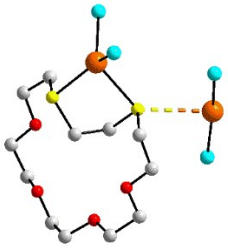
ESI Table S1. Zero-dimensional aggregates featuring Hg···S secondary bonding interactions. The asterisk indicates the sulphur atom forms a Hg–S bond and also participates in an intermolecular Hg···S interaction.

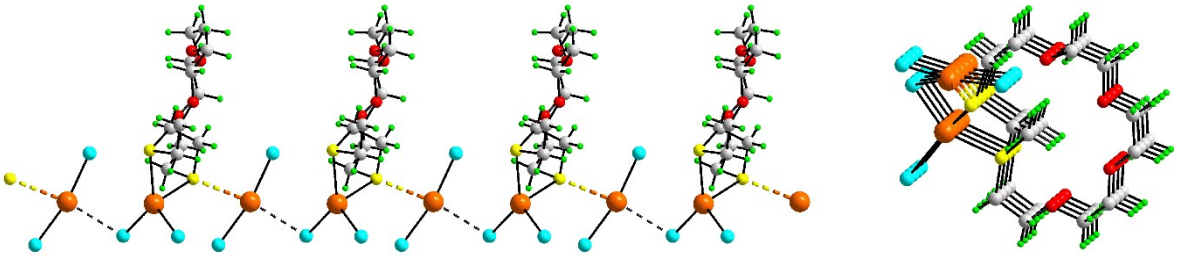
1. BARGUW dichloro-(1,4,7,10-tetraoxa-13,16-dithiacyclo-octadecane)-mercury(II)-dichloro-mercury(II)

N. K. Dalley and S. B. Larson, Structure of dichloro(1,4,7,10-tetraoxa-13,16-dithiacylooctadecane-S,S')mercury(II)-mercury dichloride. *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1981, **37**, 2225-2227; DOI: 10.1107/S0567740881008455



ZITSOK bis(bis(μ_2-Chloro)-(1,4,7,10-tetraoxa-13,16-dithiacyclo-octadecane)-dichloro-di-mercury(II))

A. J. Blake, S. Parsons, C. Radek and M. Schroder, catena-{[$HgCl_2$([18]aneS_2O_4)]$HgCl_2$} at 150K: a redetermination and reinterpretation. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 1996, **52**, 21-24. DOI: https://doi.org/10.1107/S0108270195008717



d(Hg···S) = 3.201(2) Å; Hg–S···Hg = 134.77(4)°; C–S···Hg = 99.62(3) & 115.77(3)°

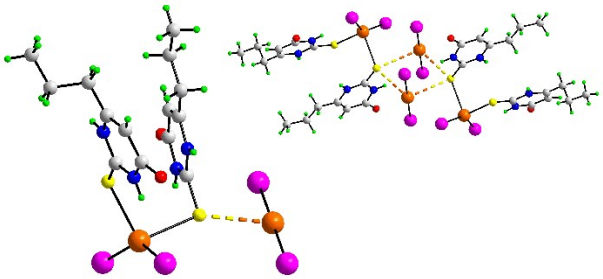
Cl–Hg···S = 79.36(18) & 94.73(18)°

{The components of the 1:1 co-crystal assemble into a zero-dimensional aggregate. A new interpretation allows for an intermolecular *d*(Hg···Cl) = 2.863(2) Å contact, resulting in a linear coordination polymer; data are presented from the earlier publication}

2. ERUXAR diiodo-bis(6-propyl-2-(thioxo)-2,3-dihydropyrimidin-4(1H)-one)-mercury diiodo-mercury

F. Isaia, M. C. Aragoni, M. Arca, C. Caltagirone, C. Castellano, F. Demartin, A. Garau, V. Lippolis and A. Pintus, Oxidative properties of iodine-adducts of propylthiouracil and

methimazole: Direct synthesis of mercury(II) complexes from the reaction with liquid mercury. *Dalton Trans.*, 2011, **40**, 4505-4513; DOI: https://doi.org/10.1039/c0dt01409e



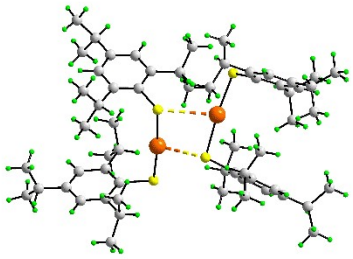
d(Hg···S) = 3.3072(15) Å; Hg–S···Hg = 153.56(5)°; C–S···Hg = 102.39(18)°

I–Hg···S = 84.17(3) & 95.56(3)°

{The co-formers of the 1:1 co-crystal assemble into a zero-dimensional aggregate. If the van der Waals criterion was relaxed, an additional Hg···S interaction [3.4669(15) Å] is apparent which leads to the formation of a centrosymmetric, four-molecule aggregate *via* a $\{\cdots Hg\cdots S\}_2$ synthon}

3. KELWED bis((2,4,6-tri-isopropyl)benzenethiolato)-mercury(II)

E. S. Gruff and S. A. Koch, Trigonal-planar $[M(SR)_3]^{1-}$ complexes of cadmium and mercury. Structural similarities between mercury-cysteine and cadmium-cysteine coordination centers. *J. Am. Chem. Soc*., 1990, **112**, 1245-1247; DOI: https://doi.org/10.1021/ja00159a054



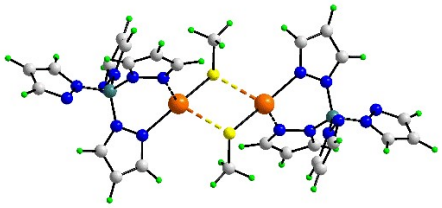
d(Hg···S) = 3.172(7) Å; Hg–S···Hg = 91.3(2)°; C–S···Hg = 133.1(8)°

S–Hg···S = *79.5(2) & 106.3(2)°; *S forming Hg···S contact

{Molecules related by 2-fold symmetry assemble into a dimeric aggregate via a $\{\cdots HgS\}_2$ synthon}

4. HESMAT methylthiolato-(tetrakis(pyrazolato)borato)mercury(II)

S. Aime, G. Digilio, R. Gobetto, P. Cecchi, G. Gioia Lobbia and M. Camalli, Solution and solid-state NMR studies of $MeHg^{II}$ and $RSHg^{II}$ (R = Me, Et) complexes with pyrazolyl-containing ligands. *Polyhedron*, 1994, **13**, 2695-2702; DOI: https://doi.org/10.1016/S0277-5387(00)81323-6



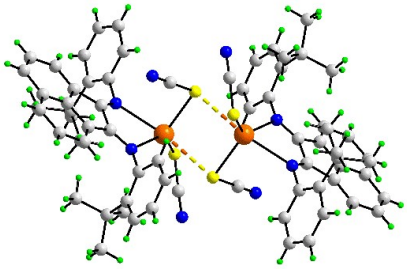
d(Hg···S) = 3.024(3) Å; Hg–S···Hg = 88.19(8)°; C–S···Hg = 92.5(3)°

S–Hg···S = 91.81(7)°; N–Hg···S = 98.21(17)° & N···Hg···S = 87.01(15)°

{Centrosymmetrically-related molecules assemble into a dimeric aggregate *via* a $\{\cdots HgS\}_2$ synthon. An intramolecular Hg···N contact = 2.434(7) Å is noted}

5. AGESAH (N-(2-t-butylphenyl)imine)acenaphthene)-thiocyanate-mercury(II)

L. C. Ferreira, C. A. L. Filgueiras, L. C. Visentin, J. Bordinhão and M. Hörner, One-pot preparation, spectroscopic and structural characterization of mercury(II) complexes of bulky diimines with halides and pseudohalides. *Z. Anorg. Allg. Chem*., 2008, **634**, 1896-1900; DOI: https://doi.org/10.1002/zaac.200800220



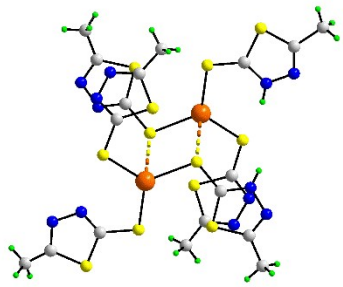
d(Hg···S) = 3.1445(9) Å; Hg–S···Hg = 96.05(3)°; C–S···Hg = 106.24(13)°

S–Hg···S = *83.95(3) & 92.71(4)°; N–Hg···S = 154.13(6) & 85.38(6)°; *S forming Hg···S contact

{Centrosymmetrically-related molecules assemble into a dimeric aggregate *via* a $\{\cdots HgS\}_2$ synthon}

6. VIMBEA bis(5-methyl-1,3,4-thiadiazole-2-thiolato)-(5-methyl-1,3,4-thiadiazole-2(3H)-thione)-mercury(II) hemikis(ethane-1,2-diamine) monohydrate

P. Bharati, A. Bharti, M. K. Bharty, S. Kashyap, U. P. Singh and N. K. Singh, Synthesis, spectral and structural characterization of Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II) complexes with 2-mercapto-5-methyl-1,3,4-thiadiazole: A Zn(II) complex acting as a new sensitive and selective fluorescent probe for the detection of Hg^{2+} in H_2O–MeOH medium. *Polyhedron*, 2013, 63, 222-231. DOI: https://doi.org/10.1016/j.poly.2013.07.027



d(Hg···S) = 3.172(6) Å; Hg–S···Hg = 102.6(2)°; C–S···Hg = 113.2(6)°

S–Hg···S = *78.91(19), 91.6(2) & 106.9(2)°; *S atom involved in Hg···S contact

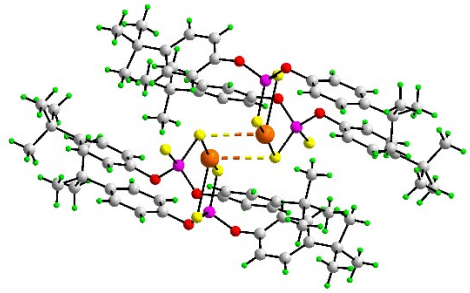
d(Hg···S) = 3.230(6) Å; Hg–S···Hg = 100.6(2)°; C–S···Hg = 112.3(9)°

S–Hg···S = *77.94(19), 90.9(2) & 106.0(2)°; *S atom involved in Hg···S contact

{Two independent Hg-containing molecules in the asymmetric-unit. These assemble to form a dimeric aggregate *via* a non-symmetric {···HgS}$_2$ synthon thiolate-S atoms}

7. EKOBAK bis[bis(4-t-butylphenyl) phosphorodithioato]-mercury(II)

P. Kumar, S. Banerjee, A. Radha, T. Firdoos, S. C. Sahoo and S. K. Pandey, Role of non-covalent interactions in the supramolecular architectures of mercury(II) diphenyldithiophosphates: An experimental and theoretical investigation. *New J. Chem.*, 2021, **45**, 2249-2263. DOI: https://doi.org/10.1039/D0NJ05709F



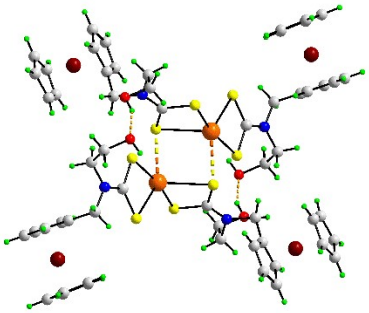
d(Hg···S) = 3.1969(10) Å; Hg–S···Hg = 91.95(3)°; P–S···Hg = 109.54(5)°

