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Lewis acid enhancement by juxtaposition with an onium ion: The case of a mercury stibonium complex

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Titration experiments

Fig. S1 ^1H NMR titration spectra of $[\text{2}]^+$ vs TBABr.

Fig. S2 ^{199}Hg titration spectra of $[\text{2}]^+$ vs TBAI, TBABr, and TBACl.

Derivation of the equation used to determine the 1:2 stability constant.

Computational section

Fig. S3 NBO plots showing $5\text{d}(\text{Hg}) \rightarrow \sigma^*(\text{Sb}-\text{C}_{\text{Ph1}})$ interactions for $[\text{2}]^+$, 2-F, $[\text{2}-\text{Cl}_2]^-$, and 2-I.

DFT optimized structural coordinates

X-ray Absorption Spectroscopy

Table S1 X-ray Absorption Spectra Fits.

Titration experiments

General considerations. NMR spectra were recorded on Varian Unity Inova 400 FT NMR (399.59 MHz for ^1H , 375.96 MHz for ^{19}F , 100.45 MHz for ^{13}C , 71.20 MHz for ^{199}Hg) spectrometers at ambient temperature. Chemical shifts (given in ppm) are referenced to residual ^1H and ^{13}C solvent signals, $\text{BF}_3\text{-Et}_2\text{O}$, and external neat HgMe_2 .

