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Mercurophilic Interactions: A Theoretical Study on the Importance of the Ligands

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SUPPORTING INFORMATION

Refcode	X	Y	Hg···Hg (Å)		τ(°)	Supp. contacts	d (Å)
doyfig*	SR	Me	3.099	Hg1···Hg1	81.8		
tmsihg01	$SiMe_3$	$SiMe_3$	3.146	Hg1···Hg1	83.5	H···H	2.5 - 2.6
pehgme10	RNH_2^+	Me	3.346	Hg2···Hg2	75.1		
duvkio	N-het†	Me	3.347	Hg2···Hg2	60.5		
lasraz	SR	SR	3.485	Hg1···Hg1	73.8	stacking	3.52
jespec	N-het	Me	3.510	Hg2···Hg3	86.6	1 N···Hg	2.82
ricliy	N-het	Ph	3.519	Hg1···Hg4	60.0		
dbezhg	Bz	Bz	3.538	Hg1···Hg1	90.0	2 Ph···Hg	3.20
hahqen	Cl	R	3.275	Hg1···Hg2	76.7	4 O···Hg	2.8 - 2.9
dojsaw	N-het	Me	3.514	Hg1···Hg2	41.9	2 O···Hg	2.99
evojad	Cb‡	Cb	3.524	Hg1···Hg2	73.9	4 O···Hg	2.8
nevdat	OOCR	OOCR	3.557	Hg5···Hg9	42.9	2 O···Hg	2.9 - 3.0
bespaq	Imino	Ph	3.582	Hg1···Hg2	86.5	2 O···Hg	2.92
kapwut	SR	Me	3.671	Hg1···Hg1	53.7	1 N···Hg	2.76
kayreh	OOCR	Ph	3.859	Hg1···Hg1	61.1	2 O···Hg	2.88
eyojeh	Cb	Cb	3.872	Hg1···Hg2	76.1	4 O···Hg	2.9
nevdat	OOCR	R	3.891	Hg4···Hg9	35.3	2 O···Hg	3.0
joptud	R	Cl	3.900	Hg1···Hg1	31.0	4 Cl···Hg	3.26, 3.87
duvkio	N-het	Me	3.924	Hg1···Hg1	38.3	2 O···Hg	3.0
eyojil	Cb	Cb	3.976	Hg1···Hg2	87.9	4 O···Hg	2.79 - 2.89
cizvem	Amido	Ph	4.096	Hg1···Hg1	79.8	1 O···Hg	2.87
nevdat	OOCR	R	4.103	Hg2···Hg6	38.2	2 O···Hg	2.9
jucfes	N-het	Me	4.114	Hg1···Hg1	72.0	2 N···Hg	3.08

*In the same compound one can find an intermolecular interaction of type **2b** (see Table 1) at 3.805 Å between two Hg2 atoms. † N-heterocycle. ‡ Carbene.

TableS1. Bimolecular association of [XHgY] complexes of type **2a**. Non-equivalent crystallographic Hg atoms are labelled with numbers.

Refcode	Xa	Yb	Ya	Xb	Xa-Yb (Å)	Ya-Xb (Å)	Hg	Hg'	Hg···Hg (Å)
ocifem	C18	C17	C17	C18	3.691	3.691	Hg2	Hg2	3.621
volfor	S2	S1	S1	S2	3.641	3.641	Hg1	Hg1	3.691
mirlaa	C1	S1	S1	C1	3.531	3.531	Hg1	Hg1	3.697
admehh	C9	N9	N9	C9	3.676	3.676	Hg9	Hg9	3.701
yulfao	C1	C9	Se1	Se2	3.984	3.637	Hg1	Hg2	3.721
vewtia	C6	C6	N4	N4	3.761	3.761	Hg1	Hg1	3.761
rocgiz	C5	N5	N5	C5	3.675	3.675	Hg1	Hg1	3.764
mehgcn01	C2	C1	C1	C2	3.839	3.839	Hg1	Hg1	3.771
qugvod	C1	C15	S1	S2	4.024	3.617	Hg1	Hg2	3.773
faknag	C7	N5	N5	C7	3.763	3.763	Hg2	Hg2	3.796
kabgoj	C7	N1	N1	C7	3.747	3.747	Hg1	Hg1	3.796
bzhgcl	Cl2	C8	C8	Cl2	3.817	3.846	Hg2	Hg2	3.805
doyfig	C6	S1	S1	C6	3.840	3.840	Hg1	Hg1	3.805
pucdew	C15	N3	N3	C15	3.801	3.801	Hg1	Hg1	3.814
bzhgcl	Cl1	C1	C1	Cl1	3.857	3.910	Hg1	Hg1	3.817
penkup	C1	C15	C2	C14	3.881	3.727	Hg1	Hg2	3.866
xemtug	Cl5	C12	C12	Cl5	3.983	3.983	Hg3	Hg3	3.890