Cl–Hg···S = *88.05(3), 95.84(3) & 102.46(3)°; S atom engaged in Hg···S contact

{Centrosymmetric dimer via {···HgS}$_2$ synthons}

8. EJAYOF bis(N-(ferrocenylmethyl)-N-(2-hydroxyethyl)dithiocarbamato)-mercury(II)

R. Yadav, M. Trivedi, G. Kociok-Köhn, R. Chauhan, A. Kumar and S. W. Gosavi, Ferrocenyl dithiocarbamate based d^{10} transition-metal complexes as potential co-sensitizers in dye-sensitized solar cells. *Eur. J. Inorg. Chem.*, 2016, **2016**, 1013-1021; DOI: https://doi.org/10.1002/ejic.201501449



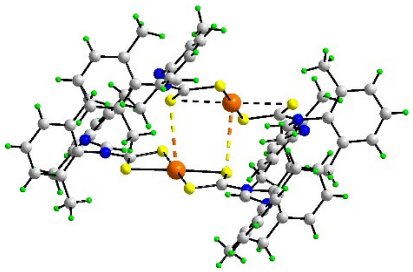
d(Hg···S) = 3.177(2) Å; Hg–S···Hg = 85.92(5)°; C–S···Hg = 92.8(2)°

S–Hg···S = non-participating dtc ligand: 87.56(6) & 152.70(5)°; participating dtc ligand: 90.77(6) & *94.08(5)°; * S atom forming Hg···S contact

{The molecules associate about a centre of inversion to form a zero-dimensional aggregate *via* a $\{\cdots HgS\}_2$ synthon. Intramolecular hydroxyl-O–H···O(hydrogen bonds are noted}

9. VUWLOR bis[(2,6-dimethylphenyl){[(2,6-dimethylphenyl)imino]methyl}-carbamodithioato]-mercury

S. D. Oladipo and B. Omondi, Mercury(II) N,N′-diarylformamidine dithiocarbamates as single-source precursors for the preparation of oleylamine-capped HgS nanoparticles. *Transition Met. Chem*., 2020, **45**, 391-402. DOI: https://doi.org/10.1007/s11243-020-00391-y



d(Hg···S) = 3.2742(9) Å; C–S···Hg = 106.93(12)°

S–Hg···S = 84.89(3) & *97.04(3)°; *S atom involved in Hg···S contact

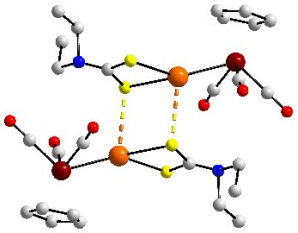
d(Hg···S) = 3.3468(10) Å; C–S···Hg = 120.07(11)°

S–Hg···S = 82.92(3) & 97.27(3)°

{Two independent Hg-containing molecules in the asymmetric-unit. These assemble to form a dimeric aggregate via a non-symmetric $\{\cdots HgS\}_2$ synthon. Intramolecular Hg···S contacts are noted: 2.9342(11) & 2.9081(11) Å and 2.8981(10) & 2.8914(10) Å. The intermolecular Hg···S contacts are formed by weakly- (entry 1) and covalently-bound S atoms, respectively, with the longer Hg···S separation involving the latter}

10. BOMVAA (diethyldithiocarbamato)-mercury-tricarbonyl-(η^5-cyclopentadienyl)-molybdenum

M. M. Kubicki, R. Kergoat, J. Le Gall, J. E. Guerchais, J. Douglade and R. Mercier, The molybdenum-mercury bond. A multinuclear (^{1}H, ^{13}C, ^{31}P, ^{95}Mo and ^{199}Hg) n.m.r. study of (η^5-C_5H_5)$(CO)_2$LMoHgX [L = CO, $P(OMe)_3$ and PPh_3; X = Cl, Br, I, S_2COEt, $S_2P(OEt)_2$, S_2CNEt_2 and $Mo(CO)_3(\eta^5$-$C_5H_5)$] complexes and the crystal and molecular structure of (η^5-C_5H_5)$(CO)_3MoHgS_2CNEt_2$. *Aust. J. Chem.*, 1982, **35**, 1543-1554; DOI: https://doi.org/10.1071/CH9821543



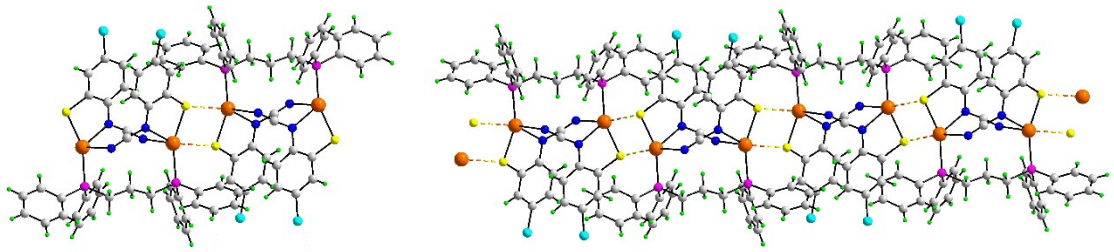
d(Hg···S) = 3.064(9) Å; Hg–S···Hg = 94.8(2)°; C–S···Hg = 100(1)°

S–Hg···S = *85.2(2) & 92.9(3)°; Mo–Hg···S = 113.32(17)°; *S forming Hg···S contact

{Centrosymmetrically-related molecules assemble into a dimeric aggregate *via* a {···HgS}$_2$ synthon. The dtc ligand is chelating, but forms long Hg–S bonds of 2.5093(7) and 2.7374(11) Å}

11. LAZFEB bis(μ-[4-chloro-2-sulfanylphenyl]cyanamidato)-(μ-propane-1,3-diylbis(diphenylphosphine))-di-mercury

S. A. Al-Jibori, A. A. Irzoqi, A. S. M. Al-Janabi, A. I. A. Al-Nassiry, S. Basak-Modi, S. Ghosh, C. Wagner and G. Hogarth, Synthesis, structure and reactivity with phosphines of Hg(II) *ortho*-cyano-aminothiophenolate complexes formed *via* C–S bond cleavage and dehydrogenation of 2-aminobenzothiazoles. *Dalton Trans.*, 2022, **51**, 7889-7898. DOI: https://doi.org/10.1039/D2DT00391K



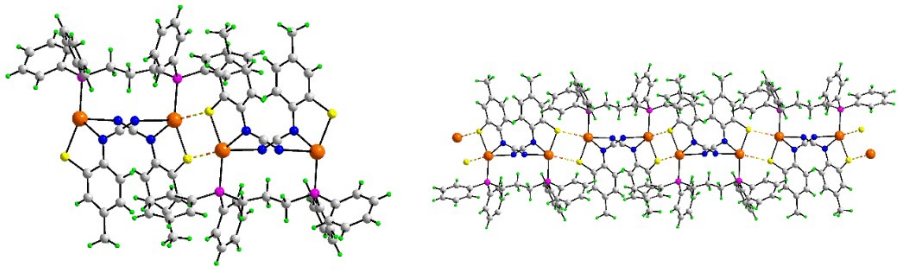
d(Hg···S) = 3.3408(19) Å; Hg–S···Hg = 100.79(7)°; C–S···Hg = 158.3(3)°

S–Hg···S = 79.21(6)°; P–Hg···S = 85.46(7)°; N–Hg···S = 159.79(17)°; N···Hg···S = 90.73(17)°

{Centrosymmetric {···HgS}$_2$ synthon leading to tetra-mercury aggregate. Should longer Hg···S interactions be considered, d(Hg···S) = 3.517(2) Å, additional centrosymmetric {···HgS}$_2$ synthons are formed, leading to a linear, supramolecular chain}

12. LAZFIF (μ-propane-1,3-diylbis(diphenylphosphine))-bis(μ-[4-methyl-2-(sulfanyl)phenyl]cyanamidato)-di-mercury

S. A. Al-Jibori, A. A. Irzoqi, A. S. M. Al-Janabi, A. I. A. Al-Nassiry, S. Basak-Modi, S. Ghosh, C. Wagner and G. Hogarth, Synthesis, structure and reactivity with phosphines of Hg(II) ortho-cyano-aminothiophenolate complexes formed via C–S bond cleavage and dehydrogenation of 2-aminobenzothiazoles. *Dalton Trans.*, 2022, **51**, 7889-7898. DOI: https://doi.org/10.1039/D2DT00391K



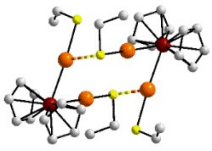
d(Hg···S) = 3.3199(17) Å; Hg–S···Hg = 99.84(6)°; C–S···Hg = 159.3(2)°

S–Hg···S = 80.16(5)°; P–Hg···S = 85.10(5)°; N–Hg···S = 160.84(13)°; N···Hg···S = 90.79(14)°

{Centrosymmetric {···HgS}$_2$ synthon leading to tetra-mercury aggregate. Should longer Hg···S interactions be considered, *d*(Hg···S) = 3.514(2) Å, additional centrosymmetric {···HgS}$_2$ synthons are formed, leading to a linear, supramolecular chain}

13. SMOHGB10 bis((η^5-cyclopentadienyl)-(ethylthio-mercury))-molybdenum

M. M. Kubicki, R. Kergoat, J. E. Guerchais, I. Bkouche-Waksman, C. Bois and P. L'Haridon, Complexes biscyclopentadienyles avec des liaisons metal de transition-mercure: III. Structure de deux phases de $(C_5H_5)_2Mo(HgSC_2H_5)_2$; etude de la distribution electronique dans les complexes $(C_5H_5)_2MoX_2$ par resonance magnetique nucleaire. *J. Organomet. Chem.*, 1981, **219**, 329-343. DOI: https://doi.org/10.1016/S0022-328X(00)90018-4



d(Hg···S) = 3.1669(15) Å; Hg–S···Hg = 78.728(12)°; C–S···Hg = 109.875(17)°

Mo–Hg···S = 109.621(13)°; S–Hg···S = 83.308(12)°

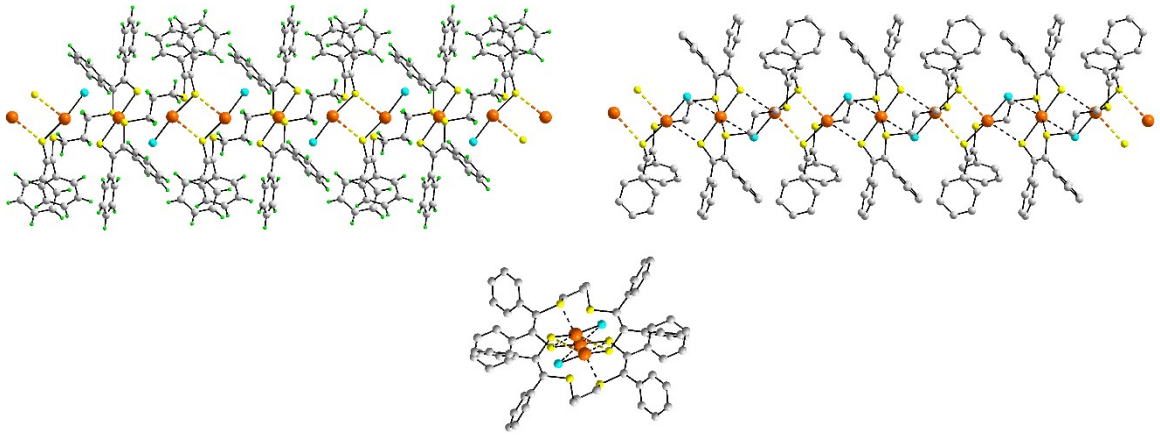
{Dimer mediated by a centrosymmetric {···HgS}$_2$ synthon; see for SMOHGB11 polymorph}

ESI Table S2. One-dimensional aggregation patterns featuring Hg···S secondary bonding interactions. The asterisk indicates the sulphur atom forms a Hg–S bond and also participates in an intermolecular Hg···S interaction.