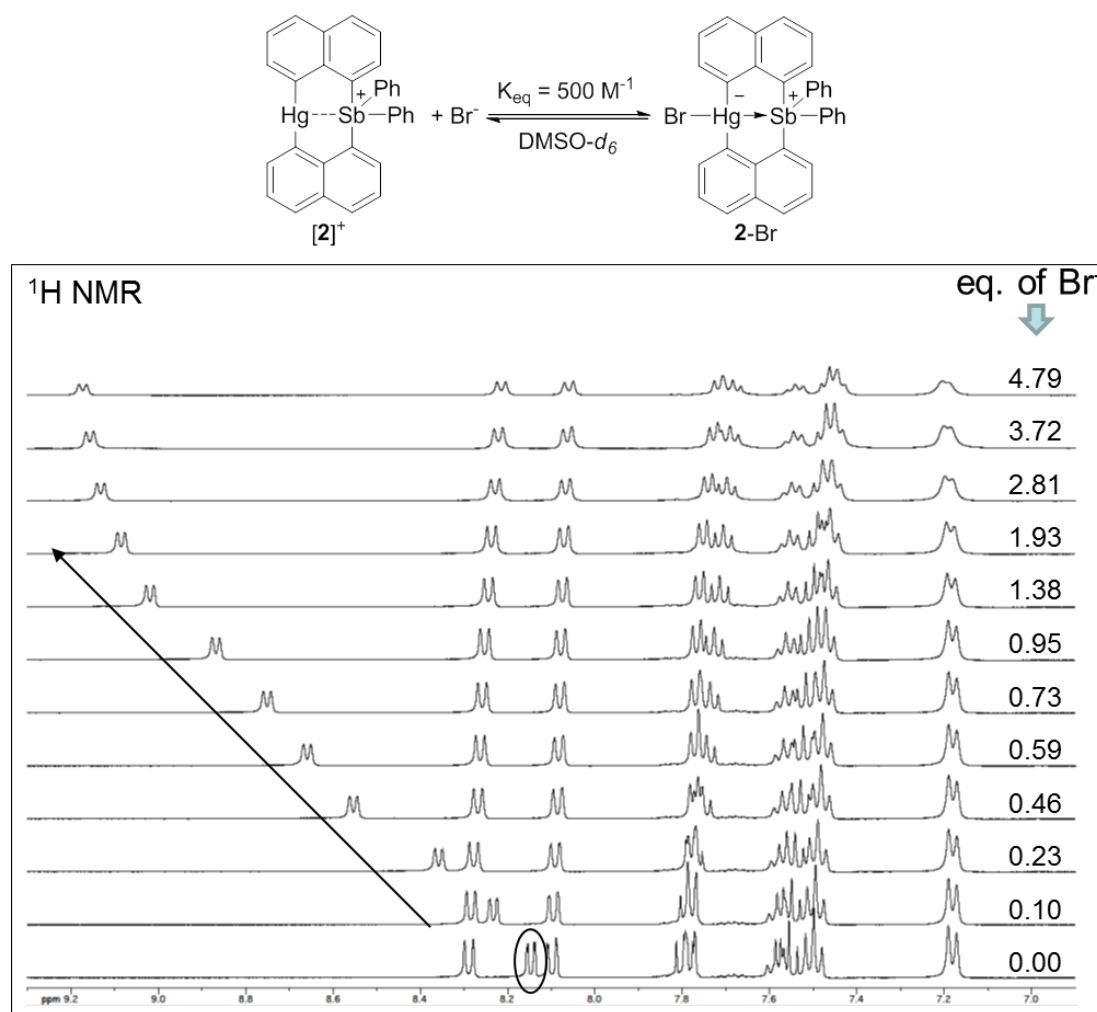


Fig. S1: ^1H Spectra obtained by titrating $[\text{2}]^+$ against TBABr in $\text{DMSO-}d_6$. The concentration in $[\text{2}]^+$ remained constant during the titration ($2.23 \times 10^{-2} \text{ M}$).

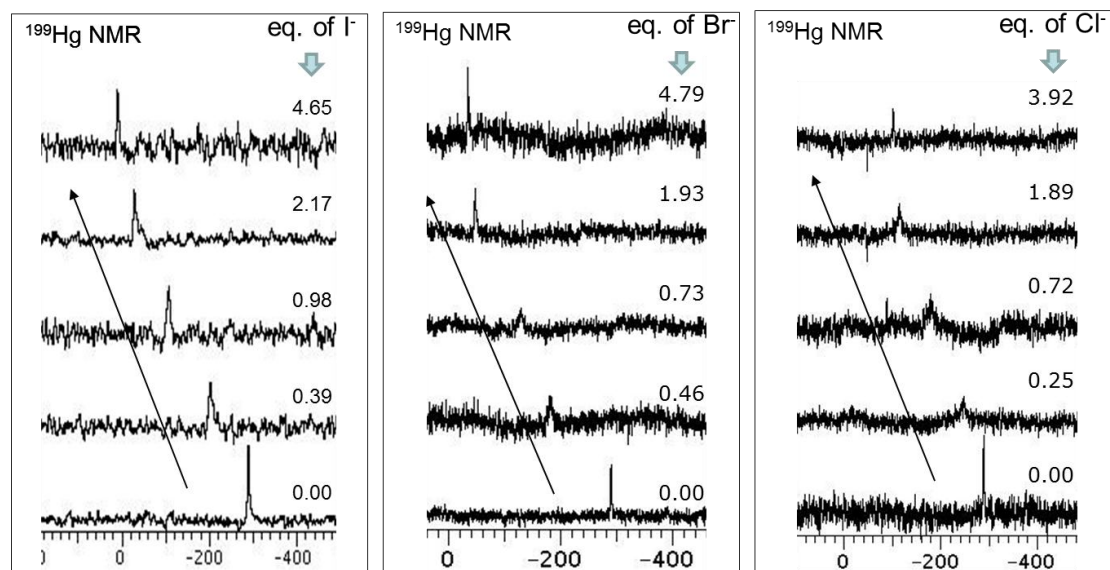


Fig. S2: ^{199}Hg spectra obtained by titrating $[2]^+$ against TBAI, TBABr, and TBACl in $\text{DMSO}-d_6$. The concentration in $[2]^+$ remained constant during the titrations (2.20×10^{-2} M (left), 2.23×10^{-2} M (middle), and 2.23×10^{-2} M (right)).

Derivation of the equation used to determine the chloride binding constants: ($R = 2^+$, $S = Cl^-$)

$$\begin{array}{c}
 R + S \xrightleftharpoons{K_1} RS + S \xrightleftharpoons{K_2} RS_2 \\
 (R-x-Y) \quad (S-x-2Y) \quad X \quad (S-x-2Y) \quad Y
 \end{array}$$

before equilibrium $\left\{ \begin{array}{l} [RS]_0 = 0 \\ [RS_2]_0 = 0 \\ [R]_0 = R \\ [S]_0 = S \end{array} \right.$ after equilibrium $\left\{ \begin{array}{l} [RS]_{eq} = X \\ [RS_2]_{eq} = Y \\ [R]_{eq} = R-x-Y \\ [S]_{eq} = S-x-2Y \end{array} \right.$

