On the nature and interplay of Hg···O/S spodium-bonding and O···S chalcogen-bonding in one-dimensional phenylmercury(II) 3-alkoxycyclobutene-1,2-dione-4-thiolate coordination polymers

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ELECTRONIC SUPPLEMENTARY INFORMATION

ESI Figure S1. ^{1}H NMR spectrum for **PhHg^{Me}** recorded in $CDCl_3$ solution.

ESI Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum for **PhHg^{Me}** recorded in $CDCl_3$ solution.

ESI Figure S3. ^{1}H NMR spectrum for **PhHg^{Et}** recorded in $CDCl_3$ solution.

ESI Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum for **PhHg^{Et}** recorded in $CDCl_3$ solution.

ESI Figure S5. Electronic absorption spectra for **PhHgL^{Me}** (black trace) and **PhHg^{Et}** recorded in 1×10^{-4}M dichloromethane solution.

ESI Figure S6. Molecular structure of the second independent molecule in the crystal of **PhHgL^{Me}** showing atom labelling scheme and displacement ellipsoids at the 35% probability level.

ESI Figure S7. Linear supramolecular chain featuring Hg···O spodium-bonding formed between Hg2-containing molecules in the crystal of **PhHgL^{Me}**.

ESI Figure S8. The molecular structure of **PhHgL^{Et}**, including the statistically disordered components indicated with hollow bonds.

ESI Figure S9. Calculated Hirshfeld surfaces for the second independent molecule of **PhHgL^{Me}**: (a) d_{norm}-plot, (b) shape-index plot and (c) curvedness plot.

ESI Figure S10. The overall and delineated two-dimensional fingerprint plots for (a) **PhHgL^{Me}**, (b) the Hg1-moleule of **PhHgL^{Me}**, (c) the Hg2-moleule of **PhHgL^{Me}** and (d) **PhHgL^{Et}**.

ESI Table S1 Percentage contributions of interatomic contacts to the calculated Hirshfeld surfaces of **PhHgL^{Me}** and **PhHgL^{Et}**.

ESI Figure S11. MEP surface plots calculated for the experimental geometries for (a) the second independent molecule of **PhHgL^{Me}** and (b) **PhHgL^{Et}**. The isosurfaces for both MEPs was 0.0004 a.u. and the plots were rendered between –0.046 to +0.046 a.u. and –0.052 to +0.052 a.u., respectively.

ESI Figure S12. Plots of the reduced density gradient (RDG) *versus* the electron density multiplied by the sign of the second Hessian eigenvalue in atomic units for (a) **PhHgL^{Me}** – first independent molecule, (b) **PhHgL^{Me}** – second independent molecule and (c) **PhHgL^{Et}**.

ESI Figure S13. The non-covalent interaction (NCI) plot for **PhHgL^{Me}** highlighting Hg···O spodium-bonding within the supramolecular chain comprising the second independent molecule.

ESI Table S2 Listing of the topographical parameters of key inter- and intra-molecular interactions calculated at the bond critical points of the interacting atom centres for **PhHgL^{Me}** and **PhHgL^{Et}**.

ESI Table S3 Listing of the Wiberg bond indices, Mayer bond orders, delocalisation indices and natural charges characterising the Hg···O/S spodium-bonding and O···S chalcogen-bonding in **PhHgL^{Me}** – first independent molecule, **PhHgL^{Me}** – second independent molecule and **PhHgL^{Et}**.

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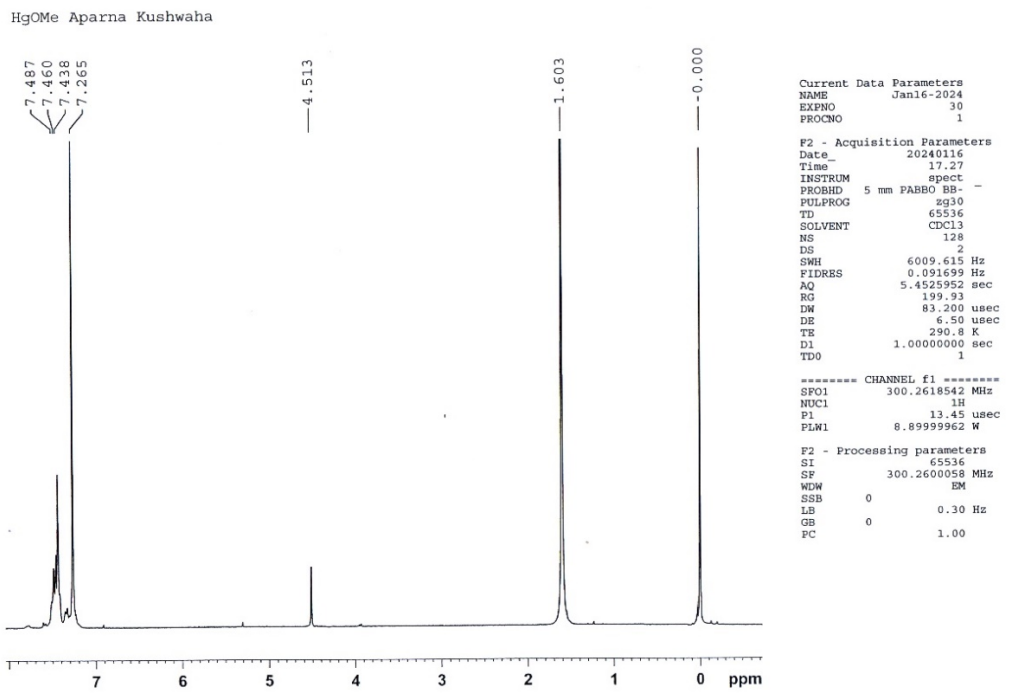
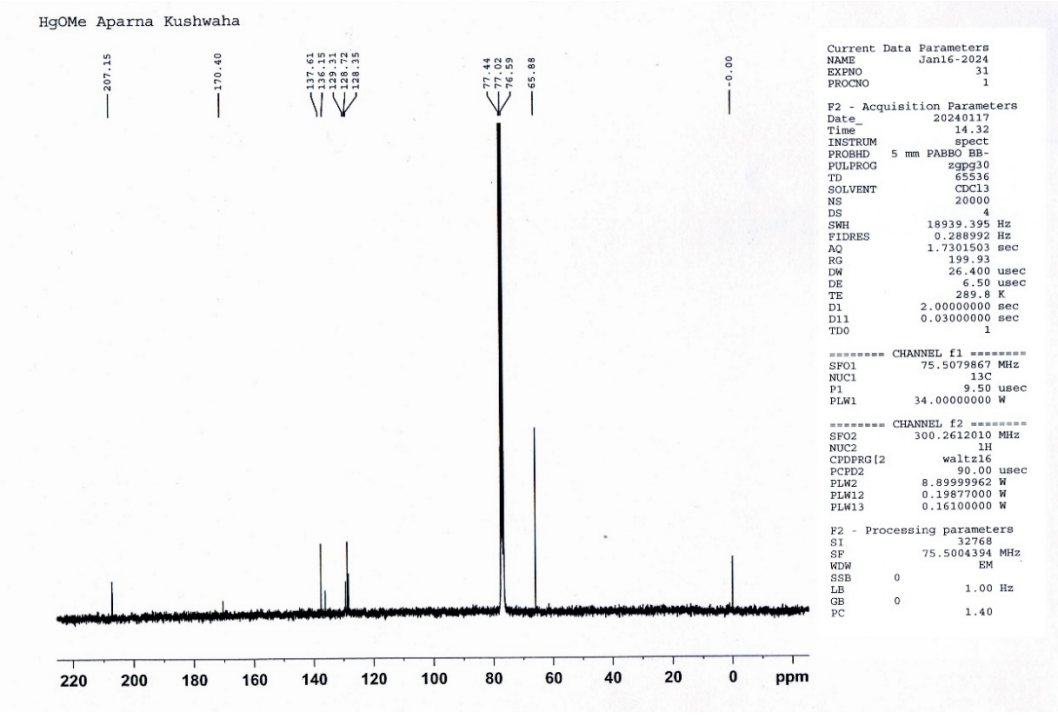
ESI Figure S15. Illustrations of the NBOs involved in the LP(O) → σ*(Hg–C) donor/acceptor interactions for the (a) first independent molecule and (b) second independent molecule of **PhHgL^{Me}**. The second-order perturbation energies are indicated and have units of kJ/mol.

