis is the e.s.d., and the second is the maximum deviation from the mean.

[b] The chemical identity of the coordinated atom or ligand is specified in these columns.

[c] There are two crystallographically independent molecules.

[20] and another containing five [123]. In all cases the molecules differ by degree of distortion. The coexistence of two or more such molecules within the same crystal is typical of the general class of distortion isomerism [194].

## 3. Dimeric mercury compounds

The structural data for these derivatives is shown in Table 2. There are fifty examples of which only one [195] has the mercury atom in the oxidation state of +1 rather than +2. This derivative [195] has a central $Hg_2^{+2}$ unit (Hg–Hg distance of 251.5 (−21) pm) which is asymmetrically complexed by hexamethylbenzene. The distorted $AlCl_4$ tetrahedron completes a molecular $[Hg(Me_6C_6)]_2[AlCl_4]_2$ unit. The Hg–Hg distance is comparable with those found in the dimeric Mercury(I) coordination compounds of 251.6 pm [3].

There are several types of bridging in these complexes between the mostly digonal Hg(II) atoms. In nine examples [196–204] a single atom of the ligand serves as a bridge, carbon [196–201], nitrogen [202], oxygen [203] and sulphur [204]. There appears to be a relationship between the Hg–Hg distance and the Hg–L–Hg bond angle in which the former elongates as the latter opens. For example, 321.3(7) pm and 98.9(5)° [196]; 344.1(1) pm and 111.6(3)° [201]; 363.9 pm and 126°

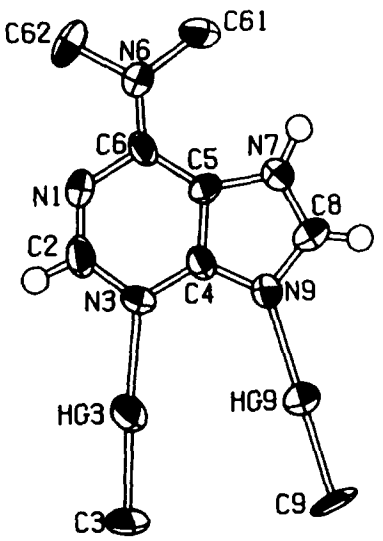


Fig. 1. Structure of $[Hg_2Me_2(6\text{-}Me_2adH)](NO_3)_2 \cdot H_2O$ [214].

[203]. However, the derivative $Hg_2Me_2(C_6H_{10}S_2)$ is an exception to this trend [204] with values of 385.9(1) pm and 100.6(1)°. Two possible reasons for this discrepancy are linked to the dimercaptocyclohexane ligand which serves as a bridge between the two Hg(II) atoms. The Hg–S distances are found to be very unsymmetrical at 236.3(4) and 285.7(3) pm, respectively, and the second S atom is coordinated to only one of the Hg(II) atoms.

There is one example of a double oxygen bridge using a pair of oxygen donors [206], one example of double chlorine bridging [206] and two examples of double iodine bridging [207,208], resulting in a geometry of distorted edge-shared bitetrahedra. In another three examples [209–211] a bidentate $C_6H_4$ ligand serves as a two atom bridge. In another example, dimethylformamide (via O atom) serves as additional weak bridging between two Hg(II) atoms.

By far the most common geometry observed in the digonal dimeric organomercury(II) structures is one in which both Hg(II) atoms sit on a N-heterocyclic ligand (usually a purine base) and the second coordination site is occupied by a methyl group. The structure of colourless $[Hg_2Me_2(6\text{-}Me_2adH)](NO_3)_2 \cdot H_2O$ [214] is shown in Fig. 1 as an example of this series.

In colourless $[HgMe(bta)]_2$ [224] two bidentate benzotriazolate ligands serve as two atom bridges with very asymmetrical Hg–N distance of 207.4 and 270.7(4) pm. Methyl groups complete the trigonal geometry about the Hg(II) atoms with the chromophore $HgN_2C$.

The structure of colourless $[Hg(C_{10}H_6)]_2$ [225] is shown in Fig. 2. The two bridging 1,8-naphthalenediyl ligands bring the mercury(II) atoms to within 279.7(1) pm with C–Hg–C angles of 173.3(6)°. This represent the shortest Hg(II)–Hg(II) distance found in the dimeric Hg(II) complexes.

There are some examples of five atom bridges via two bidentate ligands [226–228], and one example of a six atom bridge [229]. One other example [230] finds two Hg(II) atoms bridged by four $CF_3COO^-$ groups in a syn–syn arrangement. Each hexamethylbenzene molecule is $\eta^5$-bonded to the Hg(II) atoms in the apical site.