$$K_2 = \frac{Y}{X(S-x-2Y)} \Rightarrow Y = \frac{-K_2 X^2 + K_2 S X}{2K_2 X + 1}$$

$$K_1 = \frac{X}{(R-x-Y)(S-x-2Y)}$$

$$\Rightarrow \frac{X}{K_1} = (RS - RX - 2RY - SX + X^2 + 2XY - SY + XY + 2Y^2)$$

$$\Rightarrow \frac{X}{K_1} = X^2 - (R+S)X + 2Y^2 - (2R+S)Y + 3XY + RS$$

$$\Rightarrow \frac{X}{K_1} = X^2 - (R+S)X + \frac{2(-K_2 X^2 + K_2 S X)^2}{(2K_2 X + 1)^2} - \frac{(2R+S)(-K_2 X^2 + K_2 S X)}{(2K_2 X + 1)} + \frac{-3K_2 X^3 + 3K_2 S X}{(2K_2 X + 1)} + RS$$

$$\Rightarrow \frac{X(2K_2 X + 1)^2}{K_1} = X^2(2K_2 X + 1)^2 - (R+S)X(2K_2 X + 1)^2 + 2(-K_2 X^2 + K_2 S X)^2$$

$$\begin{aligned}
 & - (2R+S)(-K_2 X^2 + K_2 S X)(2K_2 X + 1) + (2K_2 X + 1)(-3K_2 X^3 + 3K_2 S X^2) \\
 & + RS(2K_2 X + 1)^2
 \end{aligned}$$

$$\begin{aligned}
 \Rightarrow \left(\frac{4K_2^2 X^3}{K_1} + \frac{4K_2 X^2}{K_1} \right) \left(\frac{X}{K_1} \right) &= \left(4K_2^2 X^4 + 4K_2 X^3 + X^2 \right) \left(-4RK_2^2 X^3 - 4RK_2 X^2 - RSX \right) \\
 & - 4SK_2^2 X^3 - 4SK_2 X^2 - RSX + (2K_2^2 X^4 + 2K_2^2 S X^2 - 4K_2^2 S X) \\
 & + 2K_2 R X^2 - 2K_2 R S X + K_2 S X^2 - K_2 S^2 X \\
 & + 4K_2^2 R X^3 - 4K_2^2 R S X^2 + 2K_2^2 S X^3 - 2K_2^2 S^2 X^2 \\
 & - 6K_2^2 X^4 + 6K_2^2 S X^3 - 3K_2 X^3 + 3K_2 S X^2 \\
 & + 4K_2^2 R S X^2 - 4K_2 R S X + RS
 \end{aligned}$$

$$\textcircled{a}x^3 + \textcircled{b}x^2 + \textcircled{c}x + \textcircled{d} = 0$$

$$\begin{aligned} a &= 4k_2 - \cancel{4Rk_2^2} - \cancel{4Sk_2^2} - \cancel{4k_2^2S} + \cancel{4k_2^2R} + \cancel{2k_2^2S} \\ &\quad + \cancel{6k_2^2S} - \cancel{3k_2^2} - \frac{4k_2^2}{k_1} \\ &= \left(k_2 - \frac{4k_2^2}{k_1} \right) \end{aligned}$$

$$\begin{aligned} b &= \cancel{1} - \cancel{4Rk_2} - \cancel{4Sk_2} + \cancel{2k_2^2S^2} + \cancel{2k_2R} + \cancel{k_2S} - \cancel{4k_2^2S} \\ &\quad - \cancel{2k_2^2S^2} + \cancel{3k_2S} + \cancel{4k_2^2RS} - \frac{4k_2}{k_1} \\ &= \left(1 - 2Rk_2 - \frac{4k_2}{k_1} \right) \end{aligned}$$

$$\begin{aligned} c &= \cancel{-R} - \cancel{S} - \cancel{2k_2RS} - \cancel{k_2S^2} + \cancel{4k_2RS} - \frac{1}{k_1} \\ &= \left(-R - S + 2k_2RS - k_2S^2 - \frac{1}{k_1} \right) \end{aligned}$$