LINEAR

14. PELBAJ bis((μ$_2$-chloro)-(μ$_3$-trimethylene)-bis(cis-stilbene-1,2-dithiolato))-tri-mercury

G. N. Schrauzer, C. Zhang, H. K. Reddy and E. O. Schlemper, Synthesis of macrocyclic mercury(II) derivatives of S,S′1-trimethylene-and S,S′1-tetramethylenebis(cis1-stilbene-α,β1-dithiol) with unusual structures. *Chem. Ber*., 1993, **126**, 1337-1340. DOI: https://doi.org/10.1002/cber.19931260611



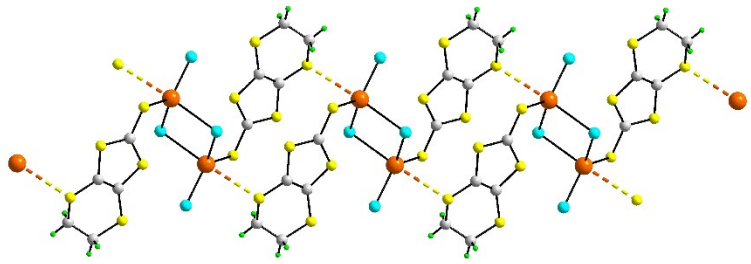
d(Hg···S) = 3.170(2) Å; Hg–S···Hg = 88.93(7)°; C–S···Hg = 105.7(3)°

Cl–Hg···S = 87.02(8)°; S–Hg···S = 91.07(6)°

{Centrosymmetric, tri-mercury molecule connected into a linear chain *via* centrosymmetric {··· HgS}$_2$ synthons involving the peripheral Hg atoms. Intramolecular *d*(Hg···S) = 2.9809(19) Å contacts are evident for the central Hg atom. Further *d*(Hg···S) = 3.157(2) Å and *d*(Hg···Cl) = 3.191(3) Å contacts provide links between the central Hg and outer Hg atoms within the repeat unit; see right-hand view}

15. FAQVEY01 bis((μ$_2$-chloro)-chloro-(4,5-ethylenedithio-1,3-dithiole-2-thione)-mercury(II))

J. Dai, M. Munakata, G.-Q. Bian, Q.-F. Xu, T. Kuroda-Sowa and M. Maekawa, Mercury(II) complexes of 4,5-ethylenedithio-1,3-dithiole-2-thione, having S···S and S···Cl contract assembled ribbon structure. *Polyhedron*, 1988, **17** 2267-2270; DOI: https://doi.org/10.1016/S0277-5387(98)00015-1



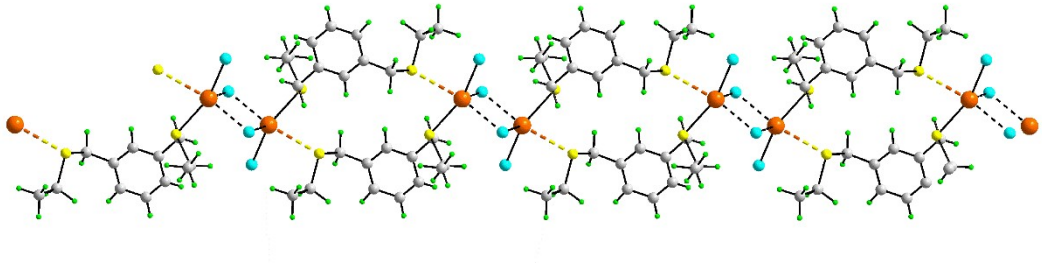
d(Hg···S) = 3.277(2) Å; methylene-C–S···Hg = 93.7(3)°; C–S···Hg = 104.9(3)°

Cl–Hg···S = 77.89(7) (terminal-Cl), 85.52(7) & 170.05(6)°; S–Hg···S = 85.54(6)°

{The binuclear molecule is disposed about a centre of inversion. The mercury atom interacts with a ring-thioether sulphur atom to generate a linear, one-dimensional chain *via* two Hg···S contacts and 12-membered, centrosymmetric {···HgSCSCS}$_2$ synthons}

16. TAZGAC bis((μ$_2$-chloro)-chloro-(1,3-bis(ethylthiomethyl)benzene)-mercury(II))

I. Romero, G. Sánchez-Castelló, F. Teixidor, C. R. Whitaker, J. Rius, C. Miravitlles, T. Flor, L. Escriche and J. Casabó, Silver(I), mercury(II) and copper(I) complexes of acyclic and macrocyclic dithioether, *meta*xylyl based ligands. *Polyhedron*, 1996, **15**, 2057-2065. DOI: 10.1016/0277-5387(95)00445-9.



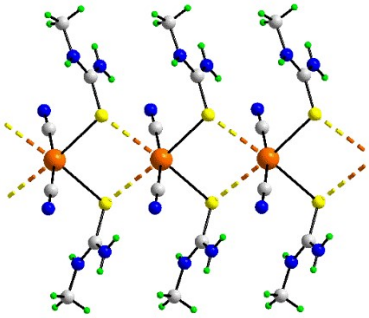
d(Hg···S) = 3.193(2) Å; C–S···Hg = 97.89(19) & 103.8(3)°

Cl–Hg···S = 93.83(5) & *83.26(5)°; S–Hg···S = 74.01(5)°; *Cl atom involved in bridging

{Centrosymmetric molecule with equal but long Hg–Cl bridges [2 × 2.731(2) Å]. Linear, supramolecular chain comprising corner (Hg)-shared, 16-membered, centrosymmetric {···HgSC$_5$S}$_2$ synthons}

17. BAFJUP dicyano-bis(methylthiourea)-mercury(II)

A. A. Isab, M. Fettouhi, M. R. Malik, S. Ali, A. Fazal and S. Ahmad, Mercury(II) cyanide complexes of thioureas and the crystal structure of [(N-methylthiourea)$_2$ Hg(CN)$_2$]. *Russ. J. Coord. Chem*., 2011, **37**, 180-185; DOI: https://doi.org/10.1134/S1070328411030055



d(Hg···S) = 3.197(2) Å; Hg–S···Hg = 86.98(5)°; C–S···Hg = 120.0(2)°

S–Hg···S = 86.98(5) & 174.48(5)°; C–Hg···S = 84.1(2) & 89.0(2)°

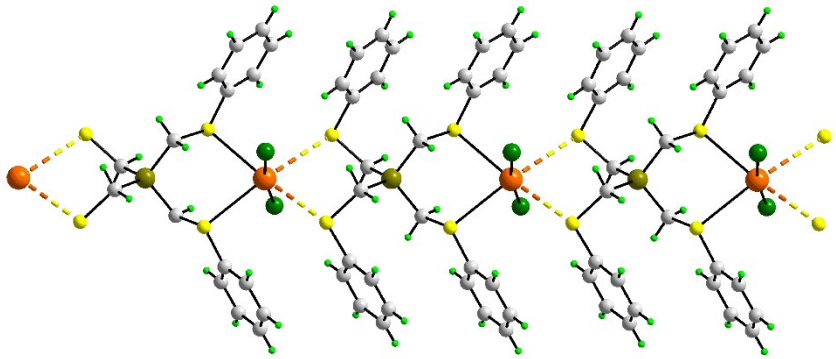
d(Hg···S) = 3.273(2) Å; Hg–S···Hg = 86.03(4)°; C–S···Hg = 122.0(2)°

S–Hg···S = 86.03(5) & 175.42(5)°; C–Hg···S = 85.6(2) & 86.1(2)°

{Molecules assemble into a linear, one-dimensional chain via two Hg···S contacts. Supporting molecular amino-N–H···N(thiourea) hydrogen bonds [2.55 & 2.56 Å] are evident}

18. WAMZAM dibromo-(tetrakis(phenylthiomethyl)silane)-mercury(II)

H. N. Peindy, F. Guyon, M. Knorr, A. B. Smith, J. A. Farouq, S. A. Islas, D. Rabinovich, J. A. Golen and C. Strohmann, Formation of extended 1D coordination polymers in tetrathioether complexes of mercury(II): Effect of the organic substituents on the crystal structures of $\{Si(CH_2SR)_4\}HgBr_2$ (R = Me, Ph). *Inorg. Chem. Commun.*, 2005, **8**, 479-482. DOI: https://doi.org/10.1016/j.inoche.2005.02.008



d(Hg···S) = 3.2013(16) Å; C–S···Hg = 105.25(14)° & phenyl 131.03(14)°

Br–Hg···S = 78.32(3) & 94.39(3)°

d(Hg···S) = 3.2036(16) Å; C–S···Hg = 105.29(14)° & phenyl 130.29(14)°

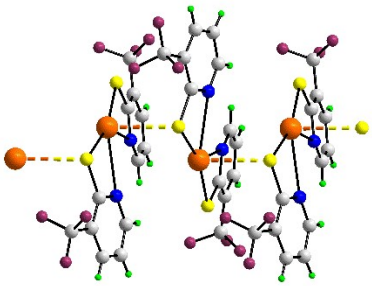
Br–Hg···S = 78.55(3) & 94.41(3)°

{Molecules assemble into a linear chain *via* two independent but equivalent Hg···S contacts and non-symmetric, six-membered {···Hg···SCSiCS} synthons}

ZIG-ZAG

19. GUYJAL bis(3-(trifluoromethyl)pyridine-2-thionato)-mercury(II)

A. Sousa-Pedrares, J. Romero, J. A. García-Vázquez, M. L. Durán, I. Casanova and A. Sousa, Electrochemical synthesis and structural characterisation of zinc, cadmium and mercury complexes of heterocyclic bidentate ligands (N, S). *Dalton Trans*., 2003, 1379-1388; DOI: https://doi.org/10.1039/b300133b



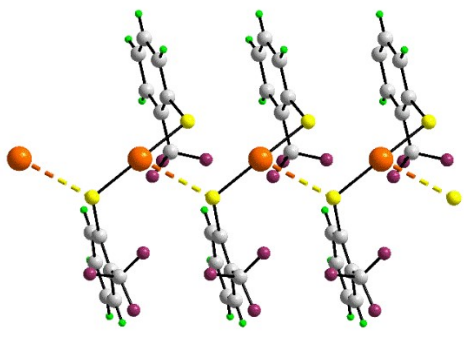
d(Hg···S) = 3.0521(17) Å; Hg–S···Hg = 94.20(5)°; C–S···Hg = 98.8(2)°

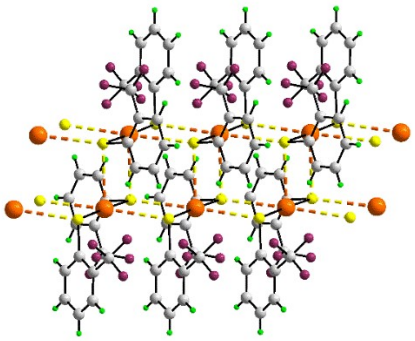
S–Hg···S = 93.06(5) & *94.70(5)°; N–Hg···S = 83.28(12) & 89.44(13)°; * S participates in the Hg···S contact

{The molecules associate into a zig-zag supramolecular chain propagated by glide symmetry}