penmhg10	C6	C6	S1	S1	3.804	3.956	Hg1	Hg1	3.917
yevcim	C1	C15	C2	C14	3.728	3.978	Hg1	Hg2	3.963
jagyar	C7	N5	N5	C7	3.881	3.881	Hg2	Hg2	3.964
cavhem10	C16	N6	N6	C16	4.136	4.136	Hg4	Hg4	3.969
yikzex	C19	C17	C17	C19	3.924	3.924	Hg2	Hg2	4.009
dofniw	C1	C1	S1	S1	4.193	3.642	Hg1	Hg1	4.013
fadvai	C12	S2	S2	C12	3.721	4.376	Hg2	Hg2	4.108
xujluj	C14	C13	C13	C14	4.110	4.110	Hg2	Hg2	4.115

Table S2. Structures showing unsupported Hg···Hg contacts with the parallel conformation **2b**.

Refcode	Hg1···X2	Hg2···X1	Hg···Hg	Hg1	X1	Hg2	X2	XHg-HgX
BUCNUJ	3.112	3.112	3.669	Hg1	S2	Hg1	S2	0.56
FEZLIF	2.923	2.934	3.732	Hg1	O1	Hg2	O3	0.80
LILWEI	3.111	3.111	3.791	Hg1	Cl2	Hg1	Cl2	0.68
FMHGIC	2.880	2.880	3.833	Hg1	N1	Hg1	N1	0.95
ISICES	2.689	2.689	3.843	Hg1	O1	Hg1	O1	1.15
AQAMOV	3.135	3.135	3.857	Hg1	N2	Hg1	N2	0.72
CBPPHG	2.858	2.858	3.857	Hg1	O1	Hg1	O1	1.00
FMHGAZ	2.739	2.739	3.859	Hg1	N1	Hg1	N1	1.12
BUCNUJ	3.037	3.037	3.869	Hg1	S1	Hg1	S1	0.83
VUDSUJ	2.953	3.060	3.889	Hg2	Cl4	Hg3	Cl5	0.83
VUDSUJ	3.044	3.104	3.890	Hg3	Cl6	Hg2	Cl3	0.79
CPCOMC	3.141	3.141	3.918	Hg1	Cl1	Hg1	Cl1	0.78
UJUHIR	2.989	3.062	3.937	Hg5	Se9	Hg4	Se6	0.88
VOFTEQ	2.798	2.798	3.939	Hg1	O1	Hg1	O1	1.14
ISICAO	2.885	2.794	3.958	Hg1	O1	Hg2	O3	1.16
HGCETS	3.058	3.058	3.963	Hg2	Cl2	Hg2	Cl2	0.91
KELWED	3.172	3.172	3.972	Hg1	S2	Hg1	S2	0.80
BITHIV10	3.102	3.102	4.000	Hg1	Cl2	Hg1	Cl2	0.90
VAVGAA	3.105	3.105	4.002	Hg1	Cl1	Hg1	Cl1	0.90
FAWKUJ	3.106	3.106	4.003	Hg4	O14	Hg4	O14	0.90
XOBTEP	3.145	3.145	4.024	Hg1	Cl1	Hg1	Cl1	0.88
PHHGAC01	2.994	2.994	4.028	Hg1	O1	Hg1	O1	1.03
PHHGAC	2.943	2.943	4.032	Hg1	O1	Hg1	O1	1.09
XAWXUP	2.907	2.907	4.074	Hg1	O1	Hg1	O1	1.17
KEZGUS	3.127	3.127	4.077	Hg1	Cl1	Hg1	Cl1	0.95
AXUDUT	3.178	3.137	4.077	Hg2	Cl2	Hg3	Cl3	0.94
ZOPZIN	2.916	2.916	4.081	Hg1	O3	Hg1	O3	1.17
JOTXIZ	3.177	3.177	4.087	Hg1	Cl2	Hg1	Cl2	0.91
VAVGAA	3.177	3.177	4.100	Hg2	Cl2	Hg2	Cl2	0.92
TEVQOA01	3.135	3.135	4.104	Hg1	S1	Hg1	S1	0.97
LEZFEB	3.123	3.123	4.122	Hg1	Cl1	Hg1	Cl1	1.00
PIFNAT	3.000	3.000	4.122	Hg1	O2	Hg1	O2	1.12
QUGVAP	3.146	3.146	4.124	Hg1	S1	Hg1	S1	0.98
PHGTFA01	2.951	2.951	4.131	Hg1	O1	Hg1	O1	1.18