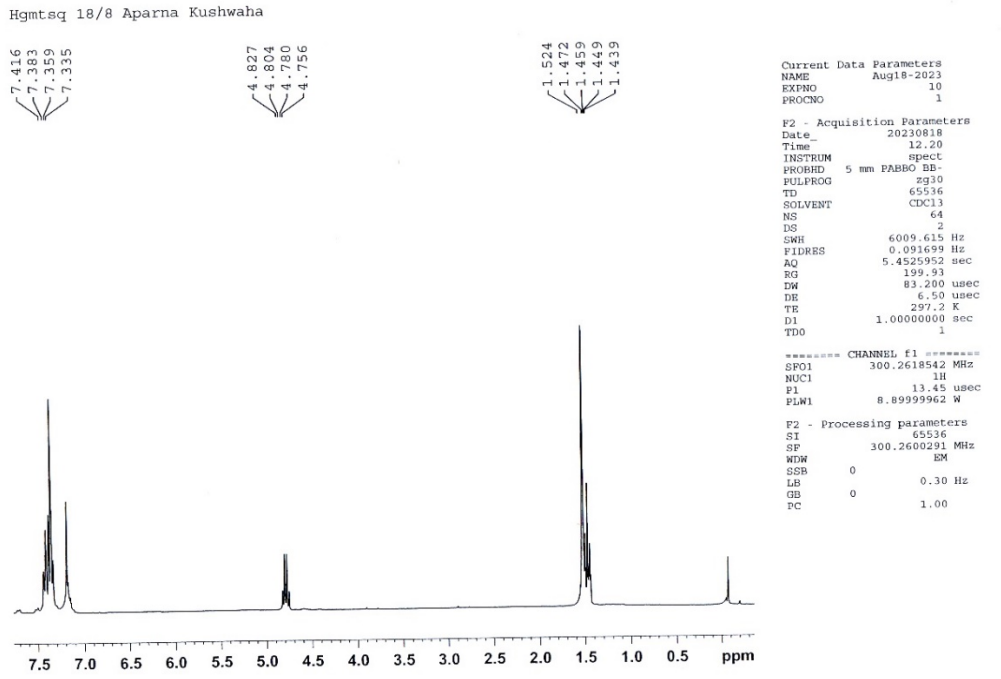
ESI Table S4 Listing of the coordinates for the calculated molecules and aggregates.



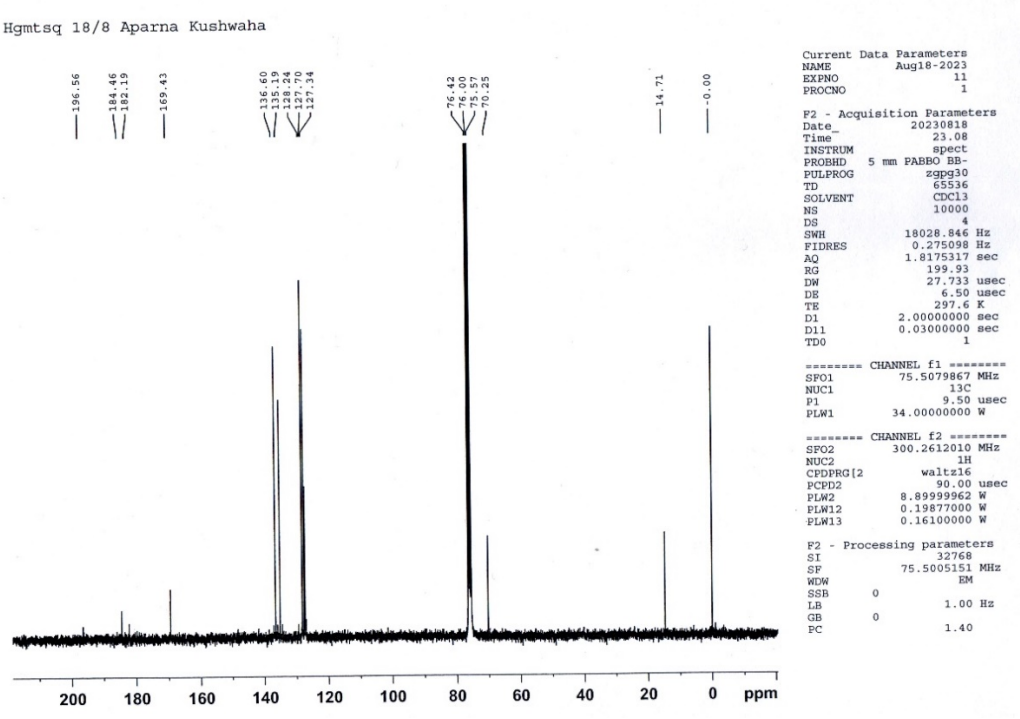
ESI Figure S1. ^{1}H NMR spectrum for **PhHg^{Me}** recorded in $CDCl_3$ solution.



ESI Figure S2. ^{13}C{^{1}H} NMR spectrum for **PhHg^{Me}** recorded in $CDCl_3$ solution.



ESI Figure S3. ^{1}H NMR spectrum for **PhHg^{Et}** recorded in $CDCl_3$ solution.



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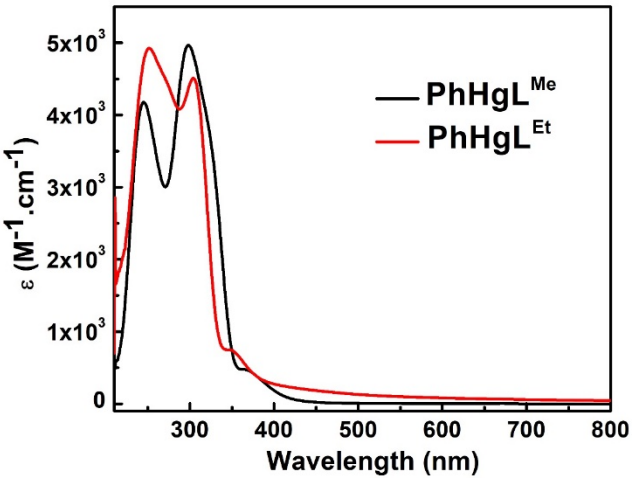
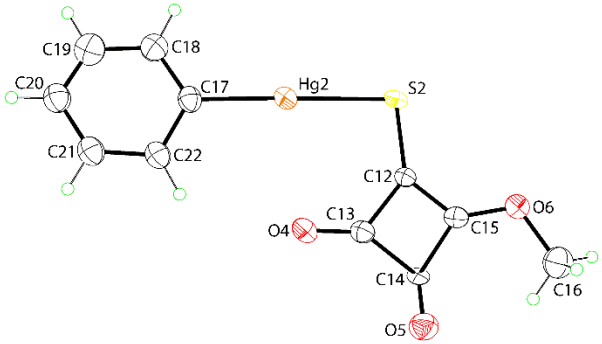
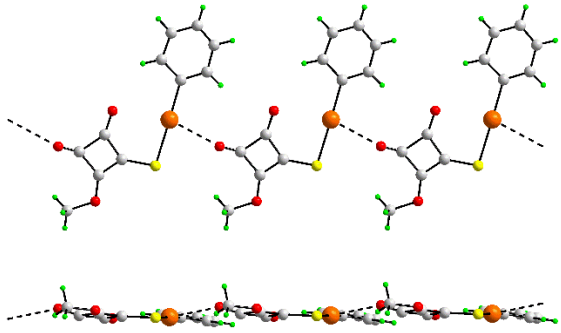


ESI Figure S5. Electronic absorption spectra for **PhHgL^{Me}** (black trace) and **PhHg^{Et}** recorded in 1×10^{-4}M dichloromethane solution.

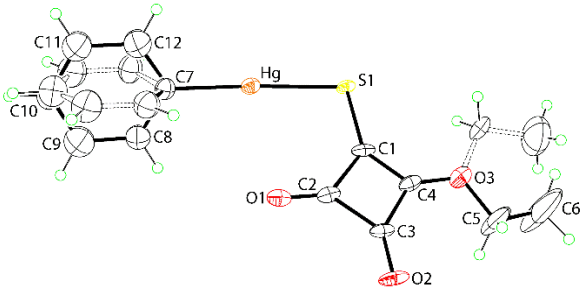
Compound	**λ_{max} (nm)**	**ε ($M^{-1}cm^{-1}$)**
PhHgL^{Me}	244	4.2×10^3
	298	4.9×10^3
	370	4.9×10^2
PhHgL^{Et}	252	4.9×10^3
	303	4.5×10^3
	351	7.6×10^2



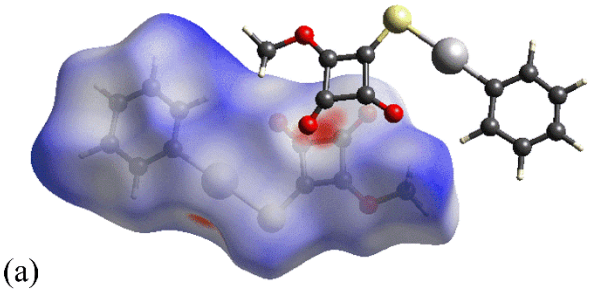
ESI Figure S6. Molecular structure of the second independent molecule in the crystal of **PhHgL^{Me}**, showing atom labelling scheme and displacement ellipsoids at the 35% probability level.