20. MIJYEL bis(2-(trifluoromethyl)phenylthiolato)-mercury(II)

G. Moreno-Alcántar, M. Arroyo, J. L. Bautista, S. Bernès, N. Esturau-Escofet and H. Torrens, Polyfluorinated mercury thiolates. ^{199}Hg NMR studies and the crystal structure of [Hg($SC_6H_4(CF_3)$-2)$_2$]. *J. Fluorine Chem*., 2013, **156**, 61-65. DOI: https://doi.org/10.1016/j.jfluchem.2013.09.001





d(Hg···S) = 3.3404(19) Å; Hg–S···Hg = 101.57(6)°; C–S···Hg = 100.1(2)°

S–Hg···S = 79.45(5) & 101.57(5)°

d(Hg···S) = 3.3812(19) Å; Hg–S···Hg = 100.17(6)°; C–S···Hg = 152.2(2)°

S–Hg···S = 78.71(5) & 100.17(5)°

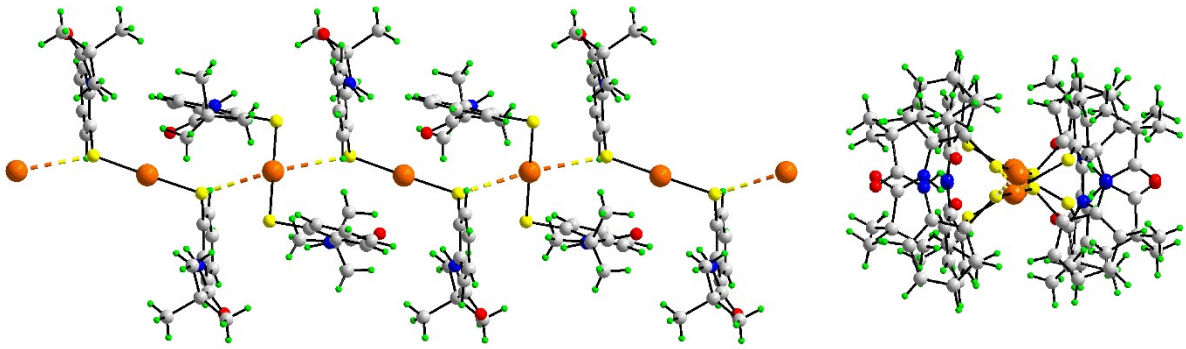
d(Hg···S) = 3.387(2) Å; Hg–S···Hg = 81.42(5)°; C–S···Hg = 106.5(2)°

S–Hg···S = 84.20(5) & 98.58(5)°

{A zig-zag chain is formed through entry 1. If a longer *d*(Hg···S) = 3.3812(19) Å contact is taken into consideration, a supramolecular tape arises through corner (Hg) shared, non-symmetric {···HgS}$_2$ synthons. Should marginally longer *d*(Hg···S) = 3.387(2) Å contacts are taken into account, centrosymmetric {···HgS}$_2$ synthons normal to the tape are formed leading to a double-tape}

21. ZURXAL bis((2-pivaloylamino)benzenethiolato)-mercury(II) hemihydrate

N. Ueyama, K. Taniuchi, T. Okamura, A. Nakamura, H. Maeda and S.Emura, Effect of the NH–S hydrogen bond on the nature of Hg–S bonding in bis[2-(acylamino)benzenethiolato]-mercury(II) and bis[2,6-bis(acylamino)benzenethiolato]mercury(II) complexes. *Inorg. Chem.*, 1996, **35**, 1945-1951. DOI: https://doi.org/10.1021/ic950472s



d(Hg···S) = 3.158(5) Å; Hg–S···Hg = 140.0(2)°; C–S···Hg = 110.9(6)°

S–Hg···S = 80.89(15) & 99.13(15)°

d(Hg···S) = 3.163(4) Å; Hg–S···Hg = 148.80(15)°; C–S···Hg = 93.5(6)°

S–Hg···S = 77.16(15) & 103.06(15)°

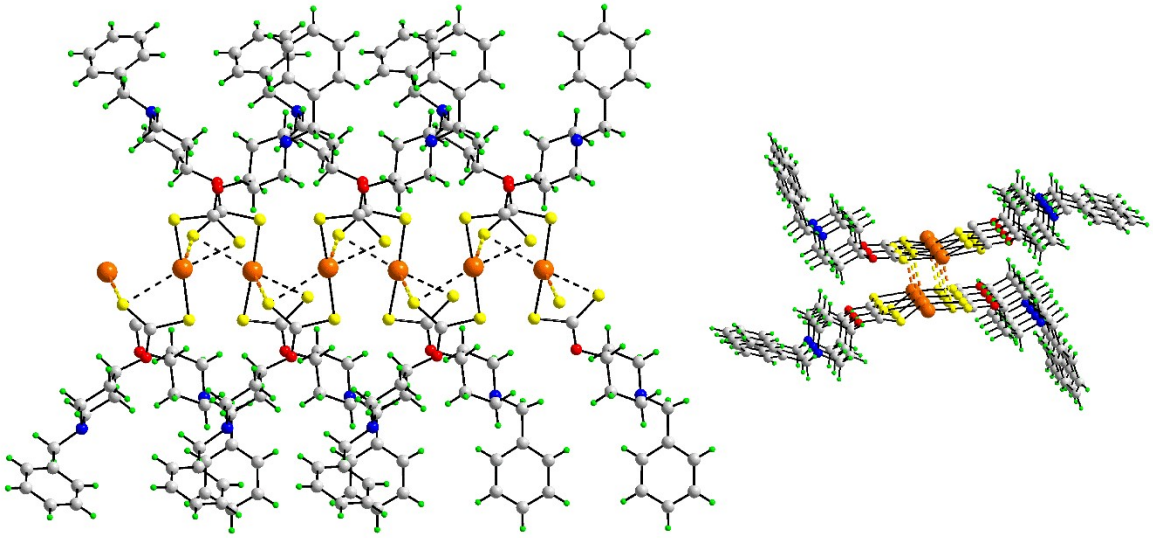
{Two independent molecules which assemble into a zig-zag (glide) chain *via* a pair of nearly equivalent Hg···S contacts involving one Hg atom only. Supporting intra-chain Hg···O contacts [2.782(14) & 2.899(14) Å] are noted. The presence of water-O–H···O hydrogen bonds connect chains into a supramolecular layer}

HELICAL

22. XOBBUN [(μ_2-O-(1-benzylpiperidin-4-yl)carbonodithioato)-(O-(1-benzylpiperidin-4-yl)carbonodithioato)-mercury]

G. Rajput, M. K. Yadav, T. S. Thakur, M. G. B. Drew and N. Singh, Versatile coordination environment and interplay of metal assisted secondary interactions in the organization of

supramolecular motifs in new Hg(II)/PhHg(II) dithiolates. *Polyhedron*, 2014, **69**, 225-233. DOI: https://doi.org/10.1016/j.poly.2013.12.005



d(Hg···S) = 3.134(2) Å; C–S···Hg = 100.4(2)°

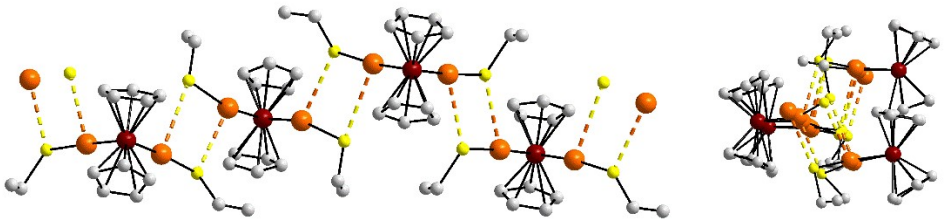
S–Hg···S = 90.52(6) & 96.49(6)°

{Molecules assemble into a helical (2_1-screw) chain *via* a Hg···S contacts involving a weakly-bound S atom; intramolecular *d*(Hg···S) = 3.0317(14) & 2.9536(19) Å with the longer separation involving the S atom forming the Hg···S contact}

TWISTED

23. SMOHGB11 bis((η^5-cyclopentadienyl)-(ethylthio-mercury))-molybdenum

M. M. Kubicki, R. Kergoat, J. E. Guerchais, I. Bkouche-Waksman, C. Bois and P. L'Haridon, Complexes biscyclopentadienyles avec des liaisons metal de transition-mercure: III. Structure de deux phases de $(C_5H_5)_2Mo(HgSC_2H_5)_2$; etude de la distribution electronique dans les complexes $(C_5H_5)_2MoX_2$ par resonance magnetique nucleaire. *J. Organomet. Chem.*, 1981, **219**, 329-343. DOI: https://doi.org/10.1016/S0022-328X(00)90018-4



d(Hg···S) = 3.3306(15) Å; Hg–S···Hg = 108.748(13)°; C–S···Hg = 134.948(15)°

Mo–Hg···S = 112.126(12)°; S–Hg···S = 71.252(11)°

d(Hg···S) = 3.3276(9) Å; Hg–S···Hg = 104.579(11)°; C–S···Hg = 126.756(15)°

Mo–Hg···S = 113.801(11)°; S–Hg···S = 81.734(11)°

d(Hg···S) = 3.5711(11) Å; Hg–S···Hg = 93.764(10)°; C–S···Hg = 164.886(17)°

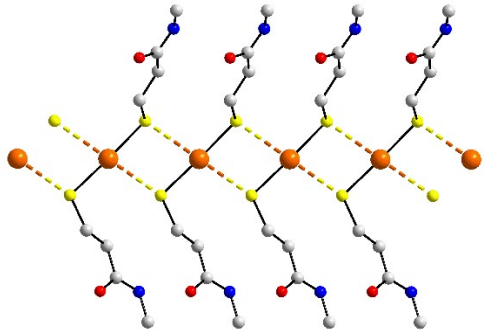
Mo–Hg···S = 106.419(10)°; S–Hg···S = 79.833(11)°

{Two independent molecules, one is disposed about a two-fold axis of symmetry. Supramolecular chain with a twisted topology. Molecules are connected *via* centrosymmetric (entry 1) and non-symmetric $\{\cdots HgS\}_2$ synthons; entry 3 has a Hg···S separation longer than the standard sum of the van der Waals radii; see for SMOHGB10 polymorph}

ESI Table S3. Supramolecular ribbons featuring Hg···S secondary bonding interactions. The asterisk indicates the sulphur atom forms a Hg–S bond and also participates in an intermolecular Hg···S interaction.

24. MECBHG bis(methylcarbamoyl-ethanethiolato)-mercury(II)

C. Perchard, G. Zuppiroli, P. Gouzerh, Y. Jeannin and F. Robert, Etude spectroscopique de derives mercuriques d'amidesthiols: Partie II. Structure cristalline et spectres de vibration du bis(méthylcarbamoyléthanethiolato)mercure(II). *J. Molec. Struct*., 1981, **72**, 119-129. DOI: https://doi.org/10.1016/0022-2860(81)85012-0



d(Hg···S) = 3.2606(16) Å; Hg–S···Hg = 100.593(9)°; C–S···Hg = 152.592(13)°

S–Hg···S = 81.763(10) & 100.593(9)°

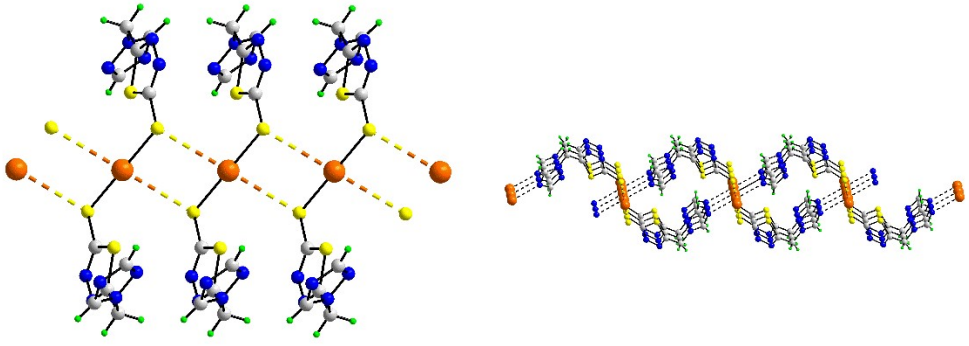
d(Hg···S) = 3.3557(17) Å; Hg–S···Hg = 97.951(9)°; C–S···Hg = 85.261(12)°

S–Hg···S = 79.692(10) & 97.951(9)°

{A supramolecular ribbon via corner-shared, non-symmetric $\{\cdots HgS\}_2$ synthons. One of the *d*(Hg···S) = 3.3557(17) Å separations is just beyond the standard van der Waals radii}