$$d = (RS)$$

Computational section

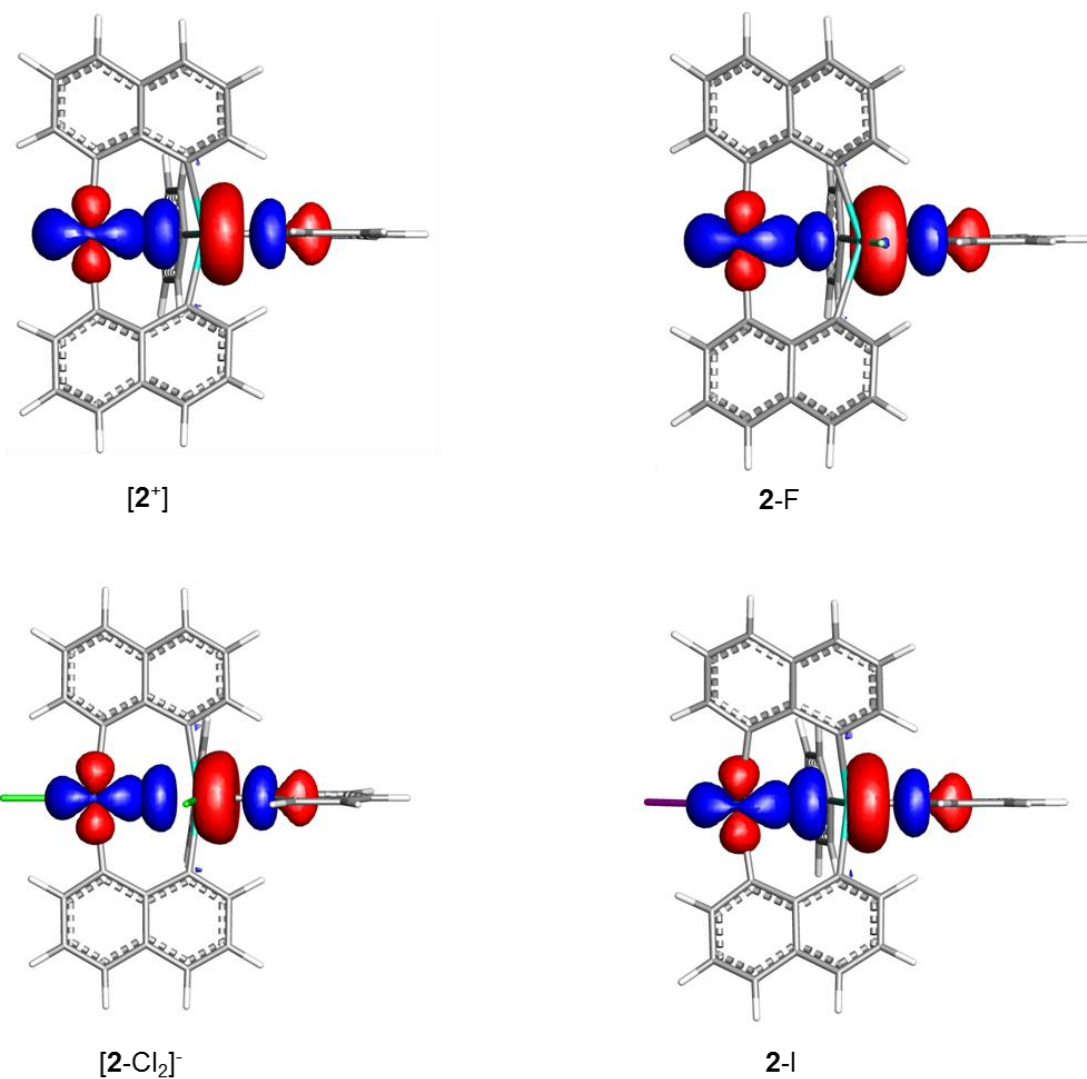
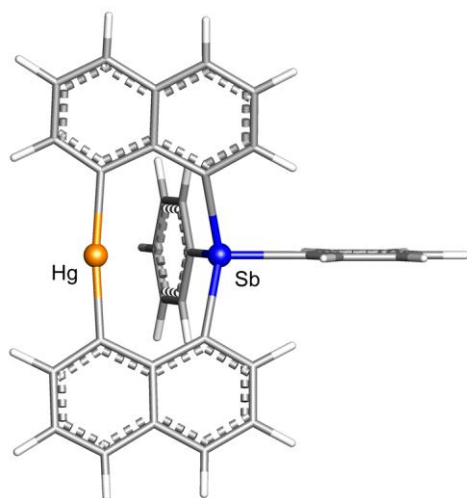


Fig. S3: NBO plots showing the $5d(\text{Hg}) \rightarrow \sigma^*(\text{Sb-C}_{\text{Ph1}})$ interactions for $[2]^+$, 2-F, $[2-\text{Cl}_2]^-$, and 2-I.