GUKHEZ	3.163	3.163	4.139	Hg1	Cl1	Hg1	Cl1	0.98
BIJDAZ	3.136	3.143	4.143	Hg2	Cl2	Hg4	Cl4	1.00
BZHGCL	3.190	3.176	4.144	Hg1	Cl1	Hg2	Cl2	0.97
CIDZOF	3.095	3.095	4.177	Hg2	Cl2	Hg2	Cl2	1.08
HALCIG	3.188	3.188	4.183	Hg1	Cl1	Hg1	Cl1	0.99
CIDZOF	3.173	3.173	4.192	Hg1	Cl1	Hg1	Cl1	1.02
KASDAJ01	3.129	3.129	4.199	Hg1	P2	Hg1	P2	1.07
KASDAJ	3.162	3.162	4.221	Hg1	P2	Hg1	P2	1.06
WUZWAP	3.156	3.156	4.245	Hg2	Cl2	Hg2	Cl2	1.09
KAYREH	3.057	3.057	4.263	Hg1	O1	Hg1	O1	1.21
HEHKEM	3.072	3.072	4.364	Hg1	O1	Hg1	O1	1.29
REWTES	2.899	2.899	4.379	Hg4	O10	Hg4	O10	1.48

Table S3. Structures showing Hg···Hg contacts with the slipped conformation **2c**. Distances are given in Angstroms and angles in degrees.

Topology	Basis set	$d_{Hg\cdots Hg}$ (Å)	$d_{H\cdots Hg}$ (Å)	DE (kcal/mol)
2a	Def2-TZVPD	3.240	3.625	1.41
	Def2-TZVPPD	3.205	3.590	2.18
	Def2-QZVPD	3.141	3.534	2.68
	Def2-QZVPPD	3.078	3.479	3.01
2b	Def2-TZVPD	3.536	3.891	0.48
	Def2-TZVPPD	3.507	3.861	0.94
	Def2-QZVPD	3.442	3.801	1.24
	Def2-QZVPPD	3.361	3.731	1.42
2c	Def2-TZVPD	3.535	3.038	1.53
	Def2-TZVPPD	3.463	2.949	2.21
	Def2-QZVPD	3.393	2.880	2.69
	Def2-QZVPPD	3.333	2.837	2.94

Table S4. Dissociation energies and key structural parameters of $(HgH_2)_2$ dimers with topologies **2a-c** calculated at the MP2 level of theory (All reported energies are BSSE corrected).

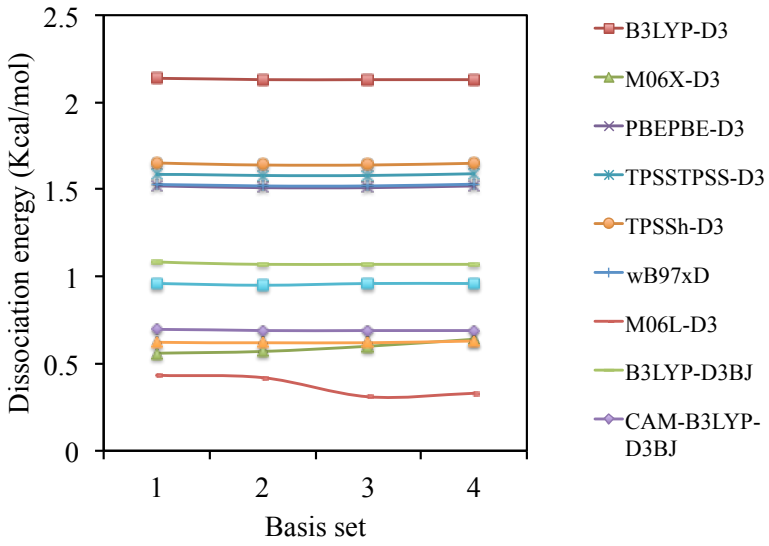

Figure S1. Effect of the basis sets on the dissociation energies for HgH_2 parallel dimers calculated at the DFT level with several functionals. Basis set 1: Def2-TZVPD; Basis set 2: Def2-TZVPPD; Basis set 3: Def2-QZVPD; Basis set 4: Def2-QZVPPD.