25. PODSAE bis(5-(1H-1,2,4-triazol-1-ylmethyl)-1,3,4-thiadiazole-2-thiolato)-mercury(II)

L.-L. Wei, L.-K. Li, L.-Y. Fan, C.-H. Wang and H.-W. Hou, Syntheses, crystal structures, and properties of six coordination complexes based on a newly designed mercapto-thiadiazole ligand. *Aust. J. Chem*., 2014, **67**, 241-249. DOI: https://doi.org/10.1071/CH13417



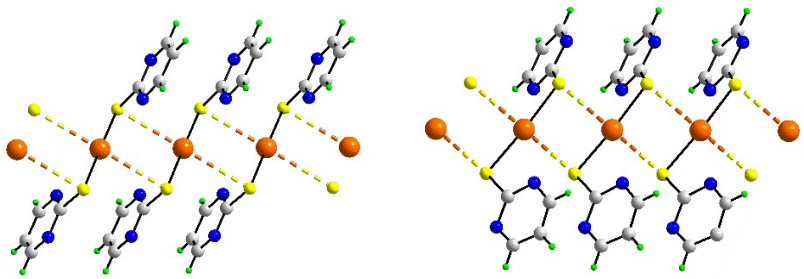
d(Hg···S) = 3.344(2) Å; Hg–S···Hg = 100.14(6)°; C–S···Hg = 127.4(2)°

S–Hg···S = 79.86(5) & 100.14(5)°

{The Hg atom is situated on a centre of inversion. Ribbons are formed by concatenated, centrosymmetric {···HgS}$_2$ synthons. Longer, intra-chain *d*(Hg···S) = 3.3525(19) Å contacts are noted. Long *d*(Hg···N) = 2.858(7) Å contacts link chains into a two-dimensional array comprising tubes}

26. MAVTAF bis(pyrimidine-2-thiolato)-mercury(II)

A. Eichhöfer and G. Buth, Synthesis and structure of the Group 12 pyrimidinethiolate complexes $_\infty^3$[Zn(S-2-$N_2C_4H_3$)$_2$], $_\infty^2$[Cd(S-2-$N_2C_4H_3$)$_2$], [Hg(S-2-$N_2C_4H_3$)$_2$] and[Cd(S-2-$N_2C_4H_3$)$_2$(tmeda)]. *Eur. J. Inorg. Chem.*, 2005, **2005**, 4160-4167. DOI: https://doi.org/10.1002/ejic.200500253



d(Hg···S) = 3.267(2) Å; Hg–S···Hg = 88.21(6)°; C–S···Hg = 83.6(3)°

S–Hg···S = 88.21(6) & 92.87(6)°

d(Hg···S) = 3.311(2) Å; Hg–S···Hg = 87.06(6)°; C–S···Hg = 81.0(3)°

S–Hg···S = 87.07(6) & 91.86(6)°

d(Hg···S) = 3.229(2) Å; Hg–S···Hg = 88.91(6)°; C–S···Hg = 105.1(3)°

S–Hg···S = 89.91(6) & 94.97(6)°

d(Hg···S) = 3.388(2) Å; Hg–S···Hg = 85.35(6)°; C–S···Hg = 77.8(3)°

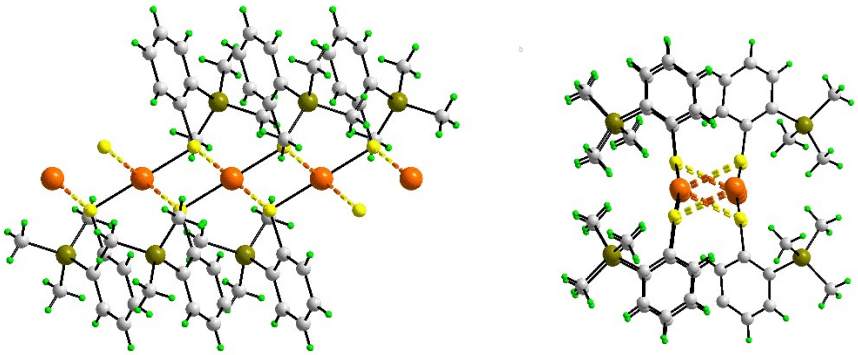
S–Hg···S = 85.35(6) & 90.76(6)°

{Two independent molecules and each self-assembles into a supramolecular ribbon *via* corner-shared, non-symmetric {···HgS}$_2$ synthons. For the right-hand image, entries 3 & 4, one of the *d*(Hg···S) = 3.388(2) Å separations is beyond the standard van der Waals radii}

27. JETYOW bis(2-(trimethylsilyl)benzenethiolato)-mercury(II)

E. Block, M. Brito, M. Gernon, D. McGowty, H. Kang and J. Zubieta, Mercury(II) and methylmercury(II) complexes of novel sterically hindered thiolates: carbon-13 and mercury-

199 NMR studies and the crystal and molecular structures of [MeHg(SC_6H_2-2,4,6-Pr-iso$_3$)], [Hg(SC_6H_4-2-$SiMe_3$)$_2$], [Hg(2-SC_5H_3N-3-$SiMe_3$)$_2$], and [Hg{(2-SC_6H_4)$_2SiMe_2$}]$_2$. *Inorg. Chem.*, 1990, **29**, 3172-3181; DOI: https://doi.org/10.1021/ic00342a024



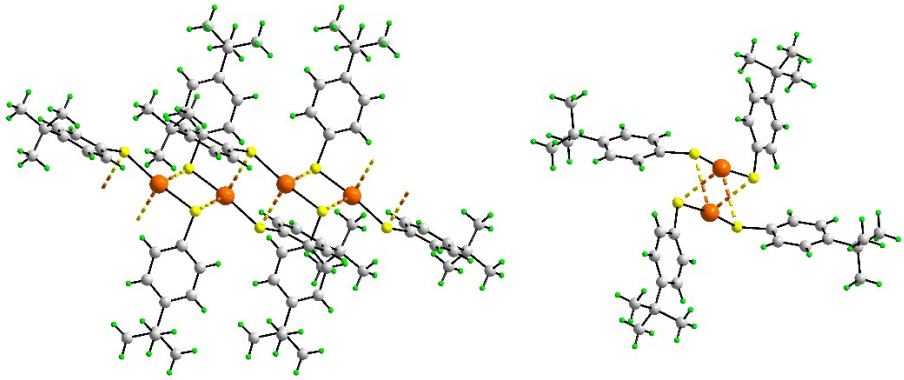
d(Hg···S) = 3.235(3) Å; Hg–S···Hg = 96.55(7)°; C–S···Hg = 125.4(3)°

S–Hg···S = *83.45(7) & 105.10(7)°)°; * S participates in the Hg···S contact

{The mercury atom lies on a 2-fold axis and forms two equivalent Hg···S interactions to associate molecules into a zig-zag supramolecular chain propagated by glide symmetry}

28. BUCNUJ bis(4-t-butylbenzenethiolato)-mercury(II)

J. G. Melnick, K. Yurkerwich and G. Parkin, Synthesis, structure, and reactivity of two-coordinate mercury alkyl compounds with sulfur ligands: Relevance to mercury detoxification. *Inorg. Chem.*, 2009, **48**, 6763-6772; DOI: https://doi.org/10.1021/ic900721g



d(Hg···S) = 3.0365(16) Å; Hg–S···Hg = 90.66(4)°; C–S···Hg = 105.69(19)°

S–Hg···S = 89.34(5) & 98.91(4)°

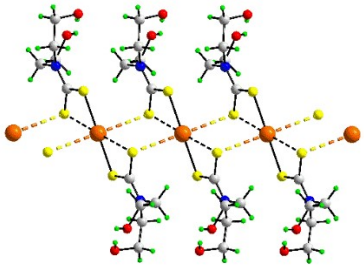
d(Hg···S) = 3.1124(18) Å; Hg–S···Hg = 83.00(4)°; C–S···Hg = 113.45(16)°

S–Hg···S = 85.75(4) & 97.00(5)°

{Molecules assemble into a twisted, one-dimensional chain *via* two distinct Hg···S contacts and two independent, centrosymmetric {···HgS}$_2$ synthons}

29. FOPWAJ bis(bis(2-hydroxyethyl)carbamodithioato)-mercury(II)

R. A. Howie, E. R. T. Tiekink, J. L. Wardell and S. M. S. V. Wardell, Complementary supramolecular aggregation via O–H···O hydrogen-bonding and Hg···S interactions in bis[N,N′-di(2-hydroxyethyl)-dithiocarbamato-S,S′]mercury(II): $Hg[S_2CN(CH_2CH_2OH)_2]_2$. *J. Chem. Crystallogr.*, 2009, **39**, 293-298; DOI: https://doi.org/10.1007/s10870-008-9473-0



d(Hg···S) = 3.182(3) Å; C–S···Hg = 93.4(3)°

S–Hg···S = 85.86(7) & 94.11(6)°

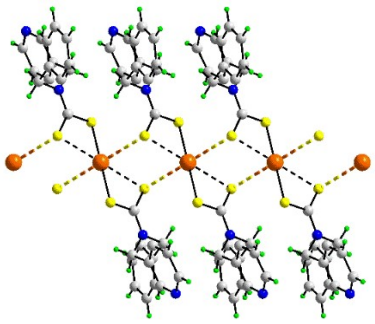
d(Hg···S) = 3.222(7) Å; C–S···Hg = 92.7(3)°

S–Hg···S = 86.19(7) & 93.8(7)°

{Molecules assemble into a linear, one-dimensional chain via two Hg···S contacts; the mercury atom occupies a general position. Intramolecular Hg···S contacts are also noted: 2.907(3) & 2.914(3) Å}

30. FODSAU bis(benzyl(pyridin-3-ylmethyl)carbamodithioato)-mercury(II)

V. Singh, V. Kumar, A. N. Gupta, M. G. B. Drew and N. Singh, Effect of pyridyl substituents leading to the formation of green luminescent mercury(II) coordination polymers, zinc(II) dimers and a monomer. *New. J. Chem.*, 2014, **38**, 3737-3748; DOI: https://doi.org/10.1039/C4NJ00435C



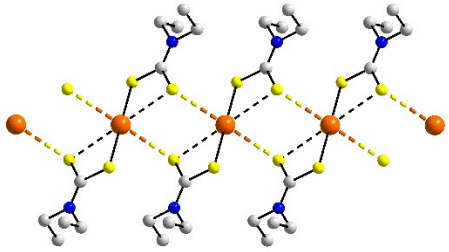
d(Hg···S) = 3.2178(19) Å; C–S···Hg = 98.9(3)°

S–Hg···S = 89.5(7) & 90.5(7)°

{Molecules assemble into a linear, one-dimensional chain via two Hg···S contacts; the mercury atom is located on a centre of inversion. An intramolecular Hg···S contact is also noted: 2.9524(18) Å}

31. HGETCB10 bis(diethyldithiocarbamato)-mercury(II)

H. Iwasaki, The crystal structure of dimeric and monomeric forms of mercury(II) N,N-diethyldithiocarbamate, $Hg_2(S_2CNEt_2)_4$ and $Hg(S_2CNEt_2)_2$. *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1973, **29**, 2115-2124; DOI: https://doi.org/10.1107/S0567740873006205



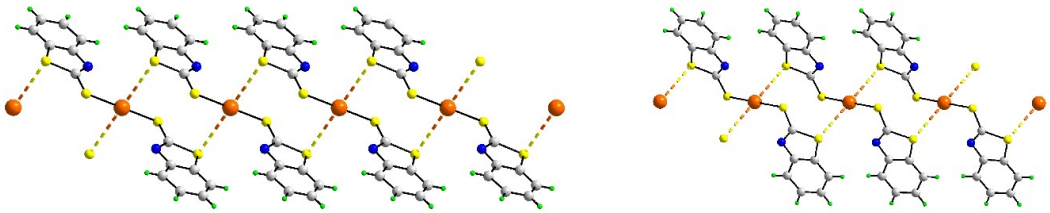
d(Hg···S) = 3.2923(18) Å; C–S···Hg = 96.031(17)°