DFT optimized structural coordinates

Complex [2]⁺



Method 1

Hg	-0.227550	-2.039756	-0.137530
Sb	0.116902	1.043079	-0.080034
C	-4.601759	-2.536969	-0.429023
H	-5.299097	-3.369892	-0.290284
C	0.430868	3.931792	-1.282871
H	0.359810	3.443372	-2.262396
C	-4.149616	-0.224987	-1.090259
C	3.931278	-3.488483	-0.412790
H	4.427621	-4.454549	-0.272586
C	-3.793228	2.094331	-1.775976
H	-4.166832	3.041993	-2.176520
C	-2.432265	1.989634	-1.389667
H	-1.806990	2.881986	-1.472930
C	-2.299814	-1.675558	-0.296006
C	-1.919564	0.795855	-0.881582
C	1.241835	0.204044	2.679389
H	2.199498	0.164893	2.148397
C	-2.743818	-0.382802	-0.743284
C	4.000382	-1.134904	-1.078410
C	1.875605	-2.140713	-0.282933
C	0.049400	0.530339	2.000994
C	2.594603	-0.978469	-0.731101
C	0.456451	3.834184	1.160723

H	0.404534	3.265013	2.095316
C	0.360121	3.184717	-0.085390
C	-5.046550	-1.320049	-0.913512
H	-6.100977	-1.174122	-1.174785
C	2.049887	0.351998	-0.874572
C	-4.634436	1.010280	-1.609092
H	-5.695927	1.084557	-1.872393
C	4.633702	-2.400500	-0.899125
H	5.694227	-2.491472	-1.160649
C	0.691411	5.973508	0.018439
H	0.820609	7.060026	0.059466
C	2.811349	1.402190	-1.387758
H	2.395948	2.409356	-1.475543
C	-3.222903	-2.710740	-0.138461
H	-2.887362	-3.696279	0.205804
C	4.744109	-0.038420	-1.602691
H	5.795494	-0.200591	-1.867145
C	0.596347	5.325513	-1.224487
H	0.651070	5.902689	-2.153593
C	2.547694	-3.353800	-0.123597
H	2.002689	-4.241230	0.219703
C	-1.184903	0.560545	2.682308
H	-2.114514	0.800347	2.153910
C	-1.218812	0.265882	4.055406
H	-2.174599	0.288044	4.589598
C	1.192472	-0.088829	4.052556
H	2.115339	-0.343493	4.584402
C	4.161638	1.203473	-1.774330
H	4.733941	2.043787	-2.179768
C	0.622007	5.229607	1.206316
H	0.696830	5.732394	2.176340
C	-0.033929	-0.058320	4.737790
H	-0.066652	-0.289493	5.807721

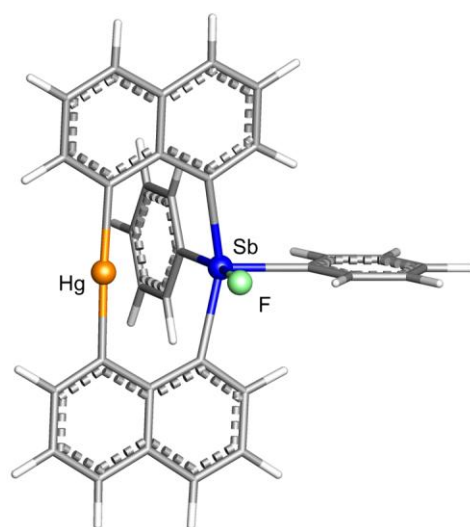
Method 2

Hg	0.133678	-2.059312	-0.207841
Sb	-0.066562	1.028608	-0.004888
C	-4.023420	-3.363333	-0.573567