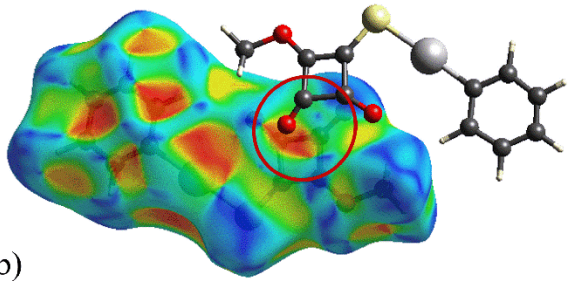
ESI Figure S7. Linear supramolecular chain featuring Hg···O spodium-bonding formed between Hg2-containing molecules in the crystal of **PhHgL^{Me}**.



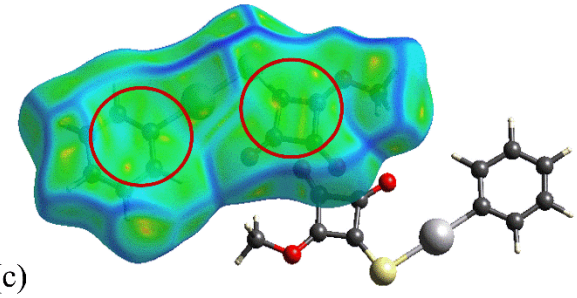
ESI Figure S8. The molecular structure of **PhHgL^{Et}**, including the statistically disordered components indicated with hollow dashed bonds.



(a)



(b)

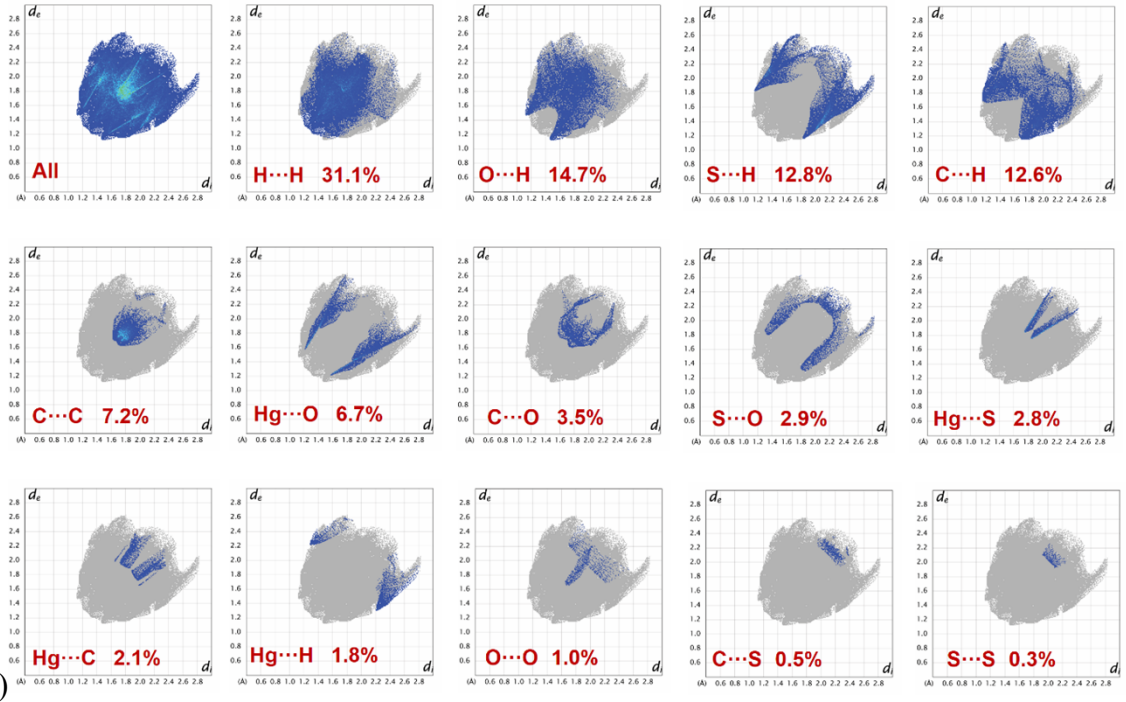


(c)

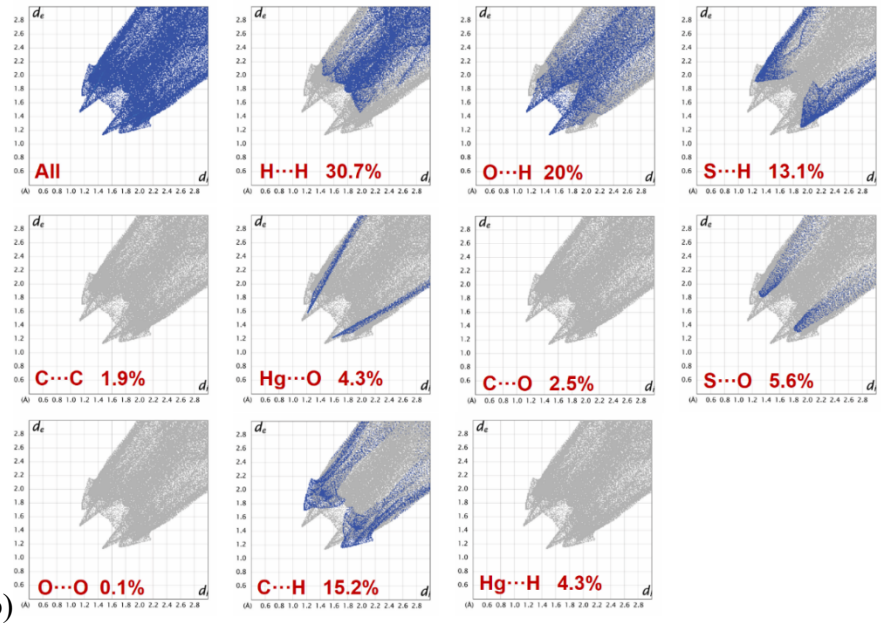
ESI Figure S9. Calculated Hirshfeld surfaces for the second independent molecule of **PhHgL^{Me}**: (a) d_{norm}-plot, (b) shape-index plot and (c) curvedness plot.

ESI Table S1 Percentage contributions of interatomic contacts to the calculated Hirshfeld surfaces of **PhHgL^{Me}** (overall and individual molecules) and **PhHgL^{Et}**

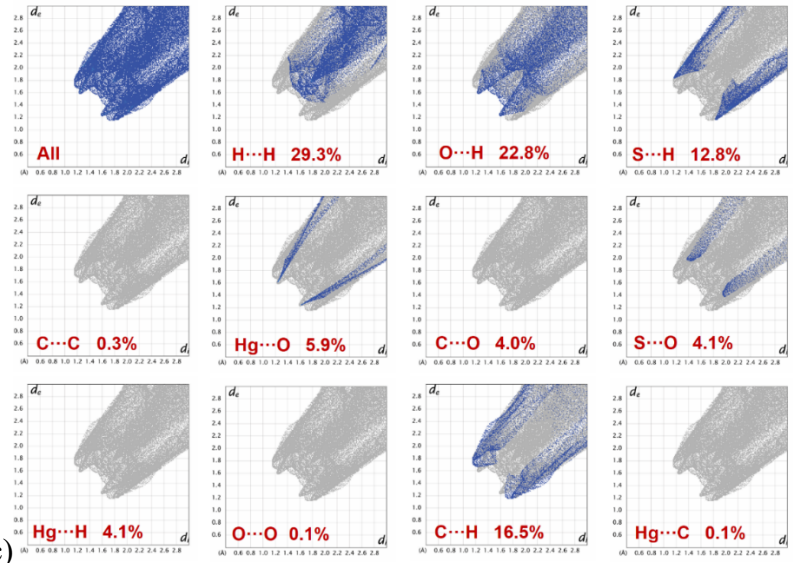
Contact	**PhHgL^{Me}** overall	**PhHgL^{Me}** Hg1-molecule	**PhHgL^{Me}** Hg2-molecule	**PhHgL^{Et}** *cf*. Fig. 3 in main text
H···H	31.1	29.3	30.5	40.6
O···H/H···O	14.7	17.3	16.6	12.3
S···H/H···S	12.8	11.2	11.5	4.7
C···H/H···C	12.6	11.9	11.1	12.3
C···C	7.2	6.6	6.7	3.7
Hg···O/O···Hg	6.7	5.6	5.9	4.8
C···O/O···C	3.5	7.7	7.8	8.6
S···O/O···S	2.9	2.7	2.1	3.9
Hg···S/Hg···S	2.8	2.5	2.6	4.6
Hg···C/C···Hg	2.1	1.7	1.8	0.0
Hg···H/H···Hg	1.8	1.7	1.6	0.8
O···O	1.0	1.1	1.1	1.9
S···C/C···S	0.5	0.4	0.5	1.7
S···S	0.3	0.2	0.2	0.0