The number of examples of the various geometries decreases in the order: digonal (majority) ≫ tetrahedral > trigonal > hexacoordinated (one only). The mean Hg–L distance increases with coordination number and with the denticity of the ligand. The mean Hg–C(Me) distance of 206 pm is similar to that found in the

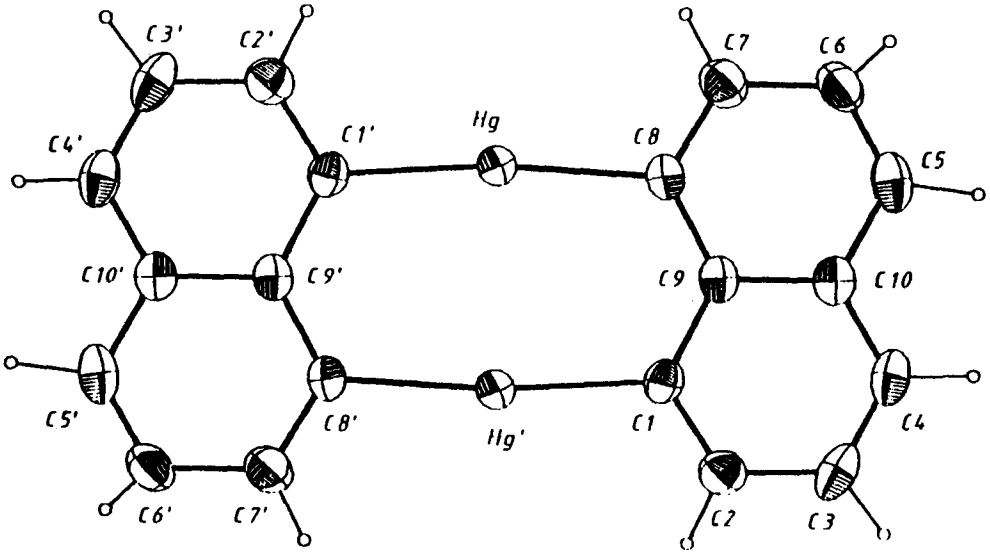


Fig. 2. Structure of $[Hg(C_{10}H_6)]_2$ [225].

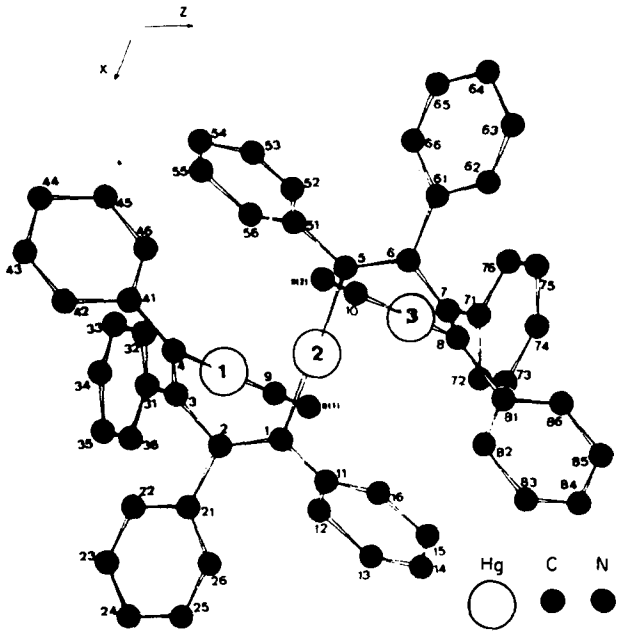


Fig. 3. Structure of $[\{Hg(C_{28}H_{20})(CN)\}_2Hg]$ [244].

monomeric organomercury derivatives (207 pm). The Hg(II)–Hg(II) distance mostly lies within 309.2 to 410.9 pm, with the exception of one case [225] which has a value of 279.7(7) pm. However, it should be noted that for several examples the relevant information was not available.

While the majority of the compounds are colourless, there are examples of white (7) and yellow (2).

Two crystallographically independent molecules in two cases [88,218] represent examples of distortion isomerism.

## 4. Trimeric mercury compounds

The structural data for these derivatives can be found in Table 3. There are twenty six species, all of which have mercury in the oxidation state +2. There are several examples where three crystallographically equivalent $(HgL)_3$ units are symmetrically linked by a triply bridging atom or ligand, for example: $(HgMe)_3$ by O atoms [231]; $(HgMe)_3$ by S atoms [232–234]; $(HgX)_3$ (X = Cl, $NO_3$, Br) by carbon-donor ligands; $[Hg(penH)]_3$ by a Cl atom. The resulting geometry is a more or less flattened trigonal bipyramid. The mean Hg–$\mu_3$L bond distance increases in the order: 207 pm (Cl) < 208 pm (O) < 237 pm (Cl) < 239 pm (S). The mean Hg–Hg distance of 340 pm is too large to indicate bonding, and the Hg–$\mu_3$L–Hg bond angles range from 99 to 120°.

The structure of two colourless isomeric forms of $[Hg(Cl_2H_8)]_3$ [237,238] has a fifteen-membered ring where three mercury(II) atoms are bridged by 2,2′-biphenylene groups $(-Hg-C-C-C-C-)_3$. The structure of another four examples [239–242] has a nine-membered ring in which three mercury(II) atoms are bridged by $\eta^2$-organic groups $(-Hg-C-C-)_3$. In another [243] a twelve membered ring is built up from three Hg(II) atoms and a 2,2,6,6-tetramethyl-3,5-hexadione group $(-Hg-C-C-N-)_3$. There are digonal coordinated mercury atoms with mean Hg–C bond distance of 210 pm and a mean value of the C–Hg–C bond angle of 177°. The mean Hg–Hg distance of 353 pm is somewhat larger than that found in the previous series. Two pairs of isomers, $Hg_3(Cl_2H_8)_3$ [237,238] and $Hg_3(o\text{-phenylene})_3$ [240,241], represent examples of distortion isomerism.