H	-4.541686	-4.319282	-0.506049
C	-0.237722	3.834899	-1.394200
H	-0.200840	3.275874	-2.329900
C	-4.035643	-0.975611	-1.054267
C	4.431920	-2.816354	-0.475146
H	5.068132	-3.696683	-0.390252
C	-4.139884	1.400751	-1.563282
H	-4.690373	2.283241	-1.886478
C	-2.780476	1.528969	-1.199728
H	-2.338357	2.522010	-1.226605
C	-1.950309	-2.087478	-0.355738
C	-2.046942	0.429719	-0.782836
C	1.167580	0.563351	2.781317
H	2.113332	0.706761	2.257053
C	-2.629148	-0.883818	-0.718457
C	4.144685	-0.449663	-0.973828
C	2.206698	-1.819391	-0.308808
C	-0.055181	0.607452	2.096586
C	2.731840	-0.539442	-0.665717
C	-0.250760	3.912739	1.040275
H	-0.223009	3.411157	2.008489
C	-0.200838	3.179077	-0.151564
C	-4.697139	-2.229654	-0.965749
H	-5.756873	-2.273566	-1.220167
C	1.986057	0.687183	-0.750276
C	-4.752921	0.173894	-1.477480
H	-5.807951	0.064625	-1.733122
C	4.961117	-1.606858	-0.862516
H	6.022555	-1.514365	-1.095733
C	-0.374235	5.965519	-0.245292
H	-0.442683	7.053374	-0.281140
C	2.578242	1.870091	-1.162635
H	2.011426	2.797084	-1.205429
C	-2.642699	-3.286632	-0.282333
H	-2.121247	-4.204417	-0.006998
C	4.714874	0.780943	-1.392764
H	5.780013	0.808262	-1.627420
C	-0.323487	5.229332	-1.434561

H	-0.351087	5.739402	-2.397526
C	3.047016	-2.918179	-0.212715
H	2.643225	-3.894700	0.058095
C	-1.271464	0.405904	2.764343
H	-2.220532	0.427024	2.227039
C	-1.257078	0.165143	4.141457
H	-2.197790	0.004821	4.668432
C	1.165406	0.321711	4.158290
H	2.111616	0.283301	4.698284
C	3.949481	1.917221	-1.500588
H	4.386905	2.861718	-1.821297
C	-0.337587	5.308874	0.987263
H	-0.376711	5.879335	1.915574
C	-0.042838	0.123043	4.835182
H	-0.037773	-0.070986	5.908333

Complex 2-F



Method 1

Hg	0.002060	-2.041331	-0.129415
Sb	0.002978	1.110999	-0.397457
F	0.015116	1.855679	-2.325271
C	-2.110002	-1.950890	-0.195829
C	-2.053668	0.493347	-0.942844
C	4.196783	-0.753863	-0.819133
C	-0.016666	0.358711	1.709720
C	-2.744532	-0.735127	-0.638203
C	2.754079	-0.736032	-0.621825
C	-4.135927	1.522349	-1.731640
H	-4.641986	2.389153	-2.170874
C	0.002423	3.194073	0.219738
C	2.114201	-1.955333	-0.196807
C	1.189961	0.180215	2.421224
H	2.152847	0.291152	1.909344
C	4.159526	1.533138	-1.672579
H	4.670823	2.404994	-2.095400
C	2.068572	0.498444	-0.914090
C	-4.848569	0.390980	-1.378940
H	-5.935457	0.345619	-1.521428
C	-2.888358	-3.074095	0.086118
H	-2.408861	-4.003088	0.419272
C	0.003019	3.552470	1.580675
H	0.003311	2.784440	2.360469