Method	DE (kcal/mol)	$d_{Hg\cdots Hg}$ (Å)
B3LYP-D3	2.99	3.707
B3LYP-D3BJ	1.46	3.532
PBEPBE-D3	2.43	3.495
PBEPBE-D3BJ	2.48	3.305
TPSSTPSS-D3	2.37	3.644
TPSSh-D3	2.45	3.663
wB97xD	2.27	3.612
M06L-D3	1.72	3.340
M062X-D3	1.99	3.385
LC-wPBE-D3BJ	1.23	3.470
CAM-B3LYP-D3BJ	1.28	3.498

Table S5. Dissociation energies and key structural parameters of $(HgH_2)_2$ dimers with topology **2a** calculated at DFT level of theory (BSSE corrected). The basis set Def2-TZVPPD was used for all functionals.

Method	DE (kcal/mol)	$d_{Hg\cdots Hg}$ (Å)
B3LYP-D3	2.13	3.822
B3LYP-D3BJ	1.07	3.838
PBEPBE-D3	1.51	3.783
PBEPBE-D3BJ	0.95	3.764
TPSSTPSS-D3	1.58	3.849
TPSSh-D3	1.64	3.840
wB97xD	1.52	4.015
M06L-D3	0.42	3.616

M062X-D3	0.57	3.655
LC-wPBE-D3BJ	0.62	3.980
CAM-B3LYP-D3BJ	0.69	3.968

Table S6. Dissociation energies and key structural parameters of $(HgH_2)_2$ dimers with topology **2b** calculated at the DFT level of theory (BSSE corrected). The basis set Def2-TZVPPD was used for all functionals.

Method	DE (kcal/mol)	$d_{Hg\cdots Hg}$ (Å)	Angle H-Hg⋯Hg (deg.)
B3LYP-D3	4.38	3.738	52.439
B3LYP-D3BJ	2.07	3.783	54.657
PBEPBE-D3	3.47	3.677	53.231
PBEPBE-D3BJ	3.07	3.588	54.138
TPSSTPSS-D3	3.89	3.691	52.120
TPSSh-D3	4.05	3.678	52.093
wB97xD	3.44	3.889	54.424
M06L-D3	2.65	3.585	54.062
M062X-D3	2.93	3.601	54.667
LC-wPBE-D3BJ	2.34	3.612	54.587
CAM-B3LYP-D3BJ	1.98	3.756	54.777

Table S7. Dissociation energies and key structural parameters of $(HgH_2)_2$ dimers with topology **2c** calculated at the DFT level of theory (BSSE corrected). The basis set Def2-TZVPPD was used for all functionals.

Topology **2a**

Method	DE (kcal/mol)	$d_{Hg\cdots Hg}$ (Å)
B3LYP	0.01	> 10
PBEPBE	0.00	4.261
TPSSTPSS	0.01	> 10
TPSSh	0.01	> 10
M06L	0.35	3.612
M062X	0.51	3.646
LC-wPBE	0.01	> 10
CAM-B3LYP	0.01	> 10

Topology **2b**

Method	DE (kcal/mol)	$d_{Hg\cdots Hg}$ (Å)
B3LYP	0.21	3.993
PBEPBE	0.85	3.402
TPSSTPSS	0.04	3.533
TPSSh	0.00	3.535
M06L	1.64	3.337
M062X	1.95	3.382

LC-wPBE	0.00	3.651
CAM-B3LYP	0.20	3.595

Topology **2c**

Method	DE (kcal/mol)	$d_{Hg\cdots Hg}$ (Å)
B3LYP	0.39	4.069
PBEPBE	1.48	3.684
TPSSTPSS	0.85	3.715
TPSSh	0.88	3.716
M06L	2.59	3.585
M062X	2.88	3.600
LC-wPBE	1.08	3.700
CAM-B3LYP	0.94	3.826

Table S8. Dissociation energies and key structural parameters of $(HgH_2)_2$ dimers with topology **2a**, **2b** and **2c** fully optimized at the DFT level of theory (BSSE corrected) without dispersion correction term.

OPTIMIZED STRUCTURES

Table S9. Optimized cartesian coordinates of $(HgH_2)_2$ dimers with topologies **2a**, **2b** and **2c**.