All
H···H 31.1%
O···H 14.7%
S···H 12.8%
C···H 12.6%
C···C 7.2%
Hg···O 6.7%
C···O 3.5%
S···O 2.9%
Hg···S 2.8%
Hg···C 2.1%
Hg···H 1.8%
O···O 1.0%
C···S 0.5%
S···S 0.3%

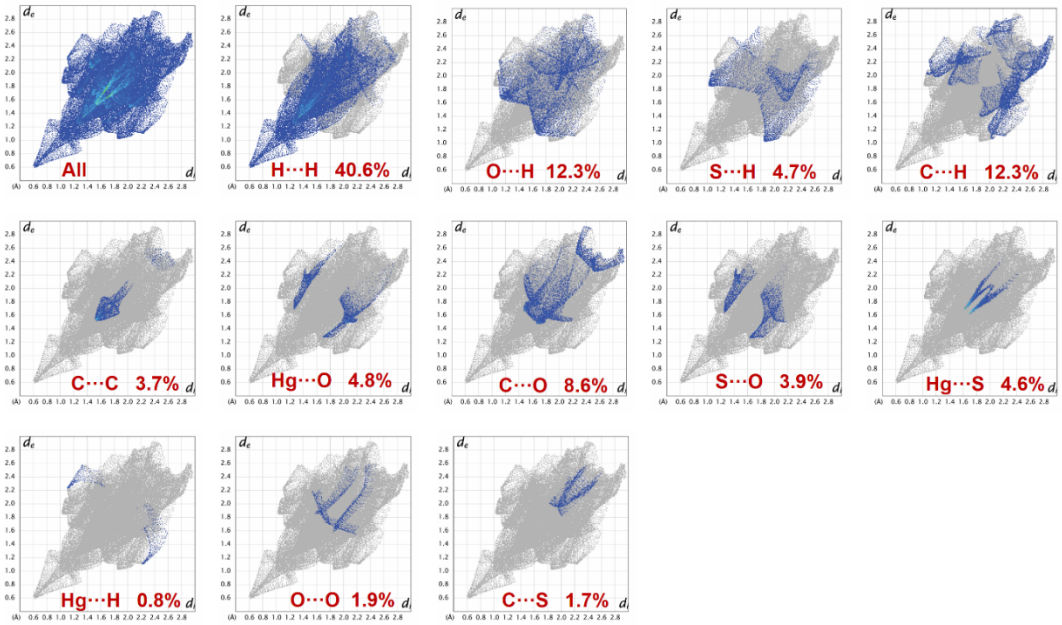
(a)


All
H···H 30.7%
O···H 20%
S···H 13.1%
C···C 1.9%
Hg···O 4.3%
C···O 2.5%
S···O 5.6%
O···O 0.1%
C···H 15.2%
Hg···H 4.3%

(b)

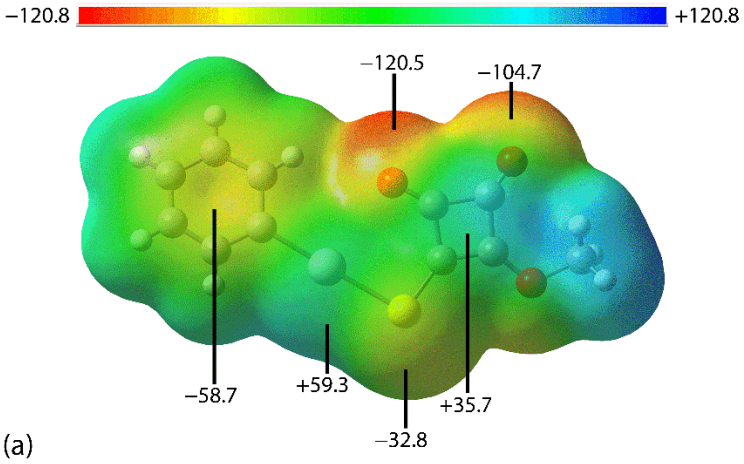


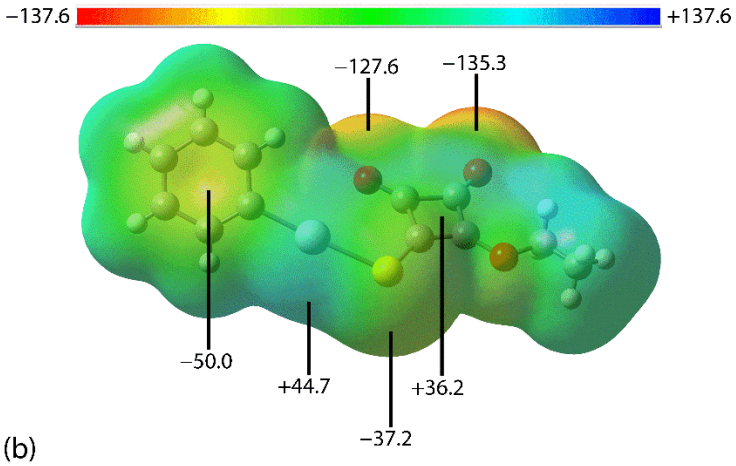
(c)



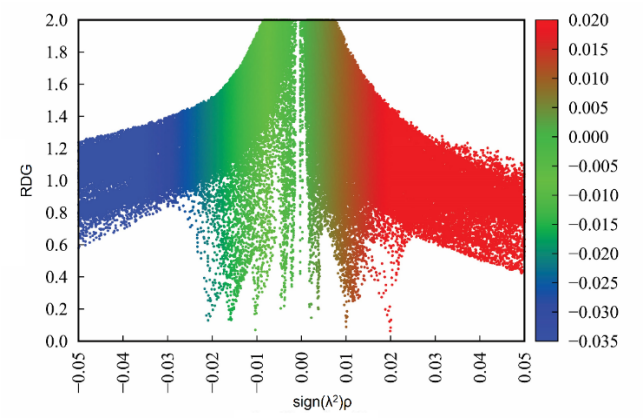
(d)

ESI Figure S10. The overall and delineated two-dimensional fingerprint plots for (a) **PhHgL^{Me}**, (b) the Hg1-molecule of **PhHgL^{Me}**, (c) the Hg2-molecule of **PhHgL^{Me}** and (d) **PhHgL^{Et}**. The squid-like shape in the fingerprint plots for **PhHgL^{Et}** arises from chemically irrelevant, impossibly short contacts between hydrogen atoms of the disordered residues.

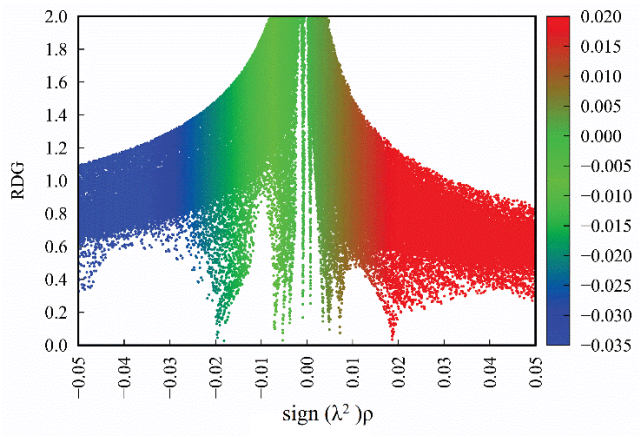




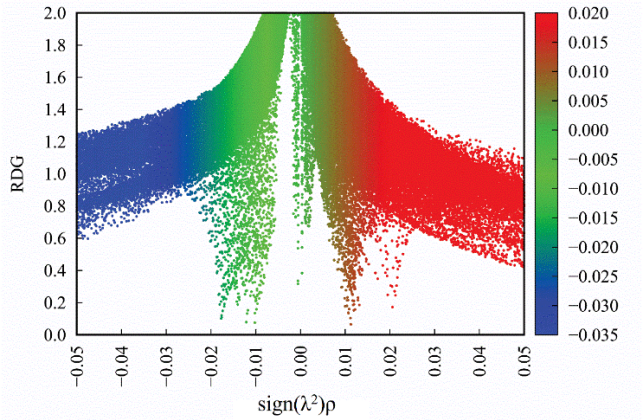
ESI Figure S11. MEP surface plots calculated for the experimental geometries for (a) the second independent molecule of **PhHgL^{Me}** and (b) **PhHgL^{Et}**. The indicated energies are in units of kJ/mol. The isosurfaces for both MEPs was 0.0004 a.u. and the plots were rendered between –0.046 to +0.046 a.u. and –0.052 to +0.052 a.u., respectively.