The structure of $[\{Hg(C_{28}H_{20})(CN)\}_2Hg]$ [244] is shown in Fig. 3. The three mercury atoms are linked by two tetraphenylbutadienyl groups, with Hg–Hg distance of 401.1 pm. The molecule is approximately centrosymmetrical with the centre of symmetry on Hg(2).

In the remaining eleven examples [86,88,90,94,202, 220,245–248] all three mercury(II) atoms are sitting on N-heterocyclic ligands (mostly purine base) and the digonal coordination is complete by a methyl group on each Hg(II) atom. The mean Hg–N and Hg–C(Me) distances of 209 and 207 pm, respectively, together with

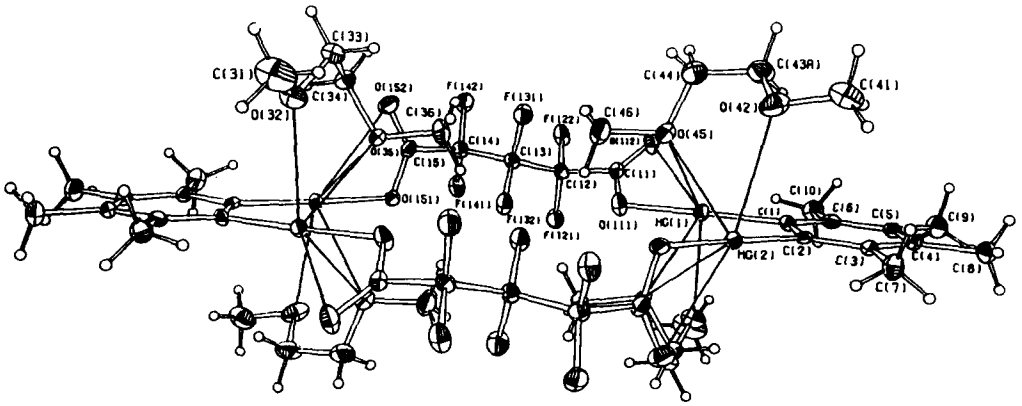

Fig. 4. $[Hg_2\{OOC(CF_2)_3COO\}(C_6Me_4)_2]_2$ [256].

Table 3
Crystallographic and structural data for trimeric organomercury(II) compounds [a]