2a

Hg	0.0181830	-0.000047	0.0005597
H	0.0188209	-1.645563	-0.0003879
H	0.0191229	1.645468	-0.0003879
Hg	3.5158170	-0.000367	0.0000720
H	3.5152582	0.000254	1.6455883
H	3.5147979	0.000254	-1.6454442

2b

Hg	0.216992	0.000000	0. 000000
H	-0.215016	-1.644959	0. 000000
H	-0.215016	1.644959	0. 000000
Hg	3.750991	0.000000	0.000001
H	3.749016	-1.644959	0. 000000
H	3.749016	1.644959	0. 000000

2c

Hg	-0.107536	-0.1128713	-0.000014
H	0.901819	-1.4201582	0.000014
H	-1.133615	1.1693399	0.000000
Hg	3.641536	0.1128713	0.000014
H	4.667613	-1.1693409	-0.000014
H	2.632181	1.4201591	-0.000000

Table S10. Optimized cartesian coordinates of $(Hg(CH_3)_2)_2$ dimers with topologies **2a**, **2b** and **2c**.

2a

Hg	0.577677	-0.342599	-0.057568
C	0.577999	-0.329760	-2.132742
H	1.459804	0.183590	-2.516909
H	0.577980	-1.342889	-2.534645
H	-0.303656	0.183701	-2.517101
C	0.577884	-0.321700	2.017540
H	-0.303793	0.193249	2.399853
H	0.577842	-1.333260	2.423375
H	1.459668	0.193137	2.399761
Hg	0.577631	3.031801	-0.064305
C	-1.497512	3.015008	-0.064304
H	-1.880780	2.499151	-0.945036
H	-1.880798	2.502594	0.818428
H	-1.901349	4.027367	-0.066285
C	2.652776	3.014879	-0.064270
H	3.036025	2.502440	0.818461
H	3.036034	2.498994	-0.944988
H	3.056674	4.027213	-0.066247

2b

Hg	0.577694	-0.541939	-0.057197
C	-1.496271	-0.547816	-0.057360
H	-1.889205	-0.040975	-0.938380
H	-1.882112	-1.567392	-0.055412
H	-1.889368	-0.037545	0.821605
C	2.651658	-0.547816	-0.057359
H	3.044755	-0.037547	0.821606
H	3.037499	-1.567392	-0.055413
H	3.044593	-0.040974	-0.938379
Hg	0.577694	3.231128	-0.064584
C	-1.496269	3.237030	-0.064694
H	-1.889233	2.726772	-0.943727
H	-1.889343	2.730100	0.816258
H	-1.882102	4.256609	-0.066698
C	2.651657	3.237030	-0.064695
H	3.044730	2.730100	0.816257
H	3.044620	2.726772	-0.943727
H	3.037489	4.256609	-0.066698

2c

Hg	0.818260	-0.574498	-0.057358
C	-0.981234	-1.603993	-0.054738
H	-1.571934	-1.352509	-0.935722
H	-0.822179	-2.682308	-0.052067
H	-1.571874	-1.348139	0.825027
C	2.631301	0.439441	-0.059946
H	2.736494	1.075428	0.819346
H	3.461569	-0.267402	-0.058842
H	2.735908	1.071983	-0.941790
Hg	0.337130	3.263686	-0.064660
C	-1.475850	2.249634	-0.063275
H	-1.580455	1.613682	-0.942664
H	-1.580975	1.617042	0.818470
H	-2.306159	2.956428	-0.064872
C	2.136562	4.293292	-0.066071
H	2.726939	4.041408	0.815015
H	2.727554	4.037910	-0.945736
H	1.977440	5.371597	-0.068264

Table S11. Optimized cartesian coordinates of $(Hg(CN)_2)_2$ dimers with topologies **2a** and **2c**.

2a

C	0.321825	-0.492275	-0.137642
Hg	0.282298	-0.502278	-2.134980
Hg	3.792960	1.534609	-2.091802
C	2.738078	3.231101	-2.082195
C	0.347269	-0.451662	-4.131030
C	4.743533	-0.222460	-2.102702
N	0.430097	-0.396247	-5.272534
N	0.390064	-0.460115	1.005718
N	5.241878	-1.254240	-2.109532
N	2.088899	4.175296	-2.077225

2c

C	1.219098	-0.038505	-0.520125
Hg	-0.347508	-1.207365	-0.109110
C	-1.969843	-2.360165	0.230232
C	-0.391759	-3.139557	2.750917
Hg	-2.013878	-4.292730	3.089941
C	-3.580196	-5.461992	3.500715
N	2.106659	0.639168	-0.776004
N	-2.811518	-3.063476	0.564493
N	0.449753	-2.435996	2.416770
N	-4.467929	-6.139307	3.756946

Table S12. Optimized cartesian coordinates of $(Hg(Cl)_2)_2$ dimers with topologies **2a** and **2c**.