(a)

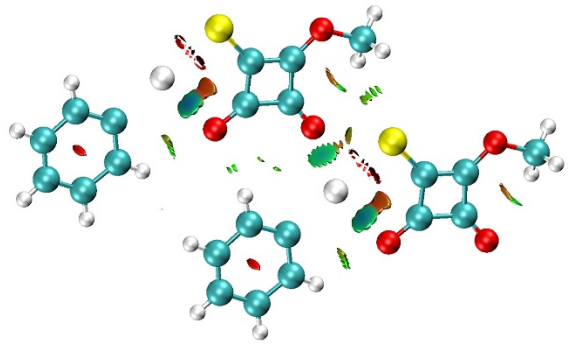


(b)



(c)

ESI Figure S12. Plots of the reduced density gradient (RDG) *versus* the electron density multiplied by the sign of the second Hessian eigenvalue in atomic units for (a) **PhHgL^{Me}** – first independent molecule, (b) **PhHgL^{Me}** – second independent molecule and (c) **PhHgL^{Et}**.



ESI Figure S13. The non-covalent interaction (NCI) plot for **PhHgL^{Me}** highlighting Hg···O spodium-bonding within the supramolecular chain comprising the second independent molecule.

ESI Table S2 The topographical parameters of inter- and intra-molecular interactions calculated at bond critical points of interacting atom centre for **PhHgL^{Me}** – first independent molecule, **PhHgL^{Me}** – second independent molecule and **PhHgL^{Et}**.

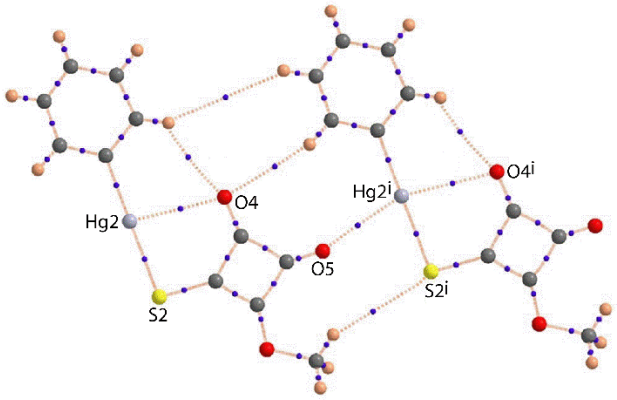
Interaction Type	P_{BCP}	$\nabla^2\rho_{BCP}$	ε	H	E (kJ/mol)
PhHgL^{Me} – first independent molecule					
Hg···O1	+0.0164	+0.0459	+0.0319	-0.0002	15.59
Hg^{i}···O1^{i}	+0.0162	+0.0449	+0.0407	–0.0003	15.44
(i: ½ + *x*, ½ + *y*, *z*)					
Hg···O2^{i}	+0.0212	+0.0787	+0.0756	+0.0010	23.30
(i: ½ + *x*, ½ + *y*, *z*)					
C14···O2	+0.0031	+0.0114	+0.6108	+0.0006	7.28
C3···O5	+0.0087	+0.0308	+0.6420	+0.0007	6.32
PhHgL^{Me} – second independent molecule					
Hg2···O4	+0.0211	+0.0624	+0.0052	–0.0004	21.67
Hg2^{i}···O4^{i}	+0.0218	+0.0636	+0.0093	-0.0004	21.92
(i: –½ + *x*, –½ + *y*, *z*)					
Hg2···O5^{i}	+0.0181	+0.0654	+0.1119	+0.0001	19.08
(i: –½ + *x*, –½ + *y*, *z*)					
PhHgL^{Et}					
Hg···O1	+0.0180	+0.0516	+0.0214	–0.0003	17.53
Hg^{i}···O1^{i}	+0.0179	+0.0509	+0.0268	–0.0003	17.74
Hg···O2^{i}	+0.0143	+0.0469	+0.2335	–0.0003	14.39
(i: *x*, –1 + *y*, *z*)					

O2···S1^{i}	+0.0122	+0.0492	+1.0737	+0.0014	12.52
(i: x, –1 + y, z)					
Hg···S1^{ii}	+0.0146	+0.0387	+0.1299	+0.0007	11.00
(ii: 1 – x, 2 – y, 1 – z)					
Hg···S1^{iii}	+0.0145	+0.0385	+0.1297	+0.00069	10.99
(iii: – x, 2 – y, 1 – z)					
C2···C3^{iv}	+0.0075	+0.0281	+1.7138	+0.0016	5.21
(iv: – x, 1 – y, 1 – z)					
C2^{i} ···C3^{v}	+0.0074	+0.0274	+1.7140	+0.0017	5.16
(v: 1 – x, 1 – y, 1 – z)					

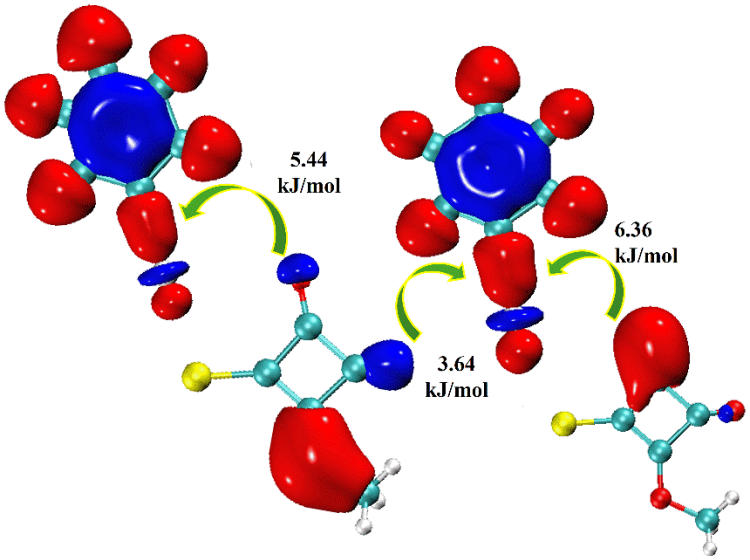
ESI Table S3 Listing of the Wiberg bond indices, Mayer bond orders, delocalisation indices and natural charges characterising the Hg···O/S spodium-bonding and O···S chalcogen-bonding in **PhHgL^{Me}** – first independent molecule, **PhHgL^{Me}** – second independent molecule and **PhHgL^{Et}**.

Bond	Wiberg bond index	Mayer bond order	Delocalisation index (basin)	Atom	Natural charge
PhHgL^{Me} – first independent molecule					
Hg1···O1	0.077	0.144	0.135	Hg1	0.787
Hg1^{i}···O1^{i}	0.078	0.142	0.136	O1	–0.565
(i: ½ + *x*, ½ + *y*, *z*)					
Hg1···O2^{i}	0.070	0.117	0.148	O2	–0.582
(i: ½ + *x*, ½ + *y*, *z*)					
PhHgL^{Me} – second independent molecule					
Hg2···O4	0.078	0.143	0.134	Hg2	0.788
Hg2^{i}···O4^{i}	0.079	0.140	0.147	O4	–0.564
(i: –½ + *x*, –½ + *y*, *z*)					
Hg2···O5^{i}	0.071	0.116	0.149	O5	–0.580
(i: –½ + *x*, –½ + *y*, *z*)					
PhHgL^{Et}					
Hg···O1	0.074	0.147	0.140	Hg	0.824
Hg^{i}···O1^{i}	0.074	0.147	0.142	O1	–0.548
(i: *x*, –1 + *y*, *z*)					
Hg···O2^{i}	0.052	0.095	0.099	O2	–0.560