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | Hg–Hg [pm] Hg–L–Hg [°] | L–Hg–Hg [°] L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|---|
| $[Hg_3(Me)_3O](NO_3)$ [c] | m | 1240.4 | | HgOC | $\mu_3O$ [b] | 208 | 344 | O,C [b] | 175 | 231 |
| (colourless) | $P2_1/c$ | 2002.9 | 115.97 | | $C_{Me}$ | 215 | 115 | | | |
| | 12 | 1404.7 | | | | | | | | |
| $[Hg_3Cl_3(CCOOH)]\cdot$ | m | 1242.7(6) | | HgCCl | $\mu_3C$ | 206(7,1) | 339.2(5,90) | C,Cl | 176(2,3) | 232 |
| (dmso) | $P2_1/c$ | 1035.1(5) | 115.4(1) | | Cl | 233(2,2) | 111(3,4) | | | |
| (colourless) | 4 | 1140(4) | | | | | | | | |
| $2[Hg_3(NO_3)_3\cdot$ | m | 1155.5(6) | | HgOC | O | 214(4,1) | 335.9(4,32) | O,C | 175(2,3) | 233 |
| $(CCOOH)]HNO_3$ [d] | $P2_1/c$ | 767.0(3) | 90.23(1) | | $\mu_3C$ | 207(5,1) | 109(2,2) | | | |
| (colourless) | 4 | 2700.4(9) | | HgOC | O | 209(5,6) | 225.1(4,95) | O,C | 175(2,2) | |
| | | | | | $\mu_3C$ | 207(5,2) | 108(2,5) | | | |
| $[Hg_3Cl_3(CCHO)]\cdot$ | m | 1276(2) | | HgCCl | $\mu_3C$ | 208(3,2) | 339.8(4,137) | C,Cl | 173(1,3) | 234 |
| (dmso) | $P2_1/c$ | 1012(1) | 115.3(1) | | Cl | 232.2(8,8) | 110(2,7) | | | |
| (colourless) | 4 | 1139(1) | | | | | | | | |
| $[Hg_3Br_3(CCHO)]\cdot$ | m | 1130(1) | | HgCBr | $\mu_3C$ | 204(5,1) | 341.2(2,136) | C,Br | 174(2,6) | 234 |
| (dmso) | $P2_1/c$ | 1038(1) | 95.7(1) | | Br | 243.5(5,7) | 113(3,6) | | | |
| (white) | 4 | 1141(1) | | | | | | | | |
| $2[\mu_3\text{-}Cl\{Hg(penH)\}_3]\cdot$ | c | 1867.9(5) | | HgClS | $\mu_3Cl$ | 237(1) | | Cl,S | 167.2(9) | 235 |
| $Cl_3(H_3O)_2(H_2O\cdot Cl)_3$ | $P4_132$ | | | | S | 232(2) | 98.5(9) | | | |
| (colourless) | 4 | | | | | | | | | |
| $[Hg_3Me_3S]\cdot ClO_4$ | tg | 964.2(3) | | HgCS | $C_{Me}$ | 207(4,3) | | C,S | 175.5(12,4.0) | 236 |
| | $P4_1$ | – | | | $\mu_3S$ | 239.6(10,13) | 100.0(4,6.5) | | | |
| | 4 | 1280.8(6) | | | | | | | | |
| $[Hg(C_{12}H_8)]_3$ [d] | tr | 1198.3(5) | 82.13(4) | $HgC_2$ | C | 211.6(16,29) | 341.9(1,22) | C,C | 177.2(6,6) | 237 |
| (colourless) | $P\bar{1}$ | 1294.7(6) | 80.28(4) | | | | | | | |
| | 4 | 2006.8(8) | 77.22(4) | $HgC_2$ | C | 212.4(16,11) | 342.2(1,28) | C,C | 176.8(7,1.8) | |
| $[Hg(C_{12}H_8)]_3$ | or | 2685.7(16) | | $HgC_2$ | C | 210(2,4) | 352.8(2,109) | C,C | 177.8(9,1.5) | 238 |
| (colourless) | Pbca | 1145.8(6) | | | | | | | | |
| | 8 | 1911.0(44) | | | | | | | | |
| $[Hg_3(o\text{-}C_6F_4)_3]\cdot$ | m | 1122 | | $HgC_2$ | C | 209(3,2) | 358.6(2,8) | C,C | 176(1,0.7) | 239 |
| $(4\text{-}PhC_6H_4N)$ | $P2_1/n$ | 2731(2) | 105.2(1) | | | | | | | |
| (colourless) | 4 | 953(1) | | | | | | | | |
| $[Hg(o\text{-phenylene})]_3$ | m | 1051.2(3) | | $HgC_2$ | C | 208(3,8) | 362(0,21) | C,C | 176.4(1.2,7) | 240 |
| (colourless) | $P2_1/c$ | 811.6(2) | 106.92(3) | | | | | | | |
| | 4 | 1912.8(7) | | | | | | | | |
| $[Hg(o\text{-phenylene})]_3$ | or | 556(2) | | $HgC_2$ | C | 210(5,3) | 362(–,35) | C,C | 177.7(1.8,1.2) | 241 |
| (colourless) | $P2_12_12_1$ | 2336(2) | | | | | | | | |
| | 4 | 1224(2) | | | | | | | | |
| $(PPh_4)[Hg_3(o\text{-}C_6F_4)_3]\cdot$ | m | 1532.6(3) | | $HgC_2$ | not given | | | | | 242 |
| $BrCH_2Br_2$ [c] | $P2_1/n$ | 2677.2(5) | 95.10(5) | | | | | | | |
| at 153K | 12 | 3158.5(6) | | | | | | | | |
| $[Hg(C_{11}H_{20}NO)]_3\cdot$ | m | 1578.0(8) | | HgNC | N | 208.3(10,12) | | N,C | 174.1(–,2.3) | 243 |