2a

Hg	0.000009	0.000006	1.793913
Hg	-0.000006	-0.000009	-1.793913
Cl	-0.000003	2.235907	1.733897
Cl	0.000011	-2.235896	1.733912
Cl	-2.235907	0.000003	-1.733897
Cl	2.235897	-0.000011	-1.733912

2b

Cl	0.740295	-0.699296	0.216317
Hg	-1.494556	-0.719863	0.241149
Hg	-1.513760	1.508972	-3.624466
Cl	-3.748614	1.488505	-3.599576
Cl	-3.729598	-0.717679	0.226424
Cl	0.721284	1.506705	-3.609786

2c

Cl	1.091208	-0.197288	-0.389036
Hg	-0.699791	-1.482397	0.002669
Cl	-2.574982	-2.724875	0.262410
Cl	0.213585	-2.775150	2.718544
Hg	-1.661634	-4.017586	2.978291
Cl	-3.452662	-5.302659	3.369989

Table S13. Optimized cartesian coordinates of $(HgBr_2)_2$ dimers with topologies **2a**, **2b** and **2c**.

2a

Br	0.560547	-0.355030	0.235237
Hg	0.513469	-0.366789	-2.133590
Hg	3.561951	1.399088	-2.093246
Br	2.310640	3.410967	-2.082022
Br	0.593769	-0.304829	-4.500731
Br	4.685898	-0.686619	-2.106178

2b

Br	0.872040	-0.689857	0.200722
Hg	-1.494853	-0.711061	0.225990
Hg	-1.513463	1.500172	-3.609303
Br	-3.880356	1.479018	-3.584009
Br	-3.861936	-0.709605	0.212029
Br	0.853620	1.498676	-3.595367

2c

Br	1.213231	-0.098648	-0.434322
Hg	-0.689580	-1.456324	-0.025819
Br	-2.694935	-2.749656	0.196996
Br	0.333472	-2.750267	2.784024
Hg	-1.671885	-4.043583	3.006844
Br	-3.574578	-5.401477	3.415144

Table S14. Optimized cartesian coordinates of $(HgI_2)_2$ dimers with topologies **2a**, **2b** and **2c**.

2a

I	0.593120	-0.336822	0.413651
Hg	0.535468	-0.354312	-2.133233
Hg	3.539815	1.386367	-2.093501
I	2.187504	3.545405	-2.081229
I	0.629522	-0.283517	-4.678094
I	4.740845	-0.860333	-2.108124

2b

I	1.049854	-0.720181	0.254202
Hg	-1.494722	-0.735718	0.268720
Hg	-1.513594	1.524841	-3.652026
I	-4.058170	1.509339	-3.637491
I	-4.039378	-0.741513	0.266536
I	1.031062	1.530576	-3.649879

2c

I	1.381440	0.053723	-0.518175
Hg	-0.663684	-1.408082	-0.076317
I	-2.839665	-2.770834	0.104167
I	0.478226	-2.729116	2.876820
Hg	-1.697747	-4.091886	3.057305
I	-3.742845	-5.553759	3.499066

Table S15. Optimized cartesian coordinates of $(Hg(CF_3)_2)_2$ dimers with topologies **2a** and **2c**.

2a

Hg	0.738556	-0.424882	0.066396
C	0.746609	-0.523976	-2.028871
F	1.872273	-1.056358	-2.534324
F	-0.278325	-1.231534	-2.533503
F	0.644794	0.723659	-2.558714
C	0.717464	-0.172995	2.149072
F	0.604732	1.145917	2.461862
F	-0.312539	-0.790570	2.751593
F	1.837250	-0.606935	2.751544
Hg	0.415917	3.112708	-0.186930
C	-1.662403	2.827089	-0.195233
F	-2.259957	3.279287	-1.310494
F	-1.955181	1.501271	-0.118334
F	-2.285344	3.409651	0.843070
C	2.509098	3.247861	-0.168317
F	3.059874	2.007723	-0.087887
F	3.017876	3.814008	-1.275866
F	2.989412	3.940991	0.877951