S–Hg···S = 87.104(11) & 92.896(12)°

{Molecules assemble into a linear, one-dimensional chain via two Hg···S contacts; the mercury atom is located on a centre of inversion. An intramolecular Hg···S contact is also noted: 2.9647(19) Å}

32. METZUG bis(1,3-benzothiazole-2-thiolato)mercury(II)

N. A. Bell, S. J. Coles, C. P. Constable, D. E. Hibbs, M. B. Hursthouse, R. Mansor, E. S. Raper and C. Sammon, Complexes of heterocyclic thiones and Group 12 metals: Part 5. Reactions of 1,3-thiazolidine-2-thione and benzo-1,3-thiazoline-2-thione with mercury(II) halides in a 2:1 ratio. Crystal structures of bis(1,3-thiazolidine-2-thione) mercury(II) bromide and bis(benzo-1,3-thiazolinato)mercury(II). *Inorg. Chim. Acta*, 2001, **323**, 69-77. DOI: https://doi.org/10.1016/S0020-1693(01)00599-0



d(Hg···S) = 3.310(3) Å; C–S···Hg = 95.1(3) & 98.9(3)°

S–Hg···S = 89.32(8) & 90.68(8)°

d(Hg···S) = 3.352(3) Å; C–S···Hg = 103.4(4) & 108.6(3)°

S–Hg···S = 87.30(9) & 94.15(8)°

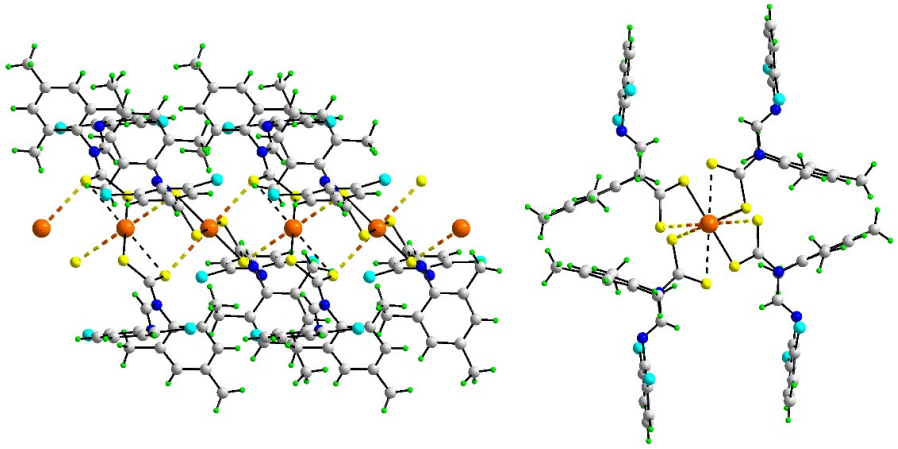
d(Hg···S) = 3.396(3) Å; C–S···Hg = 96.0(4) & 98.6(4)°

S–Hg···S = 87.03(8) & 91.49(9)°

{Two independent molecules comprise the asymmetric-unit, one with the Hg atom located on a two-fold axis. The latter assemble into a supramolecular ribbon (left-hand image, entry 1) *via* eight-membered {···HgSCS}$_2$ synthons with a chair conformation. The other molecule, with the Hg atom located in a general position assembles similarly but with one Hg···S separation longer than the standard sum of the van der Waals radii}

33. VUWMAE bis[{[(2,6-dichlorophenyl)imino]methyl}(2,4,6-trimethylphenyl)-carbamodithioato]-mercury dichloromethane solvate

S. D. Oladipo and B. Omondi, Mercury(II) N,N′-diarylformamidine dithiocarbamates as single-source precursors for the preparation of oleylamine-capped HgS nanoparticles. *Transition Met. Chem*., 2020, **45**, 391-402. DOI: https://doi.org/10.1007/s11243-020-00391-y



d(Hg···S) = 3.2198(8) Å; Hg–S···Hg = 91.12(3)°; C–S···Hg = 108.30(11)°

S–Hg···S = 88.74(2) & 91.26(2)°

d(Hg···S) = 3.2337(8) Å; C–S···Hg = 100.24(11)°

S–Hg···S = 83.41(2) & *96.59(2)°; *S atom involved in Hg···S contact

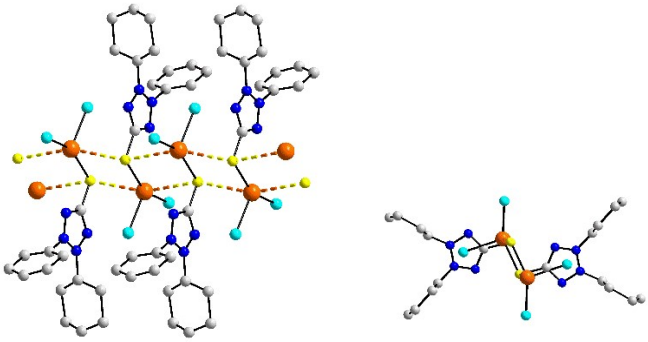
{Two independent Hg-containing molecules in the asymmetric-unit, each with the Hg atom located on a centre of inversion. Molecules assemble into a twisted ribbon *via* corner (Hg)-shared, non-symmetric {··· HgS}$_2$ synthons. Intramolecular Hg···S contacts are noted: 2.8898(9) Å and 2.9728(8) Å, respectively. The intermolecular Hg···S contacts are formed by covalently- (entry 1) and weakly-bound S atoms, respectively, with the longer Hg···S separation involving the former}

ESI Table S4. Supramolecular tape featuring Hg···S secondary bonding interactions. The asterisk indicates the sulphur atom forms a Hg–S bond and also participates in an intermolecular Hg···S interaction.

34. DTIZHG10 anhydro-5-mercapto-2,3-diphenyltetrazole-dichloro-mercury(II)

W. J. Kozarek and Q. Fernando, Crystal and molecular structure of $C_{13}H_{10}N_4S.HgCl_2$, the adduct of anhydro-5-mercapto2,3-diphenyltetrazolium hydroxide and mercury(II) chloride. *Inorg. Chem*., 1973, **12**, 2129-2131. DOI: https://doi.org/10.1021/ic50127a038

R. E. Marsh and F. H. Herbstein, Some additional changes in space groups of published crystal structures. *Acta Crystallogr., Sect. B: Struct. Sci*., 1983, **39**, 280-287. DOI: https://doi.org/10.1107/S0108768183002402



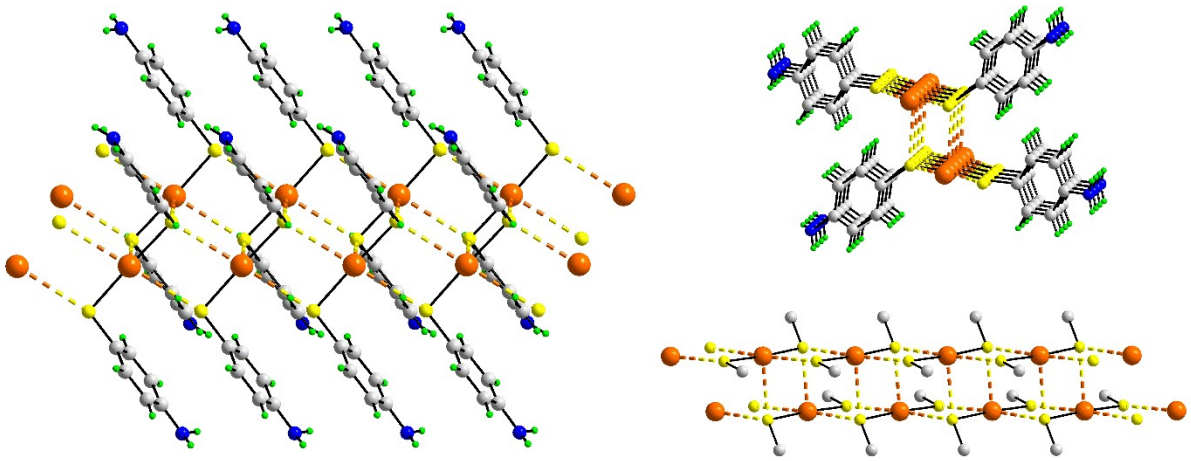
d(Hg···S) = 3.280(3) Å; Hg–S···Hg = 96.719(10)°; C–S···Hg = 82.630(11)°

Cl–Hg···S = 93.119(10) & 96.895(10)°; S–Hg···S = 83.281(9)°

{The molecule is bisected by a mirror plane; molecules assemble into a supramolecular tape *via* edge-shared (Hg–S) $\{\cdots HgS\}_2$ synthons}

35. QUGVAP bis(4-aminophenylthiolato)-mercury(II)

X. Almagro, W. Clegg, L. Cucurull-Sánchez, P. González-Duarte and M. Traveria, Schiff bases derived from mercury(II)–aminothiolate complexes as metalloligands for transition metals. *J. Organomet. Chem*., 2001, **623**, 137-148. DOI: https://doi.org/10.1016/S0022-328X(00)00672-0



d(Hg···S) = 3.185(3) Å; Hg–S···Hg = 100.84(10)°; C–S···Hg = 132.2(4)°

S–Hg···S = 80.67(9) & 100.84(9)°

d(Hg···S) = 3.252(3) Å; Hg–S···Hg = 99.17(10)°; C–S···Hg = 157.4(4)°

S–Hg···S = 79.12(9) & 99.17(9)°

d(Hg···S) = 3.146(3) Å; Hg–S···Hg = 95.95(10)°; C–S···Hg = 124.6(4)°

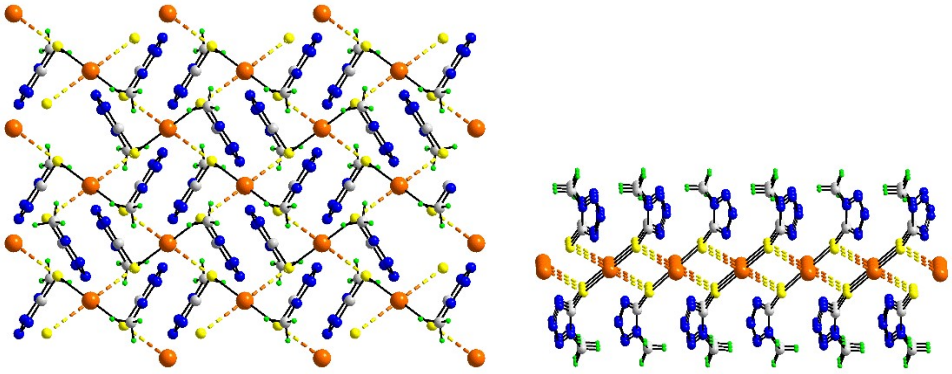
S–Hg···S = 84.06(10) & 100.02(10)°

{A supramolecular double-tape. Non-symmetric {···HgS}$_2$ synthons link molecules into a corner-shared ribbon (entries 1 & 2) and these are connected into a double ribbon *via* centrosymmetric {···HgS}$_2$ synthons. N–H···N hydrogen bonds link chains into a three-dimensional architecture}

ESI Table S5. Two-dimensional arrays featuring Hg···S secondary bonding interactions. The asterisk indicates the sulphur atom forms a Hg–S bond and also participates in an intermolecular Hg···S interaction.