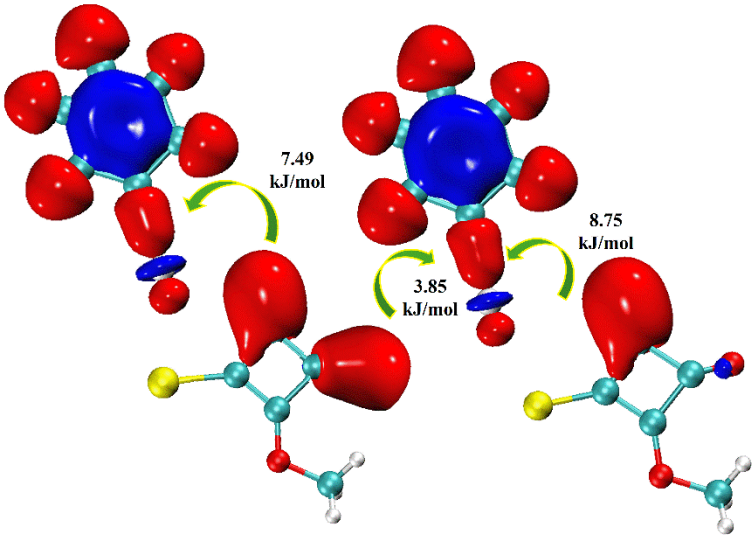
(i: x, $-1 + y$, z)					
O2···S1[i]	0.0122	0.029	0.096	S1	–0.156
(i: x, $-1 + y$, z)					
Hg···S1[ii]	0.075	0.084	0.127	S1	–0.157
(ii: $1 - x$, $2 - y$, $1 - z$)					
Hg···S1[iii]	0.074	0.083	0.126	S1[i]	–0.156
(iii: $- x$, $2 - y$, $1 - z$)					
C2···C3[iv]	0.0038	0.0067	0.012	C2	0.452
(iv: $- x$, $1 - y$, $1 - z$)					
C2···C3[v]	0.0039	0.0071	0.011	C3	0.399
(v: $1 - x$, $1 - y$, $1 - z$)					



ESI Figure S14. QTAIM analysis (BCPs are represented as blue spheres and bond paths as dotted orange lines) highlighting the Hg···O spodium bonding involving the second independent molecule of **PhHgL^{Me}**.



(a)



(b)

ESI Figure S15. Illustrations of the NBOs involved in the LP(O) → σ*(Hg–C) donor/acceptor interactions for the (a) first independent molecule and (b) second independent molecule of **PhHgL^{Me}**. The second-order perturbation energies are indicated and have units of kJ/mol.

ESI Table S4 Listing of the coordinates for the calculated molecules and aggregates.

Coordinates for the calculated monomer of PhHgL^{Me}

0 1

O	-0.22252500	-0.29795000	10.47676200
C	-4.09103800	-5.60070200	7.56110500
C	-4.85597500	-6.64879800	7.43040900
H	-5.42741500	-6.89541600	8.15127100
C	-4.87485700	-7.43439000	6.22532200
H	-5.56184200	-8.05501800	6.00058400
C	-3.64273000	-7.16613900	5.34889500
H	-3.44099200	-7.75759500	4.63624100
C	-2.82211500	-6.09313400	5.56031400
H	-2.12608400	-5.88100500	4.94916000
C	-3.03870600	-5.30754200	6.69621000
H	-2.45803300	-4.57952700	6.88325800
C	-2.99596300	-2.23606500	11.11101800
C	-1.89258000	-2.21211400	10.02509500
C	-1.15964100	-1.06629900	10.67664900
C	-2.16035300	-1.21287900	11.79909000
C	-1.47298600	0.38321600	13.29439800
H	-1.36267000	0.40902600	14.26786600
H	-1.82980600	1.24022100	12.98257400
H	-0.60933500	0.21122900	12.86985000
O	-1.58785500	-2.91723200	9.05833400
O	-2.39363500	-0.66967000	12.94844000
S	-4.25258400	-3.20560200	11.37048700
Hg	-4.15460100	-4.44846700	9.35470500

Coordinates for the calculated PhHgL^{Me} dimer featuring Hg···O spodium-bonding

0 1

C	2.29501	-0.8105	7.56111
C	1.53008	-1.8586	7.43041
H	0.95864	-2.10522	8.15127
C	1.51119	-2.64419	6.22532
H	0.82421	-3.26482	6.00058
C	2.74332	-2.37594	5.3489
H	2.94506	-2.9674	4.63624
C	3.56394	-1.30293	5.56031
H	4.25997	-1.09081	4.94916
C	3.34734	-0.51734	6.69621
H	3.92802	0.21067	6.88326
C	3.39009	2.55414	11.11102
C	4.49347	2.57809	10.0251
C	5.22641	3.7239	10.67665
C	4.2257	3.57732	11.79909
C	4.91306	5.17342	13.2944
H	5.02338	5.19923	14.26787
H	4.55624	6.03042	12.98257
H	5.77672	5.00143	12.86985
O	4.7982	1.87297	9.05833
O	6.16352	4.49225	10.47676
O	3.99242	4.12053	12.94844
S	2.13347	1.5846	11.37049
Hg	2.23145	0.34173	9.35471
O	-0.22253	-0.29795	10.47676
C	-4.09104	-5.6007	7.56111
C	-4.85598	-6.6488	7.43041
H	-5.42741	-6.89542	8.15127
C	-4.87486	-7.43439	6.22532
H	-5.56184	-8.05502	6.00058
C	-3.64273	-7.16614	5.3489
H	-3.44099	-7.7576	4.63624

C	-2.82212	-6.09313	5.56031
H	-2.12608	-5.88101	4.94916
C	-3.03871	-5.30754	6.69621
H	-2.45803	-4.57953	6.88326
C	-2.99596	-2.23607	11.11102
C	-1.89258	-2.21211	10.0251
C	-1.15964	-1.0663	10.67665
C	-2.16035	-1.21288	11.79909
C	-1.47299	0.38322	13.2944
H	-1.36267	0.40903	14.26787
H	-1.82981	1.24022	12.98257
H	-0.60934	0.21123	12.86985
O	-1.58786	-2.91723	9.05833
O	-2.39364	-0.66967	12.94844
S	-4.25258	-3.2056	11.37049
Hg	-4.1546	-4.44847	9.35471

Coordinates for the calculated PhHgL^{Me} dimer featuring C···O interactions

0 1

C	2.29501	-0.8105	7.56111
C	1.53008	-1.8586	7.43041
H	0.95864	-2.10522	8.15127
C	1.51119	-2.64419	6.22532
H	0.82421	-3.26482	6.00058
C	2.74332	-2.37594	5.3489
H	2.94506	-2.9674	4.63624
C	3.56394	-1.30293	5.56031
H	4.25997	-1.09081	4.94916
C	3.34734	-0.51734	6.69621
H	3.92802	0.21067	6.88326
C	3.39009	2.55414	11.11102
C	4.49347	2.57809	10.0251
C	5.22641	3.7239	10.67665

C	4.2257	3.57732	11.79909
C	4.91306	5.17342	13.2944
H	5.02338	5.19923	14.26787
H	4.55624	6.03042	12.98257
H	5.77672	5.00143	12.86985
O	4.7982	1.87297	9.05833
O	6.16352	4.49225	10.47676
O	3.99242	4.12053	12.94844
S	2.13347	1.5846	11.37049
Hg	2.23145	0.34173	9.35471
Hg	8.6175	5.13193	9.35471
C	6.85387	10.4618	11.73567
C	7.83893	11.50606	12.05279
H	8.62142	11.65029	11.5381
C	7.52246	12.24375	13.14448
H	7.93482	13.09458	13.1895
C	6.75794	11.96592	14.11124
H	6.7617	12.44604	14.93197
C	5.93622	10.93124	13.87292
H	5.32367	10.69989	14.56297
C	5.885	10.17439	12.70243
H	5.23529	9.50222	12.5714
C	5.61219	7.14027	8.31452
C	4.68236	7.16614	9.39468
C	3.99723	5.99925	8.7143
C	5.10659	6.06535	7.74754
C	4.49339	4.23454	6.32334
H	4.79248	3.80095	5.49996
H	4.49873	3.59009	7.05891
H	3.57652	4.5736	6.19676
O	4.70158	7.80515	10.46139
O	3.21361	5.22228	9.07563
O	5.39175	5.36694	6.64624
S	7.07252	8.08969	8.01277

Hg	6.9874	9.35957	10.02548
O	9.59966	10.01248	9.07563
C	13.23992	15.252	11.73567
C	14.22498	16.29626	12.05279
H	15.00747	16.44049	11.5381
C	13.90851	17.03395	13.14448
H	14.32087	17.88478	13.1895
C	13.14399	16.75612	14.11124
H	13.14775	17.23624	14.93197
C	12.32227	15.72144	13.87292
H	11.70972	15.49009	14.56297
C	12.27105	14.96459	12.70243
H	11.62134	14.29242	12.5714
C	11.99824	11.93047	8.31452
C	11.06841	11.95634	9.39468
C	10.38328	10.78945	8.7143
C	11.49264	10.85555	7.74754
C	10.87944	9.02474	6.32334
H	11.17853	8.59115	5.49996
H	10.88478	8.38029	7.05891
H	9.96257	9.3638	6.19676
O	11.08763	12.59535	10.46139
O	11.7778	10.15714	6.64624
S	13.45857	12.87989	8.01277
Hg	13.37345	14.14977	10.02548
C	8.68106	3.9797	7.56111
C	7.91613	2.9316	7.43041
H	7.34469	2.68498	8.15127
C	7.89724	2.14601	6.22532
H	7.21026	1.52538	6.00058
C	9.12937	2.41426	5.3489
H	9.33111	1.82281	4.63624
C	9.94998	3.48727	5.56031
H	10.64602	3.6994	4.94916