| $(ClO_4)_3\cdot C_4H_8O_2$ | $P2_1/n$ | 1698.9(6) | 100.23(3) | | C | 210.4(12,8) | | | | |
| (colourless) | 4 | 1961.4(6) | | | | | | | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $[\{Hg(C_{28}H_{20})(CN)\}_2Hg]$ | m | 2389(2) | | $HgC_2$ | C | 218(4,1) | 401.1(2,26) | C,C | 177(1) | 244 |
| | $P2_1/c$ | 847(3) | 114.4(5) | | | | | | | |
| | 4 | 2791(2) | | $HgC_2$ | C | 209(4,6) | | C,C | 177(2,2) | |
| | | | | (×2) | NC | 204(4,4) | | | | |
| $[Hg_3Me_3(ad2H)]\frac{1}{2}H_2O$ | m | 2080.9(7) | | HgNC | N | 205(3) | | N,C | 178(1) | 202 |
| (colourless) | C2/c | 726.3(1) | 104.91(4) | | $C_{Me}$ | 211(4) | | | | 245 |
| | 8 | 1878.8(1) | | HgNC | $\mu$N | 204(3,4) | | N,C | 177(1,2) | |
| | | | | (×2) | $C_{Me}$ | 206(4,3) | 128(1) | | | |
| $[Hg_3Me_3(Mecy2H)]\cdot$ | or | 717.5(5) | | HgNC | N | 209(5) | 305.7(3) | N,C | 176(3) | 202 |
| $(NO_3)$ | Pbca | 1798(1) | | | $C_{Me}$ | not given | | | | |
| (colourless) | ? | 2343.4(9) | | HgMC | $\mu$N | 209(5,11) | | N,C | 174(3,2) | |
| | | | | (×2) | $C_{Me}$ | not given | | | | |
| $[Hg_3Me_3(5aw)](NO_3)$ | m | 696.1(1) | | HgNC | N | not given | | | | 94 |
| (colourless) | $P2_1/c$ | 2130.7(4) | 99.58(1) | | $C_{Me}$ | not given | | | | |
| | 8 | 1872.8(5) | | | | | | | | |
| $[Hg_3Me_3(7\text{-}MeguH_{-1})]\cdot$ | tr | 1110.1(3) | 90.51(5) | HgNC | N | 209(2,2) | | N,C | 176(1,3) | 90 |
| | $P\bar{1}$ | 1574.6(5) | 91.62(4) | | $C_{Me}$ | 205(3,7) | | | | |
| $(NO_3)$ [d] | 4 | 1104.2(5) | 73.12(4) | HgNC | N | 207(2,1) | | N,C | 176(1,1) | |
| (colourless) | | | | | $C_{Me}$ | 205(3,5) | | | | |
| $[Hg_3(Me)_3(ad)](NO_3)_2$ | m | 2093.9(7) | | HgNC | N | 211(2,2) | | N,C | 175(1,3) | 246 |
| | C2/c | 2397.6(3) | 94.29(4) | | $C_{Me}$ | 209(2,2) | | | | |
| (colourless) | 8 | 707.3(6) | | | | | | | | |
| $[Hg_3Me_3(ad)](NO_3)_2\cdot H_2O$ | tr | 701.7(3) | 64.91(3) | HgNC | N | 211(2,1) | | N,C | 176(1,2) | 220 |
| | $P\bar{1}$ | 1134.5(6) | 87.50(3) | | $C_{Me}$ | 205(4,3) | | | | |
| (colourless) | 2 | 1272.2(3) | 89.59(4) | | | | | | | |
| $[Hg_3Me_3(ad)](ClO_4)_2$ [d] | tr | 630.4(7) | 85.76(2) | HgNC | N | 208(3) | 329.0(2,20) | N,C | 177(1) | 247 |
| | $P\bar{1}$ | 1192.5(4) | 89.78(5) | | $C_{Me}$ | 205(4) | | | | |
| (colourless) | 4 | 2594.6(4) | 83.57(6) | | | | | | | |
| $[Hg_3Me_3(ad)]\cdot$ | m | 1071.7(7) | | HgNC | N | 210(2,2) | | N,C | 177(1,1) | 220 |
| | $P2_1/c$ | 2668.0(8) | 102.59(4) | (×3) | C | 211(4,3) | | | | |
| $[Hg_2Me_2(ad)](NO_3)\cdot 3H_2O$ | 4 | 1177.8(2) | | HgNC | N | 211(4,4) | | N,C | 178(1,1) | |
| | | | | (dimer) | $C_{Me}$ | 208(3,1) | | | | |
| (colourless) | | | | | | | | | | |
| $[Hg_3(Me)_3(xanH)]NO_3\cdot$ | tr | 731.9(3) | 96.06(5) | HgNC | N | 208(2,5) | | N,C | 176.6(9,2.9) | 248 |
| | $P\bar{1}$ | 946.6(8) | 95.00(3) | | $C_{Me}$ | 207(3,4) | | | | |
| $H_2O$ | 2 | 1200.4(3) | 97.69(5) | | | | | | | |
| (white) | | | | | | | | | | |
| $[(HgMe)_3(app)](NO_3)_2$ | m | 1724.1(4) | | HgNC | *not given* | | | | | 88 |
| | $P2_1/c$ | 2829.8(5) | 100.47(2) | | | | | | | |
| (colourless) | 8 | 788.4(3) | | | | | | | | |
| $[Hg_3(Me)_3(aadH_{-1})]\cdot$ | m | 2941.8(3) | | HgNC | N | 213(1,4) | 347.4(1) | N,C | 174.1(5,4.9) | 86 |
| | C2/c | 1261.7(4) | 96.06(1) | | $C_{Me}$ | 208(2,3) | | | | |
| $(NO_3)$ | 8 | 805.7(1) | | | | | | | | |
| (colourless) | | | | | | | | | | |