2c

Hg	0.343658	-1.004668	-0.056429
C	-1.367994	-2.213143	-0.053947
F	-2.146490	-1.999273	-1.132370
F	-1.066521	-3.528387	-0.054977
F	-2.142661	-2.000091	1.027422
C	2.075723	0.188747	-0.058889
F	2.139394	1.013751	1.018130
F	3.215646	-0.518911	-0.057248
F	2.139498	1.008957	-1.139536
Hg	0.811733	3.693837	-0.065486
C	-0.920308	2.500399	-0.063606
F	-0.983935	1.675998	-1.141070
F	-0.984109	1.679583	1.016599
F	-2.060240	3.208043	-0.064855
C	2.523361	4.902366	-0.067592
F	3.297084	4.694865	1.015529
F	3.302811	4.683029	-1.144227
F	2.221844	6.217577	-0.075594

Table S16. Optimized cartesian coordinates of $(Hg(SiH_3)_2)_2$ dimers with topologies **2a**, **2b** and **2c**.

2a

Hg	0.578004	-0.251717	-0.057734
Si	0.578021	-0.211901	-2.523345

H	1.774657	0.494774	-3.045919
H	0.577931	-1.581268	-3.096862
H	-0.618503	0.494942	-3.045954
Si	0.577546	-0.202065	2.407712
H	-0.619079	0.506828	2.927303
H	0.577350	-1.569140	2.986664
H	1.774073	0.506671	2.927738
Hg	0.577787	2.940938	-0.064191
Si	-1.887743	2.896121	-0.063928
H	-2.409014	2.186407	-1.259333
H	-2.408819	2.190218	1.133819
H	-2.464032	4.264321	-0.066058
Si	3.043322	2.896274	-0.064226
H	3.564596	2.190410	1.133458
H	3.564491	2.186591	-1.259693
H	3.619519	4.264512	-0.066433

2b

Hg	0.577694	-0.637832	-0.057293
Si	-1.885688	-0.703897	-0.057055
H	-2.462153	-0.048209	-1.256683
H	-2.353397	-2.114386	-0.054318
H	-2.462081	-0.043556	1.140053
Si	3.041076	-0.703898	-0.057056
H	3.617470	-0.043559	1.140053
H	3.508785	-2.114387	-0.054321
H	3.617541	-0.048208	-1.256683
Hg	0.577693	3.327034	-0.064879
Si	-1.885689	3.393095	-0.064991
H	-2.462081	2.732783	-1.262116
H	-2.462149	2.737369	1.134620
H	-2.353405	4.803582	-0.067722
Si	3.041075	3.393094	-0.064990
H	3.617535	2.737366	1.134620
H	3.617468	2.732784	-1.262116
H	3.508792	4.803581	-0.067720

2c

Hg	0.303291	-0.967514	-0.056418
Si	-1.690087	-2.404262	-0.050724
H	-2.533696	-2.154517	-1.247051
H	-1.338327	-3.847473	-0.048955
H	-2.530364	-2.150825	1.147204
Si	2.310027	0.464277	-0.062416
H	2.344474	1.368074	1.122470
H	3.586544	-0.292871	-0.060284
H	2.343562	1.360346	-1.253097
Hg	0.852066	3.656749	-0.065398
Si	-1.154769	2.225083	-0.065872
H	-1.188316	1.324400	-1.253062

H	-1.189346	1.325900	1.122518
H	-2.431233	2.982325	-0.066754
Si	2.845601	5.093289	-0.065047
H	3.684375	4.846257	1.135265
H	3.690644	4.836906	-1.258964
H	2.494050	6.536536	-0.071560

Table S17. Optimized cartesian coordinates of $(Hg(SiMe_3)_2)_2$ dimers with topologies **2a** and **2c**.