C	9.73339	4.27286	6.69621
H	10.31407	5.00087	6.88326
C	9.77614	7.34434	11.11102
C	10.87952	7.36829	10.0251
C	11.61246	8.5141	10.67665
C	10.61175	8.36752	11.79909
C	11.29911	9.96362	13.2944
H	11.40943	9.98943	14.26787
H	10.94229	10.82062	12.98257
H	12.16277	9.79163	12.86985
O	11.18425	6.66317	9.05833
O	12.54958	9.28245	10.47676
O	10.37847	8.91073	12.94844
S	8.51952	6.3748	11.37049

Coordinates for the calculated PhHgL^{Me} dimer featuring π(cyclobutene)···π(phenyl) interactions

0 1

Hg	6.98800300	9.35995500	10.02567100
S	7.06433400	8.09064800	8.00892800
O	4.58849000	7.85592800	10.39988200
O	3.21134900	5.22227600	9.08716400
O	5.39340400	5.36598200	6.64431600
C	5.68925500	7.14793600	8.33182200
C	4.61829300	7.15847500	9.36969600
C	3.93368500	5.98487600	8.69315600
C	5.07445900	6.06535100	7.72255200
C	4.49264000	4.24411700	6.32718800
H	4.86705300	3.41388900	6.68654200
H	4.39826200	4.16688000	5.35450800
H	3.61415400	4.40866100	6.72848000
C	6.86400500	10.45221600	11.74911900
C	7.69269100	11.50606000	12.01050900

H	8.35942000	11.74091400	11.37529200
C	7.58216700	12.23417100	13.16562500
H	8.16046000	12.98537000	13.27786900
C	6.75831300	11.96592000	14.10932100
H	6.74212400	12.45311200	14.92395600
C	5.91067300	10.94081700	13.87291700
H	5.28894700	10.71570600	14.55332000
C	5.88688600	10.17438500	12.69281500
H	5.23262400	9.49846800	12.54999200
Hg	2.23226700	9.92213300	9.35508900
S	2.12234900	11.16787200	11.36856500
O	4.67578400	11.49743800	8.99875300
O	6.15345300	14.06977500	10.48252800
O	3.99520200	13.70859400	12.94075200
C	3.48291800	12.12782800	11.14561400
C	4.43947800	12.15369500	9.99434300
C	5.15198100	13.31579800	10.64589700
C	4.17861300	13.15101500	11.77218300
C	4.92432700	14.75381600	13.30208600
H	5.80597700	14.54294200	12.92768200
H	4.98764700	14.80656600	14.27747600
H	4.60963900	15.60576300	12.94350000
C	2.30145700	8.77852100	7.58032500
C	1.38766500	7.72180200	7.38812600
H	0.67866200	7.56114900	7.99756900
C	1.58367500	6.92662900	6.24646400
H	0.97699200	6.22307300	6.04448200
C	2.75722400	7.21404100	5.34312900
H	2.94214000	6.62824800	4.61694400
C	3.54553200	8.28704600	5.55647000
H	4.23635100	8.50507700	4.93991500
C	3.34885300	9.05347800	6.68852200
H	3.92172500	9.78678100	6.86234600

Coordinates for the calculated PhHgL^{Et} monomer

0 1

Hg	0.00706200	6.08089600	8.21029200
S	0.00704500	5.53071200	5.88977100
C	0.00337200	3.82714300	6.00873700
C	0.00887300	2.93815500	7.21213300
O	-0.00064000	3.14277600	8.41415500
C	0.00091800	1.76045700	6.23540400
O	0.00596100	0.55172600	6.34805100
C	0.01020700	2.73978400	5.15839200
O	0.00556800	2.60487300	3.86295600
C	0.02171900	1.29860500	3.46182400
H	-0.75225100	0.81074900	3.84501500
H	0.85301600	0.85431300	3.75945800
C	-0.05329000	1.30713000	2.08945800
H	0.08481300	0.40074900	1.74826200
H	0.63821200	1.90224600	1.73039000
H	-0.93680600	1.63088100	1.81255300
C	-0.08543700	6.48233100	10.23710800
C	-0.92683300	5.73749400	11.05585600
H	-1.47103300	5.05596200	10.68093500
C	-0.96644000	5.98542000	12.42135400
H	-1.54258500	5.48019600	12.98104300
C	-0.17106700	6.98970700	12.96947600
H	-0.19776200	7.15822000	13.90367300
C	0.67002600	7.73032500	12.15210100
H	1.21861600	8.41203200	12.52621100
C	0.71604900	7.47874700	10.78523000
H	1.29018600	7.98781400	10.22610400

Coordinates for the calculated PhHgL^{Et} dimer featuring Hg···O spodium-bonding

0 1

Hg	0.00706	6.0809	8.21029
S	0.00705	5.53071	5.88977
C	0.00337	3.82714	6.00874
C	0.00887	2.93816	7.21213
O	-0.00064	3.14278	8.41416
C	0.00092	1.76046	6.2354
O	0.00596	0.55173	6.34805
C	0.01021	2.73978	5.15839
O	0.00557	2.60487	3.86296
C	0.02172	1.29861	3.46182
H	-0.75225	0.81075	3.84502
H	0.85302	0.85431	3.75946
C	-0.05329	1.30713	2.08946
H	0.08481	0.40075	1.74826
H	0.63821	1.90225	1.73039
H	-0.93681	1.63088	1.81255
C	-0.08544	6.48233	10.23711
C	-0.92683	5.73749	11.05586
H	-1.47103	5.05596	10.68094
C	-0.96644	5.98542	12.42135
H	-1.54259	5.4802	12.98104
C	-0.17107	6.98971	12.96948
H	-0.19776	7.15822	13.90367
C	0.67003	7.73033	12.1521
H	1.21862	8.41203	12.52621
C	0.71605	7.47875	10.78523
H	1.29019	7.98781	10.2261
O	0.00569	8.42303	6.34805
Hg	0.00679	13.9522	8.21029
S	0.00677	13.40201	5.88977
C	0.0031	11.69844	6.00874
C	0.0086	10.80946	7.21213

O	-0.00092	11.01408	8.41416
C	0.00064	9.63176	6.2354
C	0.00993	10.61108	5.15839
O	0.00529	10.47617	3.86296
C	0.02144	9.16991	3.46182
H	-0.75253	8.68205	3.84502
H	0.85274	8.72561	3.75946
C	-0.05357	9.17843	2.08946
H	0.08454	8.27205	1.74826
H	0.63794	9.77355	1.73039
H	-0.93708	9.50218	1.81255
C	-0.08571	14.35363	10.23711
C	-0.92711	13.60879	11.05586
H	-1.47131	12.92726	10.68094
C	-0.96672	13.85672	12.42135
H	-1.54286	13.3515	12.98104
C	-0.17134	14.86101	12.96948
H	-0.19804	15.02952	13.90367
C	0.66975	15.60163	12.1521
H	1.21834	16.28333	12.52621
C	0.71577	15.35005	10.78523
H	1.28991	15.85911	10.2261

Coordinates for the calculated PhHgL^{Et} dimer featuring π(cyclobutene)···π(cyclobutene) interactions

0 1

Hg	0.00706	6.0809	8.21029
S	0.00705	5.53071	5.88977
C	0.00337	3.82714	6.00874
C	0.00887	2.93816	7.21213
O	-0.00064	3.14278	8.41416
C	0.00092	1.76046	6.2354
O	0.00596	0.55173	6.34805

C	0.01021	2.73978	5.15839
O	0.00557	2.60487	3.86296
C	0.02172	1.29861	3.46182
H	-0.75225	0.81075	3.84502
H	0.85302	0.85431	3.75946
C	-0.05329	1.30713	2.08946
H	0.08481	0.40075	1.74826
H	0.63821	1.90225	1.73039
H	-0.93681	1.63088	1.81255
C	-0.08544	6.48233	10.23711
C	-0.92683	5.73749	11.05586
H	-1.47103	5.05596	10.68094
C	-0.96644	5.98542	12.42135
H	-1.54259	5.4802	12.98104
C	-0.17107	6.98971	12.96948
H	-0.19776	7.15822	13.90367
C	0.67003	7.73033	12.1521
H	1.21862	8.41203	12.52621
C	0.71605	7.47875	10.78523
H	1.29019	7.98781	10.2261
O	0.00569	8.42303	6.34805
Hg	0.00679	13.9522	8.21029
S	0.00677	13.40201	5.88977
C	0.0031	11.69844	6.00874
C	0.0086	10.80946	7.21213
O	-0.00092	11.01408	8.41416
C	0.00064	9.63176	6.2354
C	0.00993	10.61108	5.15839
O	0.00529	10.47617	3.86296
C	0.02144	9.16991	3.46182
H	-0.75253	8.68205	3.84502
H	0.85274	8.72561	3.75946
C	-0.05357	9.17843	2.08946
H	0.08454	8.27205	1.74826