[a] Where more than one chemically equivalent distance or angle is present, the mean value is tabulated. The first number in parenthesis is the e.s.d., and the second is the maximum deviation from the mean.

[b] The chemical identity of the coordinated atom or ligand is specified in these columns.

[c] There are three crystallographically independent molecules.

[d] There are two crystallographically independent molecules.

Table 4
Crystallographic and structural data for oligo- and polymeric organomercury(II) compounds [a]

| COMPOUND (colour) | Crys.cl Sp.Gr. Z | a [pm] b [pm] c [pm] | α [°] β [°] γ [°] | Chromo-phore | Hg–L [pm] | | Hg–Hg [pm] Hg–L–Hg [°] | L–Hg–Hg [°] L–Hg–L [°] | | Ref |
|---|---|---|---|---|---|---|---|---|---|---|
| $[\{Hg(CF_3CO_2)\}_4\cdot$ | tg | 1286.6(4) | | HgOC | O | 206.5(11) | 334.9(−,44) | O,C | 175.2(3) | 249 |
| $(\mu_4\text{-C})$ | $P4_2/n$ | – | | | $\mu_4$C | 204.2(4) | 110.2(1,2.2) | | | |
| (colourless) | 2 | 611.1(2) | | | | | | | | |
| $[\{Hg(CN)\}_4\cdot$ | m | 852.0(5) | | $HgC_2$ | NC | 204(10,2) | 335.2(4,72) | C,C | 177(3,2) | 250 |
| $(\mu_4\text{-C})]\cdot H_2O$ | $P2_1/n$ | 1362.2(8) | 92.48(5) | | $\mu_4$C | 206(5,6) | 109(2,5) | | | |
| (colourless) | 4 | 1078.3(6) | | | | | | | | |
| $\{\{Hg(MeCO_2)\}_4\cdot$ | m | 726.2(7) | | HgOC | O | 207(2,2) | 335.5(−,104) | O,C | 176.7(8,2.2) | 251 |
| $(\mu_4\text{-C})]\cdot 2H_2O$ | $P2_1/c$ | 2181.6(12) | 98.8(8) | | $\mu_4$C | 206(2,1) | 109.5(10,4.9) | | | |
| (colourless) | 4 | 1200.3(8) | | | | | | | | |
| $[(HgCl)_4(\mu_4\text{-C})]\cdot$ | m | 1854(1) | | HgCCl | $\mu_4$C | 207.0(27,56) | 338.0(2,69) | C,Cl | 174.3(3,4.0) | 252 |
| dmso | $P2_1/n$ | 727.3(5) | 94.82(3) | | Cl | 233.2(9,18) | 109.5(4,2.2) | | | |
| (colourless) | 4 | 1049.1(6) | | | | | | | | |
| $Li[\{Hg(C_2H_{10}B_{10})\}_4\cdot$ | tg | 1432.33(8) | | $HgC_2Cl$ | C | 209.3(13,13) | 412.9(1) | C,C | 162.0(3) | 253 |
| $(\mu_4\text{-Cl})]$ | P4/mcc | – | | | $\mu_4$Cl | 294.4(2) | | C,Cl | ca 90. | |
| | 2 | 1126.40(7) | | | | | | | | |
| $(PPh_4)[\{Hg_2\cdot$ | tr | 1335.1(8) | 108.43(6) | $HgCl_2$ | Cl | 232.6(4,38) | $d_1$ | $\mu_4$Cl,Cl | 90.9(1,4.6) | 254 |
| $(o\text{-}C_6H_4)Cl_2\}_2\cdot$ | $P\bar{1}$ | 1642.0(8) | 94.48(6) | | $\mu_4$Cl | 307.6(4,259) | | $\mu_4$Cl,C | 101.3(4,7.7) | |
| $(\mu_4\text{-Cl})]\cdot\frac{1}{2}CH_2Cl_2$ [c] | 4 | 2020.0(17) | 105.41(6) | | C | 205.6(14,45) | | Cl,C | 167.3(4) | |
| (colourless) | | | | $HgCl_2$ | Cl | 233.4(4,24) | $d_2$ | $\mu_4$Cl,Cl | 91.3(4,5.3) | |
| | | | | | $\mu_4$Cl | 301.7(4,107) | | $\mu_4$Cl | 96.5(4,1.6) | |
| | | | | | C | 206.2(13,12) | | Cl,C | 172.0(4,4.9) | |
| $[Hg_2(OOC(CF_3)_3\cdot$ | or | 1226.1(9) | | HgOC | not given | | | O,C | 174(2) | 255 |
| $COO)(C_6H_4)]_2\cdot$dmf | Pnnm | 2411.6(14) | | | | | | | | |
| (colourless) | ? | 1695.4(2) | | | | | | | | |
| $[Hg_2\{OOC(CF_2)_3\cdot$ | tr | 914.1(3) | 97.34(4) | HgOC | O | 209.3(6,1) | 344.4 | O,C | 177.5(3,1.0) | 256 |
| $COO\}(C_6Me_4)_2]_2\cdot$ | $P\bar{1}$ | 1120.3(4) | 96.70(4) | | C | 205.2(8,6) | | | | |
| (dme) | 1 | 1456.3(11) | 97.45(3) | | | | | | | |
| (colourless) | | | | | | | | | | |
| $[Hg_4Me_4(ad2H)]NO_3$ | m | 1445.8(2) | | HgNC | N | 212(4,2) | | N,C | 177(2,2) | 245 |
| | $P2_1/c$ | 747.8(1) | 126.34(2) | (×2) | C | 206(6,2) | | | | |
| | 4 | 2017.4(5) | | HgNC | $\mu$N | 209(4,4) | | N,C | 177(2,1) | |
| | | | | (×2) | $C_{Me}$ | 211(5,1) | 123(2) | | | |
| $[Hg_4Me_4(appH_{-1})]\cdot$ | or | 752.4(1) | | HgNC | not given | | | | | 88 |
| $(NO_3)_2\cdot 2H_2O$ | $Pna2_1$ | 1569.8(2) | | | | | | | | |
| (colourless) | 4 | 1801.5(1) | | | | | | | | |
| $[Hg_4Me_4(app)]\cdot$ | or | 2853.6(5) | | HgNC | not given | | | | | 88 |
| $(NO_3)_3\cdot H_2O$ | Pccn | 2105.6(4) | | | | | | | | |
| (colourless) | 8 | 762.4(2) | | | | | | | | |
| $[Hg_4Me_4(xan)]NO_3$ [c] | m | 2455(2) | | HgNC | N | 207(4,5) | 335.3(4) | N,C | 175(2,5) | 248 |
| (white) | C2/c | 1701.6(4) | 110.26(5) | | $C_{Me}$ | 206(7,3) | 363.9(4) | | | |
| | 16 | 1910.8(9) | | | | | | | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $(Hg(C)(CF_3)_2)_5 \cdot$ | m | 1651.1(6) | | $HgC_4$ | $\mu C$ | 211(3,4) | 333.3(2,21) | not given | | 257 |
| $(py)_2 \cdot 2H_2O$ | $P2_1/c$ | 1403.8(4) | 91.18(3) | | $F_3C$ | 211 | 105(1,5) | | | |
| (colourless) | 4 | 1825.6(5) | | | | | | | | |
| $Hg_3(O)(CCHO)NO_3 \cdot$ | tg | 1075.5(3) | | HgOC | $\mu_3O$ | 205(2,1) | not given | O,C | 176.4(9,1) | 258 |
| $H_2O$ (colourless) | $P4_2/n$ | – | | | $\mu_3C$ | 207(2,1) | e | | | |
| | 4 | 676.3(2) | | | | | | | | |
| $2[Hg_3(O)(CCHO)] \cdot$ | or | 685.3(2) | | HgOC | $\mu_3O$ | 217(−,1) | not given | O,C | 178.3(−,1.0) | 259 |
| $(NO_3)_2 \cdot HNO_3$ [c] | $Cmc2_1$ | 1204.3(3) | | | $\mu_3O$ | 208(−,3) | $f_1$ | | | |
| (colourless) | 4 | 1850.8(12) | | HgOC | $\mu O$ | 215(−,2) | not given | O,C | 175.8(−,9) | |
| | | | | | $\mu C$ | 211(−,1) | $f_2$ | | | |
| $[HOHg_2(NO_3Hg) \cdot$ | m | 721.5 | | HgOC | $\mu O$ | 208(2,4) | not given | O,C | 173.7(9,2) | 259 |
| $(CCHO)](NO_3)$ | $P2_1/c$ | 1164.3 | 105.00(3) | | $\mu_3C$ | 206(2,2) | g | | | |
| (colourless) | 4 | 1082.1 | | HgOC | O | 218(3) | | O,C | 170.9(9) | |
| | | | | | $\mu_3C$ | 204(3) | | | | |
| $[Hg(H_2OHg)(NO_3Hg) \cdot$ | m | 923.3(9) | | HgOC | O | 213(3,4) | 334.4(3,177) | O,C | 173(1,2) | 233 |
| $CCOO](NO_3)$ | $P2_1/c$ | 1070.6(4) | 104.24(4) | | $\mu_3C$ | 208(3,3) | 107(1,10) | | | |
| (colourless) | 4 | 960.8(4) | | | | | | | | |
| $[Hg_7(OH)_2O_4] \cdot$ | or | 729.5 | | $HgO_x$ | O | 204(−,2) | not given | | | 231 |
| $(ClO_4)_4 \cdot H_2O$ | Pnma | 2057.6 | | | $\mu O$ | 273(−,18) | | | | |
| (pale yellow) | 8 | 1424.2 | | | | | | | | |