2a

C	18.866075	-11.621055	14.773972
C	16.662888	-8.539042	13.246504
C	22.987708	-8.704818	14.646081
C	20.656940	-5.476480	13.733488
C	18.684602	-12.106537	11.789627
C	15.973853	-8.691964	16.191216
C	22.484865	-7.242122	17.249954
C	22.020575	-6.280641	11.152011
C	21.370374	-12.266107	13.203220
C	16.693122	-6.023335	14.927822
C	22.073072	-10.248065	17.082259
C	19.022573	-5.785666	11.206073
H	18.679193	-12.687537	14.915988
H	15.601654	-8.381085	13.043105
H	24.025098	-8.834922	14.961356
H	20.861490	-4.436484	13.470633
H	19.469113	-11.277617	15.615782
H	17.227027	-8.041088	12.456475
H	22.733553	-9.543506	13.996224
H	19.750220	-5.490330	14.340147
H	17.905907	-11.106315	14.815044
H	16.858738	-9.609376	13.177833
H	22.931780	-7.790857	14.054333
H	21.481533	-5.832012	14.351604
H	17.712215	-11.618045	11.717435
H	16.147225	-9.768075	16.226914
H	22.409230	-6.274927	16.751826
H	22.898847	-6.658445	11.676671
H	19.166846	-12.029844	10.814517
H	16.133310	-8.297379	17.195268
H	21.912146	-7.183207	18.176126
H	21.950752	-6.808612	10.200373
H	18.514129	-13.164745	11.997721
H	14.926491	-8.529501	15.928899
H	23.532340	-7.403365	17.512554
H	22.186753	-5.222965	10.937853
H	21.192143	-13.329669	13.374232
H	15.636174	-5.870593	14.700445
H	23.115143	-10.382086	17.379425
H	19.213622	-4.737708	10.966314
H	21.927605	-12.165420	12.271241

H	16.898214	-5.561270	15.894088
H	21.461489	-10.271790	17.984816
H	18.863024	-6.320153	10.269016
H	22.005299	-11.900967	14.010947
H	17.275881	-5.491669	14.175166
H	21.790217	-11.102334	16.466551
H	18.095103	-5.832639	11.777372
Hg	20.101886	-8.920565	12.656636
Hg	19.481970	-8.243330	15.545805
Si	19.742145	-11.333104	13.135158
Si	17.101223	-7.856149	14.943089
Si	21.861726	-8.631398	16.150475
Si	20.460896	-6.508089	12.173319

2c

C	-13.728758	-9.298642	-16.262308
C	-19.412831	-12.680525	-16.741858
C	-20.253089	-4.786820	-19.081324
C	-25.935284	-8.168780	-19.570844
C	-14.986053	-7.080442	-17.906345
C	-19.098794	-7.076684	-17.473106
C	-20.567499	-10.392212	-18.352076
C	-24.681580	-10.387269	-17.924498
C	-23.858401	-9.991733	-20.822244
C	-21.081685	-5.185455	-16.186154
C	-15.803999	-7.476422	-15.007170
C	-18.585587	-12.285220	-19.637857
H	-12.945380	-8.606172	-15.947474
H	-19.428741	-4.155466	-18.743529
H	-20.237468	-13.312099	-17.078536
H	-26.718318	-8.861024	-19.887028
H	-13.853122	-10.043308	-15.475276
H	-18.557628	-13.326335	-16.539725
H	-25.809321	-7.424174	-20.357679
H	-21.108303	-4.140946	-19.283204
H	-13.378909	-9.815175	-17.156859
H	-19.709025	-12.217222	-15.799971
H	-19.956316	-5.249051	-20.023555
H	-26.286541	-7.652117	-18.676920
H	-14.653143	-7.542401	-18.836598
H	-18.780648	-7.592835	-18.380528
H	-20.885317	-9.875202	-17.445031
H	-25.015964	-9.925155	-16.994851
H	-15.875394	-6.489959	-18.128452
H	-19.262885	-7.825713	-16.696509
H	-20.403545	-9.643907	-19.129402
H	-23.792839	-10.978054	-17.700802
H	-14.202814	-6.396123	-17.573828
H	-18.284337	-6.426256	-17.150084
H	-21.382127	-11.042829	-18.674287
H	-25.464472	-11.071328	-18.258367
H	-24.649727	-10.681956	-21.121740

H	-20.249928	-4.550084	-15.875037
H	-15.012359	-6.785969	-14.709035
H	-19.417600	-12.920806	-19.947847
H	-22.941545	-10.567592	-20.693706
H	-21.285961	-5.888914	-15.378079
H	-16.721265	-6.900839	-15.134016
H	-18.381608	-11.582695	-20.446819
H	-23.698218	-9.290838	-21.642408
H	-21.961035	-4.551365	-16.304420
H	-15.962492	-8.177425	-14.186772
H	-17.706278	-12.919317	-19.519329
Hg	-22.514334	-7.569976	-18.516155
Hg	-17.151301	-9.898433	-17.311250
Si	-24.333274	-9.093343	-19.241756
Si	-20.664991	-6.080974	-17.783834
Si	-15.331626	-8.374559	-16.588553
Si	-19.001338	-11.387861	-18.040962