36. CABSAC bis(μ-1-methyl-1H-tetrazole-5-thiolato)-mercury

M. Taheriha, M. Ghadermazi and V. Amani, Dimeric and polymeric mercury(II) complexes of 1-methyl-1,2,3,4-tetrazole-5-thiol: Synthesis, crystal structure, spectroscopic characterization, and thermal analyses. *J. Molec. Struct.*, 2016, **1107**, 57-65. DOI: https://doi.org/10.1016/j.molstruc.2015.11.012



d(Hg···S) = 3.125(2) Å; Hg–S···Hg = 119.78(9)°; C–S···Hg = 108.5(3)°

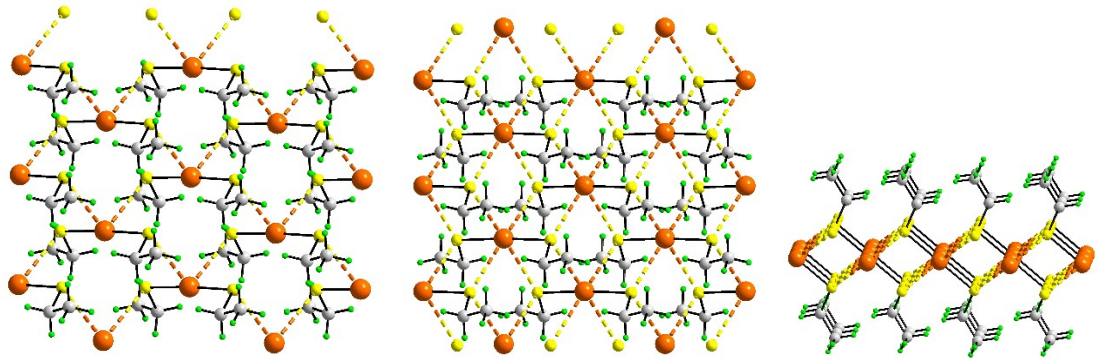
S–Hg···S = 88.02(7) & 91.98(7)°

{The Hg is located on a centre of inversion and forms two Hg···S interactions to generate a flat grid}

37. MERSET bis(ethanethiolato)-mercury(II)

K. A. Fraser, W. Clegg, D. C. Craig, M. L. Scudder and I. G. Dance, New crystal data for $[Hg(SC_2H_5)_2]$. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 1995, **51**, 406-408. DOI: https://doi.org/10.1107/S0108270194009510

D. C. Bradley and N. R. Kunchur, Structures of mercury mercaptides: Part II. X-ray structural analysis of mercury ethylmercaptide. *Can. J. Chem.*, 1965, **43**, 2786-2792. DOI: https://doi.org/10.1139/v65-389



d(Hg···S) = 3.285(2) Å; Hg–S···Hg = 100.18(5)°; C–S···Hg = 97.21(19)°

S–Hg···S = 82.29(5) & 100.18(5)°

d(Hg···S) = 3.387(2) Å; Hg–S···Hg = 97.40(5)°; C–S···Hg = 155.52(19)°

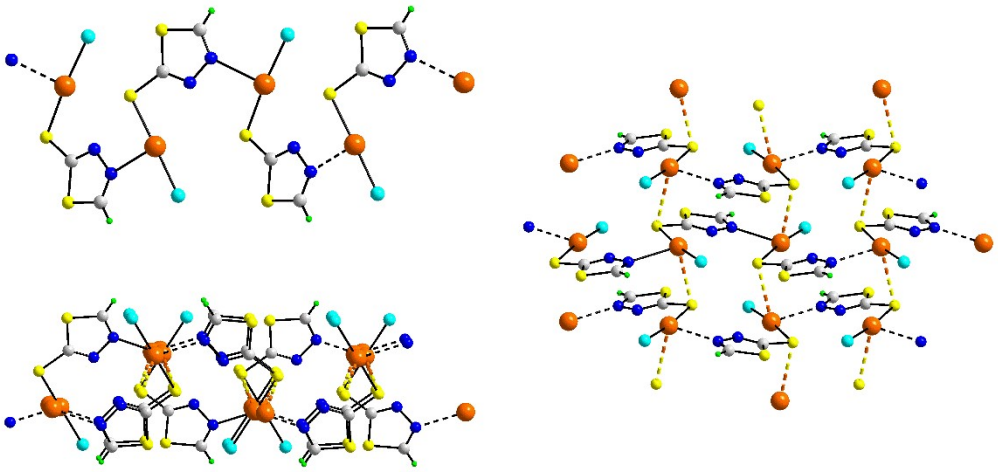
S–Hg···S = 80.05(5) & 97.40(5)°

{The Hg atom is located on a two-fold axis of symmetry. A two-dimensional array constructed from eight-membered {···SHgS···HgS···Hg···HgS} synthons. If a longer *d*(Hg···S) = 3.387(2) Å contact is taken into consideration, a supramolecular grid arises as the original grid now encompasses non-symmetric $\{\cdots HgS\}_2$. The topology of the layer is flat}

ESI Table S6. Aggregation patterns featuring Hg···S secondary bonding interactions in supramolecular coordination polymers. The asterisk indicates the sulphur atom forms a Hg–S bond and also participates in an intermolecular Hg···S interaction.

38. NAKGUD *catena*-((1,3,4-thiadiazole-2-thiolato)-chloro-mercury(II))

P.-Z. Hu, J.-G. Wang, J. Liu and B.-T. Zhao, Two novel crystal structures of 2-mercapto-1,3,4-thiadiazole complexes with mercury (II) chloride. *J. Chem. Crystallogr.*, 2010, **40**, 825-830. DOI: https://doi.org/10.1007/s10870-010-9747-1



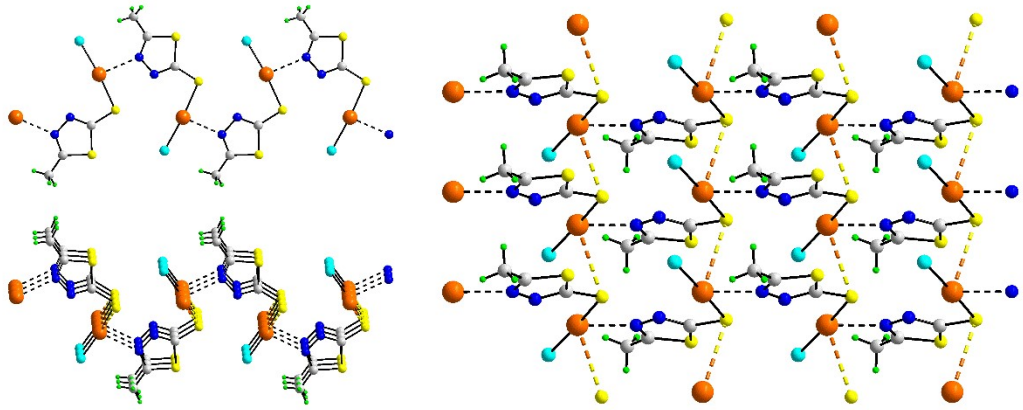
d(Hg···S) = 3.1313(16) Å; Hg–S···Hg = 86.75(4)°; C–S···Hg = 93.02(16)°

Cl–Hg···S = 88.85(4)°; S–Hg···S = 96.90(4)°

{A helical (2_1-screw) one-dimensional coordination polymer is formed through *d*(Hg···N) = 2.623(5) Å contacts. These are linked into a flat, two-dimensional array by Hg···S contacts}

39. PILTEM *catena*-[(μ-5-methyl-1,3,4-thiadiazole-2-thiolato)-chloro-mercury(II)]

L.-W. Liu and B.-T. Zhao, The crystal structure of catena-poly[chlorido-(μ_2-5-methyl-1,3,4-thiadiazole-2-thiolato-κ^2S:N)mercury(II)], $C_3H_3ClHgN_2S_2$. *Z. Kristallogr. - New Cryst. Struct.*, 2018, **233**, 547-548. DOI: https://doi.org/10.1515/ncrs-2017-0277



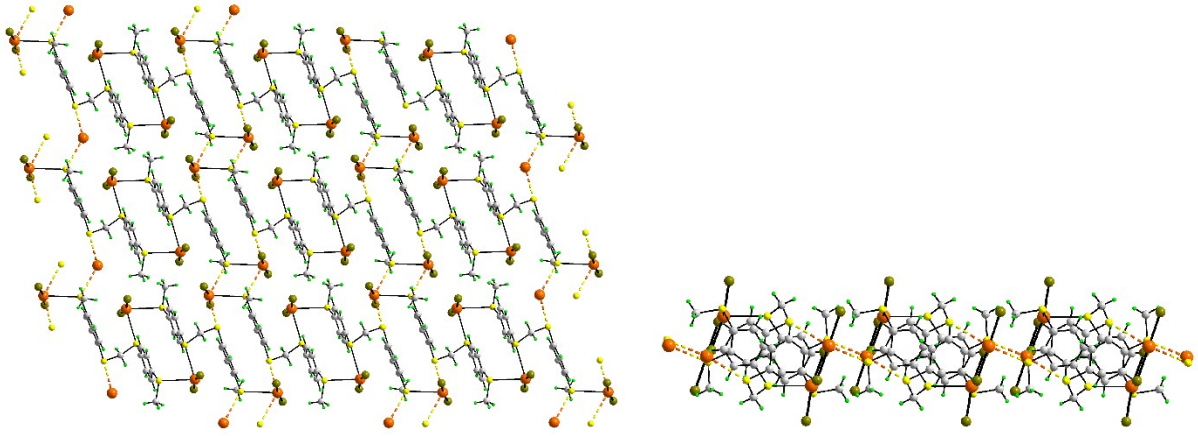
d(Hg···S) = 3.331(6) Å; Hg–S···Hg = 89.60(16)°; C–S···Hg = 80.6(6)°

Cl–Hg···S = 88.31(18)°; S–Hg···S = 89.60(16)°

{A flattened, helical (2_1-screw axis) one-dimensional coordination polymer. Connected into a two-dimensional array by strings of zig-zag $\{\cdots HgS\}_n$ chains}

40. ASAMEO *catena*-[(μ-1-(methylsulfanyl)-4-((((4-(methylsulfanyl)phenyl)sulfanyl)methyl)-sulfanyl)benzene)-tetrabromo-di-mercury]

M. Chaabéne, A. Khatyr, M. Knorr, M. Askri, Y. Rousselin and M. M. Kubicki, Bis{(4-methylthio)phenylthio}methane as assembling ligand for the construction of Cu(I) and Hg(II) coordination polymers. Crystal structures and topological (AIM) analysis of the bonding. *Inorg. Chim. Acta*, 2016, **451**, 177-186; DOI: https://doi.org/10.1016/j.ica.2016.07.023



d(Hg···S) = 3.169(2) Å; Hg–S···Hg = 112.13(8)°; methyl-C–S···Hg = 106.3(4)°; C–S···Hg = 115.6(4)°

Br–Hg···S = 86.8(6) & 97.0(6)°; S–Hg···S = 67.9(7)°

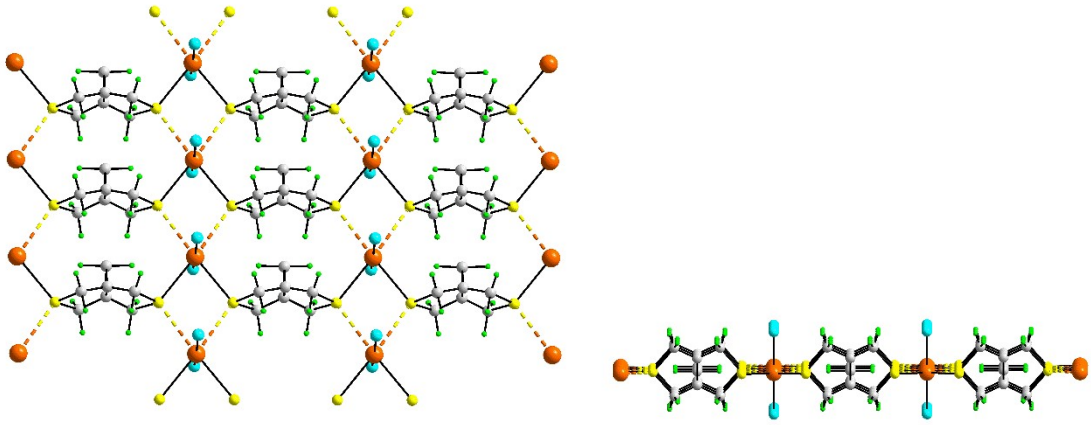
d(Hg···S) = 3.185(3) Å; methylene-C–S···Hg = 110.6(4)°; C–S···Hg = 125.3(4)°