[a] Where more than one chemically equivalent distance or angle is present, the mean value is tabulated. The first number in parenthesis is the e.s.d., and the second is the maximum deviation from the mean.

[b] The chemical identity of the coordinated atom or ligand is specified in these columns.

[c] There are two crystallographically independent molecules.

[d1] Hg–Cl–Hg = 81.9(1,10.9) and 157.7(1)°.

[d2] Hg–Cl–Hg = 81.1(1,11.6) and 159.0(1)°.

[e] Hg–O–Hg = 115.7(6,3.1)°, Hg–C–Hg = 109.1(2,2.1)°.

[f1] Hg–O–Hg = 108.1(−,4)°; Hg–C–Hg = 110.4(−,3)°.

[f2] Hg–O–Hg = 109.3(−,1.0)°; Hg–C–Hg = 107.1(−,1.3)°.

[g] Hg–O–Hg = 121(2)°; Hg–C–Hg = 110(1,2)°.

the mean value of 176° for the N–Hg–C angle, are exactly the same as those found in the dimeric species despite the difference in denticity of the N-heterocyclic ligand. This is quite unique in organometallic chemistry.

As in the other series most of the compounds are colourless, with just a few white ones. There are two crystallographically independent molecules found in several cases [90,233,237,247], with one example with three such molecules [231], all of which are examples of distortion isomerism.

## 5. Oligo- and polymeric mercury compounds

The structural data for these derivatives are given in Table 4. Mercury is found only in the oxidation state of +2. There are twelve tetramers, and in four of them [249–252] a carbon atom is bonded to four Hg(II) atoms in a distorted tetrahedron. The tetrahedral angles range from 104.6 to 113.6° and the Hg–Hg distance is 336 pm. The mean Hg–$\mu_4$C distance is 206 pm, and mean C–Hg–L angle is 176°. In another two examples [253,254] the real centre is a chlorine atom with a mean Hg–$\mu_4$Cl distance of 299.5 pm. An orthorhombic [255] and triclinic [256] derivative contains a twisted 22-membered cyclic aggregate and is shown in Figure 4. In the remaining four examples [88,245,248] all four Hg(II) atoms are sitting on purine bases with a mean Hg–N bond distance of 209 pm. Digonal coordination about the mercury is completed by methyl groups with a mean Hg–C distance of 207 pm and mean N–Hg–C angle of 176°.