H	0.63794	9.77355	1.73039
H	-0.93708	9.50218	1.81255
C	-0.08571	14.35363	10.23711
C	-0.92711	13.60879	11.05586
H	-1.47131	12.92726	10.68094
C	-0.96672	13.85672	12.42135
H	-1.54286	13.3515	12.98104
C	-0.17134	14.86101	12.96948
H	-0.19804	15.02952	13.90367
C	0.66975	15.60163	12.1521
H	1.21834	16.28333	12.52621
C	0.71577	15.35005	10.78523
H	1.28991	15.85911	10.2261
Hg	-3.04991	6.81866	5.5271
S	-3.04989	7.36884	7.84763
C	-3.04622	9.07241	7.72866
C	-3.05172	9.9614	6.52526
O	-3.04221	9.75678	5.32324
C	-3.04377	11.1391	7.50199
O	-3.04881	12.34783	7.38935
C	-3.05306	10.15977	8.579
O	-3.04841	10.29468	9.87444
C	-3.06457	11.60095	10.27557
H	-2.2906	12.0888	9.89238
H	-3.89586	12.04524	9.97794
C	-2.98956	11.59242	11.64794
H	-3.12766	12.4988	11.98913
H	-3.68106	10.99731	12.00701
H	-2.10604	11.26867	11.92484
C	-2.95741	6.41722	3.50029
C	-2.11601	7.16206	2.68154
H	-1.57182	7.84359	3.05646
C	-2.07641	6.91413	1.31604
H	-1.50026	7.41936	0.75635

C	-2.87178	5.90985	0.76792
H	-2.84509	5.74133	-0.16628
C	-3.71287	5.16923	1.5853
H	-4.26146	4.48752	1.21119
C	-3.7589	5.42081	2.95217
H	-4.33303	4.91174	3.51129
O	-3.04853	4.47653	7.38935
Hg	-3.04963	-1.05264	5.5271
S	-3.04962	-0.50246	7.84763
C	-3.04594	1.20111	7.72866
C	-3.05145	2.0901	6.52526
O	-3.04193	1.88548	5.32324
C	-3.04349	3.2678	7.50199
C	-3.05278	2.28847	8.579
O	-3.04814	2.42338	9.87444
C	-3.06429	3.72965	10.27557
H	-2.29032	4.2175	9.89238
H	-3.89559	4.17394	9.97794
C	-2.98928	3.72112	11.64794
H	-3.12739	4.6275	11.98913
H	-3.68078	3.12601	12.00701
H	-2.10577	3.39737	11.92484
C	-2.95714	-1.45408	3.50029
C	-2.11574	-0.70924	2.68154
H	-1.57154	-0.02771	3.05646
C	-2.07613	-0.95717	1.31604
H	-1.49999	-0.45194	0.75635
C	-2.87151	-1.96145	0.76792
H	-2.84481	-2.12997	-0.16628
C	-3.7126	-2.70207	1.5853
H	-4.26119	-3.38378	1.21119
C	-3.75862	-2.45049	2.95217
H	-4.33276	-2.95956	3.51129

Coordinates for the calculated PhHgL^{Et} dimer featuring Hg···S spodium-bonding

0 1

Hg	0.00706	6.08098	8.21029
S	0.00772	5.53156	5.8895
C	0.00398	3.82692	6.00599
C	0.00826	2.93501	7.21213
O	-0.00187	3.1402	8.41141
C	0.00091	1.75845	6.22991
O	0.00627	0.55223	6.34942
C	0.00868	2.73928	5.15702
O	0.00251	2.60015	3.86296
C	0.03419	1.31026	3.4055
H	0.8786	0.87774	3.68228
H	-0.72017	0.80043	3.79467
C	-0.05293	1.31966	2.14303
H	-0.95302	1.60777	1.8848
H	0.10657	0.41097	1.80728
H	0.61083	1.92945	1.77546
C	-0.07573	6.52309	10.16567
C	-0.92501	5.76596	11.04761
H	-1.47114	5.08562	10.67842
C	-0.97496	6.00107	12.45982
H	-1.5333	5.47213	13.02066
C	-0.19214	7.01863	12.98184
H	-0.25273	7.22346	13.91469
C	0.6554	7.73338	12.19056
H	1.20173	8.40723	12.5694
C	0.72429	7.45948	10.77561
H	1.34578	7.94359	10.24668
Hg	-3.04991	6.81858	5.5271
S	-3.05056	7.368	7.8479
C	-3.04683	9.07263	7.73141
C	-3.05111	9.96455	6.52526
O	-3.04098	9.75936	5.32599

C	-3.04376	11.14111	7.50749
O	-3.04912	12.34732	7.38797
C	-3.05153	10.16027	8.58038
O	-3.04536	10.2994	9.87444
C	-3.07704	11.58929	10.3319
H	-3.92145	12.02181	10.05512
H	-2.32268	12.09913	9.94273
C	-2.98992	11.5799	11.59436
H	-2.08983	11.29179	11.8526
H	-3.14942	12.48859	11.93012
H	-3.65368	10.97011	11.96193
C	-2.96712	6.37646	3.57172
C	-2.11784	7.13359	2.68978
H	-1.5717	7.81393	3.05898
C	-2.06789	6.89848	1.27758
H	-1.50954	7.42742	0.71674
C	-2.85071	5.88092	0.75556
H	-2.79012	5.67609	-0.1773
C	-3.69824	5.16617	1.54683
H	-4.24458	4.49233	1.168
C	-3.76714	5.44007	2.96178
H	-4.38863	4.95597	3.49071

Coordinates for the calculated PhHgL^{Et} dimer featuring C=O···π(cyclobutene) interactions

0 1

Hg	0.00706200	6.08097500	8.21029200
S	0.00771700	5.53155600	5.88949600
C	0.00398000	3.82692400	6.00599000
C	0.00826100	2.93500700	7.21213300
O	-0.00186500	3.14019600	8.41140800
C	0.00091200	1.75844600	6.22990900
O	0.00626800	0.55222900	6.34942400

C	0.00867800	2.73928100	5.15701800
O	0.00251200	2.60015000	3.86295600
C	0.03419200	1.31026200	3.40550000
H	0.87859700	0.87773900	3.68228200
H	-0.72016700	0.80042800	3.79466700
C	-0.05293200	1.31965600	2.14303400
H	-0.95301900	1.60776700	1.88479800
H	0.10656900	0.41096900	1.80727800
H	0.61083400	1.92944900	1.77546200
C	-0.07573000	6.52309000	10.16567300
C	-0.92500900	5.76596200	11.04761400
H	-1.47114300	5.08562200	10.67842100
C	-0.97496000	6.00107400	12.45981800
H	-1.53330400	5.47213000	13.02066100
C	-0.19214200	7.01863400	12.98183900
H	-0.25273100	7.22346000	13.91469100
C	0.65539500	7.73338400	12.19056500
H	1.20172800	8.40722600	12.56940100
C	0.72429100	7.45948500	10.77561300
H	1.34577800	7.94358500	10.24668300
Hg	3.06236500	-1.05272200	5.52710400
S	3.06171100	-0.50330300	7.84790000
C	3.06544700	1.20132900	7.73140700
C	3.06116600	2.09324700	6.52526300
O	3.07129300	1.88805800	5.32598800
C	3.06851500	3.26980800	7.50748700
O	3.06315900	4.47602400	7.38797200
C	3.06074900	2.28897200	8.58037800
O	3.06691500	2.42810400	9.87444000
C	3.03523500	3.71799200	10.33189600
H	2.19083000	4.15051400	10.05511500
H	3.78959400	4.22782500	9.94272900
C	3.12235900	3.70859700	11.59436200
H	4.02244600	3.42048700	11.85259800

H	2.96285900	4.61728500	11.93011800
H	2.45859300	3.09880500	11.96193400
C	3.14515700	-1.49483700	3.57172300
C	3.99443600	-0.73770800	2.68978200
H	4.54057100	-0.05736900	3.05897500
C	4.04438700	-0.97282000	1.27757800
H	4.60273100	-0.44387700	0.71673500
C	3.26157000	-1.99038000	0.75555700
H	3.32215800	-2.19520700	-0.17729500
C	2.41403300	-2.70513100	1.54683100
H	1.86769900	-3.37897300	1.16799500
C	2.34513600	-2.43123100	2.96178300
H	1.72364900	-2.91533200	3.49071400