Br–Hg···S = 79.9(6) & 101.7(6)°; S–Hg···S = 71.2(7)°

{Two $HgBr_2$ molecules and one organic molecule comprise the asymmetric-unit. One $HgBr_2$ molecule forms one Hg–S bond while the other forms two Hg–S bonds so one-dimensional coordination polymer eventuates (running across the page). These are connected into a flat layer by Hg···S interactions involving the same mercury atom leading to centrosymmetric $\{\cdots Hg–S\}_2$ synthons (entry 1) and stand-alone Hg···S contacts; the second independent mercury atom does not form Hg···S contacts}

41. FAJNUZ *catena*-((μ_4-dithia(3.3.1)propellane)-dichloro-mercury)

F. H. Herbstein, P. Ashkenazi, M. Kaftory, M. Kapon, G. M. Reisner and D. Ginsburg, Propellanes LXXIX. Comparison of the geometries of dithia[n.3.3]propellanes (n = 1, 2, 3) and dithia(and oxathia)[4.3.3]propellanes. Study of the influence of complexation with $HgCl_2$, I_2, $CdCl_2$ and $PdCl_2$ and of formation of sulfoxides on some of these compounds. Demonstration of the 'Klammer' effect. Structures of eighteen crystals. *Acta Crystallogr., Sect. B: Struct. Sci.*, 1986, **42**, 575-601; DOI: https://doi.org/10.1107/S0108768186097689



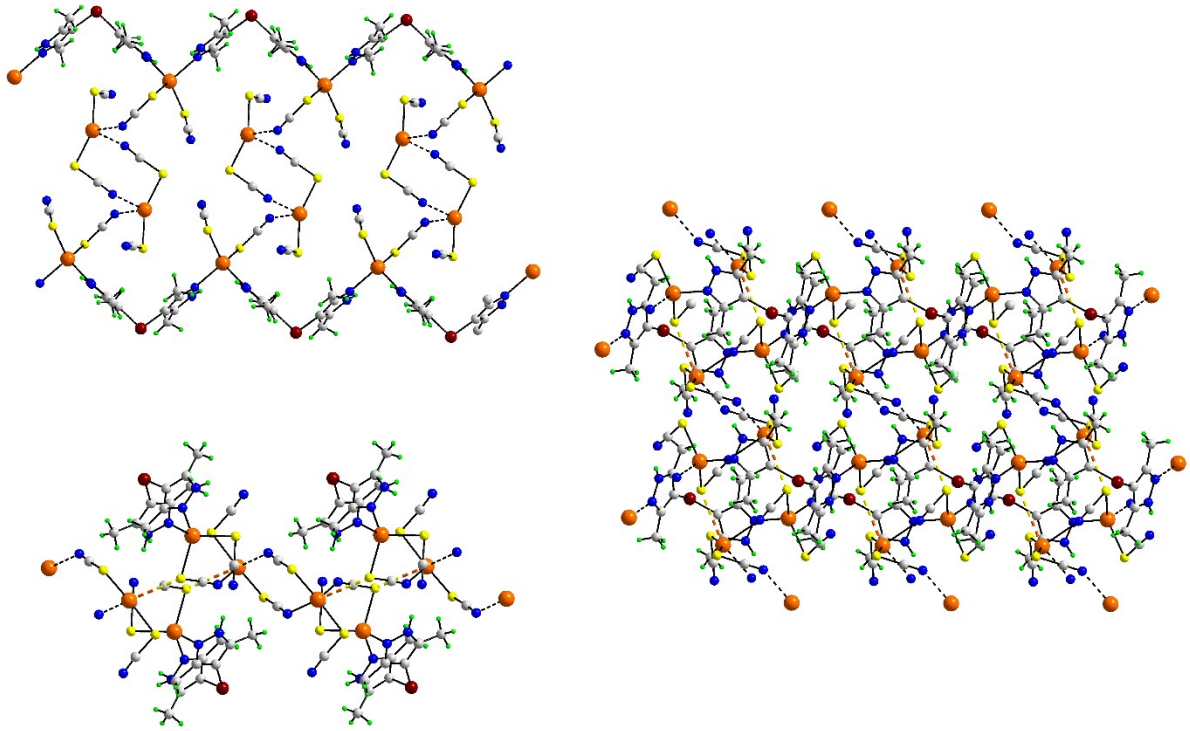
d(Hg···S) = 3.212(3) Å; Hg–S···Hg = 107.69(6)°; 2 × methylene-C–S···Hg = 114.7(3)°

Cl–Hg···S = 2 × 86.36(16)°; S–Hg···S = 107.69(6) & 176.85(6)°

{The $HgCl_2$ molecule lies on a site of symmetry mm2 and is connected into a linear chain (across the page) through Hg–S [2.979(3) Å] bonds, and forms two equivalent Hg···S interactions to a form a flat layer through {···HgSHgS···} synthons}

42. PIHCEP *catena*-((μ_2-trans-bis(3,5-dimethyl-1H-pyrazol-4-yl)selenide)-bis(μ_2-thiocyanato)-bis(thiocyanato)-di-mercury(II))

M. Seredyuk, M. Haukka, I. O. Fritsky, H. Kozłowski, R. Krämer, V. A. Pavlenko and P. Gütlich, Bis(3,5-dimethyl-1H-pyrazolyl)selenide – a new bidentate bent connector for preparation of 1D and 2D co-ordination polymers. *Dalton Trans.*, 2007, 3183-3194. DOI: https://doi.org/10.1039/b702574b



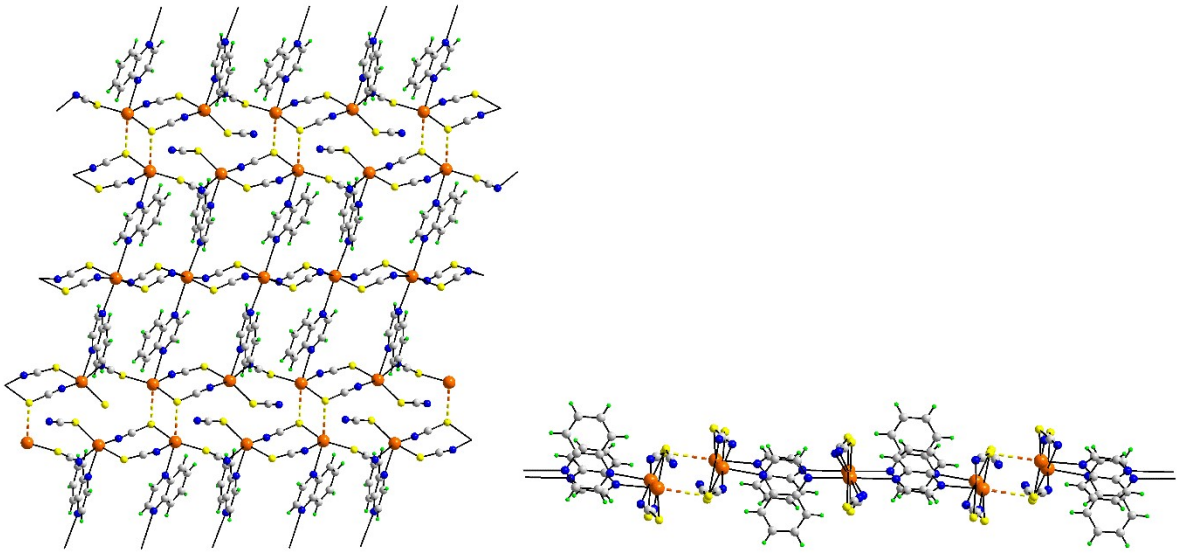
d(Hg···S) = 3.3471(9) Å; Hg–S···Hg = 130.35(3)°; C–S···Hg = 108.46(15)°

S–Hg···S = 75.89(3) & 96.23(3)°

{A double-chain is formed through *d*[Hg···N(pyrazolyl)] = 2.252(3) & 2.258(3) Å and *d*[Hg···N(nitrile)] = 2.491(3) & 2.514(3) Å and non-symmetric, eight-membered {··· $HgSCN\}_2$ synthons. These are connected into a two-dimensional array *via* Hg···S(terminal thiocyanate) interactions and centrosymmetric, eight-membered {··· $Hg{\cdots}SCN\}_2$ synthons}

43. GUVKOZ *catena*-[pentakis(μ-isothiocyanato)-(μ-quinoxaline)-(isothiocyanato)-(quinoxaline)-tri-mercury]

Y. Hou, M. Y. Masoomi, M. Bagheri, A. Morsali and S. W. Joo, Two reversible transformable mercury(II) coordination polymers as efficient adsorbents for removal of dibenzothiophene. *RSC Advances*, 2015, **5**, 81356-81361; DOI: https://doi.org/10.1039/C5RA12686J



d(Hg···S) = 3.298(1) Å; Hg–S···Hg = 96.78(4)°; C–S···Hg = 93.44(15)°

S–Hg···S = 83.22(4) & 88.06(4)°; N···Hg···S = 79.48(9) & 163.29(9)°

{There are three independent mercury atoms in the asymmetric unit. One forms a chain comprising concatenated $\{Hg(NCS)\}_2$ eight-membered rings, Chain_1; the rings are centrosymmetric. The other two mercury atoms are connected into an independent chain, Chain_2, with $\{Hg(NCS)\}_2$ eight-membered rings connected by –NCS– bridges and with one thiocyanate molecule being S-monodentate. The chains are bridged by μ-quinoxaline molecules leading to a supramolecular tape, formulated as Chain_2(μ-quinoxaline)Chain_1(μ-quinoxaline)Chain_2. The outer chains are connected to centrosymmetrically-related tapes *via* centrosymmetric $\{\cdots HgS\}_2$ synthons to form a supramolecular layer with a flattened-step topology}

ESI Table S7. QTAIM parameters (a.u.) for the bond critical points that characterise the spodium bonds. [a]

Cmpd	Interaction	ϱ	G	V	H	$\nabla^2\varrho$	ϵ
4	Hg···S	0.0279	0.0180	-0.0196	-0.0016	0.0654	0.0862
6	Hg···S	0.0171	0.0108	-0.0105	0.0003	0.0441	0.1013
	Hg···S	0.0198	0.0124	-0.0125	-0.0001	0.0494	0.0667
16	Hg···S	0.0204	0.0125	-0.0128	-0.0002	0.0491	0.0424
	Hg···S	0.0161	0.0103	-0.0097	0.0005	0.0432	0.0620
	Hg···S	0.0188	0.0121	-0.0119	0.0002	0.0495	0.0602
	Hg···Cl	0.0436	0.0353	-0.0394	-0.0041	0.1246	0.0164
18	Hg···S	0.0184	0.0118	-0.0115	0.0003	0.0482	0.1095
20	Hg···S	0.0155	0.0090	-0.0086	0.0004	0.0376	0.1176
	Hg···S	0.0116	0.0074	-0.0064	0.0009	0.0333	0.1027
38	Hg···N	0.0356	0.0311	-0.0323	-0.0012	0.1197	0.0528
39	Hg···N	0.0347	0.0294	-0.0306	-0.0011	0.1133	0.0534
	Hg···S	0.0149	0.0091	-0.0086	0.0005	0.0384	0.0324
	Hg···Cl	0.0145	0.0101	-0.0090	0.0011	0.0447	0.0458
42	Hg···N	0.0442	0.0413	-0.0438	-0.0024	0.1558	0.0185

a Abbreviations: electron-density (ϱ), total, Lagrangian kinetic and potential energy densities (H, G and V, respectively) and the Laplacian of the electron-density ($\nabla^2\varrho$) and ellipticity (ϵ)