The monoclinic colourless pentamer $[Hg(C)(CF_3)_2]_5(py)_2 \cdot 2H_2O$ [257] has a $Hg_5C_5$ core with a ten-membered ring of alternating mercury and carbon atoms. An additional two terminal $CF_3$ groups complete the tetrahedral coordination about each mercury atom. This is the only example of a pentameric organomercury compound.

In the remaining five examples [231,233,258,259] digonal coordinated Hg(II) atoms are linked via O and C donor ligands to form infinite chain polymers.

In two examples [254,259] two crystallographically independent molecules present in one crystal are examples of distortion isomerism.

Table 5
Summary of the Hg(II)-ligand(atom) bond distances [a]

| COORD. ATOM | Covalent Radius [pm] | 2-Coordination [pm] | 3-Coordination [pm] | 4-Coordination [pm] |
|---|---|---|---|---|
| LO | 73 | 208(9,8) | | |
| $\mu$LO | | 204 | 272.9 | 273.7 |
| LN | 75 | 211(15,17) | | 214.8 |
| | | 209(6,4) [b] | 232(4,4) [b] | |
| | | 209(9,11) [c] | | |
| | | 209(7,4) [d] | | |
| $\mu$LN | | 205 | | |
| LC | 77 | 207(15,25) | 212 | 216(11,14) |
| | | 210(10,7) [b] | | |
| $\mu$LC | | 211(7,6) | | |
| Cl | 99 | 233.2(22,23) | 233.5(47,29) | |
| LS | 102 | 237.6(46,70) | | |
| | | 239(2,2) [b] | 236.7 [b] | |
| LP | 106 | 243 | | |
| Br | 114 | 243.0(70,30) | | |
| I | 133 | 259.4(27,16) | | 269.4(13,12) |
| $\mu$I | | | | 296.2(66,70) |

[a] The first number in parenthesis is the deviation from the mean of the shortest value and the second is the deviation from the mean of the highest value.l
[b] Bidentate ligands.
[c] Tridentate ligands.
[d] Tetradentate ligands.

## 6. Conclusions

The data presented in this review covers the more than three hundred and twenty organomercury structures available to the end of 1992. By comparison, there are over five hundred and fifty for mercury coordination compounds [3]. The number of examples of the various geometries put the vast majority in the digonal class, with the remaining few being tetrahedral and trigonal. Monomeric species are by far the most common, but there are di-, tri-, tetra-, penta- and polymeric examples observed. Except for one example [195] where mercury is in the +1 oxidation state, all of the compounds are found with mercury in the +2 state.

The compounds are for the most part colourless, but examples of white, yellow and red-brown are observed.

The ligands in use are uni-, bi-, tri- and tetradentate, the most common unidentate ligand being methyl and the most common tetradentate the purine bases.

Distortion isomerism has been observed in several cases with differing Hg–L and L–Hg–L values [6,7,26,27,62,118,126,127,187,237,238,240,241]. In a larger number of examples, two crystallographically independent molecules, differing by degree of distortion, have been found in one crystal [12,20,44,49,53, 88,90,96,97,99,101,107,110,118,120,124,131,139,140, 151,157,163,166,170,183,186,218,233,237,247,254]. In some cases three such molecules have been found [93, 113,163,231], in one case four [20] and in one other five [123]. These are all examples of distortion isomerism [197].

A summary of the Hg–L(atom) distances for mercury(II) organometallics with different types of geometry is given in Table 5. In general, these distances increase with coordination number and covalent radius of the coordinating donor atom with the exception of the C donor ligands.

The Hg(I)–Hg(I) distance of 251.5(1) pm [195] is the only example of a metal bonding interaction in the

organometallic derivatives, however, it compares well with the values found for the dimeric Hg(I) coordination compounds (mean value 252 pm) [3]. In the series of mercury(II) derivatives there is only one example [225] where the Hg–Hg distance (279.7(2) pm) is less than 300 pm. and this is the shortest value observed for the mercury(II) organometallics. Relationships between bond angles and distances are discussed in each section.

These examples together with the coordination compounds [3] represent an overview of more than nine hundred known structures for the complexes of mercury. During the collection and organisation of the data it was clear that, despite the increasing use of data retrieval systems, the tracing of relevant material is not always straightforward. Some of the data is only available as supplementary material and some is not mentioned. The listing of interatomic distances depends on the author, some of whom give values well over 300 pm and others cut off data over 240 pm. It is thus often possible to overlook relevant structural features. One of the uses of a review such as this might be to point out these variations by comparing examples in which information that might be relevant is missing. A related overview of the structural chemistry of heterometallic mercury compounds [260], in which two different metal atoms occur together, has been recently completed and also contains several examples of organo-metal derivatives.

## Acknowledgements

The authors wish to thank those who gave permission for reproduction of original figures, the Chemical Faculty of the Slovak Technical University for their cooperation in allowing M.M. to participate, and the Faculty of Pure and Applied Science of York University and the Ministry of Education of the Slovak Republic for financial support.

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