C	-4.302262	-3.064941	-0.057919
H	-4.882690	-3.964030	0.179643
C	1.176719	-0.152441	3.787435
H	2.123594	-0.291916	4.322329
C	-4.186032	-0.751276	-0.843235
C	0.002643	4.198859	-0.770153
H	0.003843	3.894951	-1.820990
C	-2.735217	1.569728	-1.509483
H	-2.178682	2.461753	-1.806816
C	-4.931480	-1.926615	-0.529100
H	-6.017370	-1.910190	-0.684484
C	4.866257	0.393960	-1.333751
H	5.953744	0.346913	-1.470960
C	2.887791	-3.084948	0.072472
H	2.403984	-4.016601	0.391680
C	2.757477	1.581099	-1.459452
H	2.207191	2.479987	-1.747630
C	4.937022	-1.935937	-0.518290
H	6.023745	-1.920328	-0.667689
C	-1.237413	0.215498	2.404842
H	-2.189620	0.353857	1.879774
C	0.002652	5.552378	-0.395271
H	0.002622	6.329670	-1.168339
C	0.003337	4.909531	1.948189
H	0.003805	5.182933	3.009730
C	4.302169	-3.078956	-0.066549
H	4.878648	-3.983252	0.160630
C	0.002827	5.909550	0.962990
H	0.002853	6.966373	1.254068
C	-1.252691	-0.116752	3.770847
H	-2.210409	-0.228253	4.292799
C	-0.045069	-0.304617	4.463741
H	-0.056095	-0.564766	5.528461

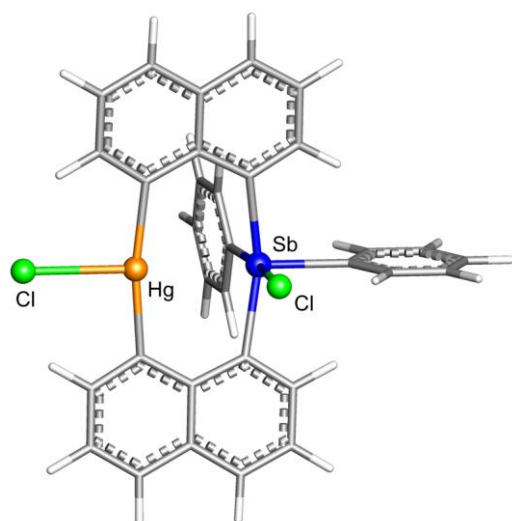
Method 2

Hg	1.183400	-0.191889	-3.659187
Sb	3.304930	1.841171	-2.743737
F	1.822159	2.013554	-1.321460

C	2.115364	-1.642186	-2.468643
C	3.830039	0.008267	-1.572583
C	0.037658	3.682638	-5.453287
C	4.624773	1.344538	-4.458105
C	3.222286	-1.289773	-1.633064
C	0.762181	2.666583	-4.717115
C	5.401657	-0.765361	0.129169
H	6.231185	-0.534124	0.797872
C	4.506627	3.347399	-1.764287
C	0.283223	1.319751	-4.795235
C	4.514907	2.053021	-5.663369
H	3.762590	2.835374	-5.776002
C	1.539167	5.410763	-4.640478
H	1.855697	6.452830	-4.587013
C	1.902061	3.093999	-3.959226
C	4.857526	-2.025380	0.090667
H	5.247393	-2.821257	0.728291
C	1.610358	-2.934271	-2.453086
H	0.763688	-3.200859	-3.089252
C	5.751321	3.724995	-2.282455
H	6.136020	3.263673	-3.193603
C	2.157400	-3.935859	-1.618235
H	1.735616	-4.941369	-1.625066
C	5.363622	1.756836	-6.736429
H	5.266769	2.312111	-7.670611
C	3.771206	-2.319419	-0.774969
C	4.013209	3.941972	-0.595129
H	3.040875	3.634646	-0.208699
C	4.881791	0.251004	-0.708115
H	5.336946	1.237716	-0.650646
C	3.215182	-3.626790	-0.794667
H	3.645766	-4.382779	-0.135571
C	0.450507	5.041273	-5.393381
H	-0.118164	5.785517	-5.954554
C	-0.825232	1.014383	-5.571177
H	-1.190149	-0.013275	-5.627470
C	2.264247	4.427660	-3.923957
H	3.124620	4.752542	-3.340769

C	-1.093673	3.316088	-6.231984
H	-1.622434	4.100252	-6.777035
C	5.583476	0.327252	-4.343450
H	5.670919	-0.246263	-3.419462
C	4.773993	4.918038	0.056595
H	4.392067	5.381354	0.967500
C	6.506779	4.702617	-1.624173
H	7.477379	4.996178	-2.026627
C	-1.519352	2.008777	-6.297241
H	-2.389524	1.738291	-6.895835
C	6.018610	5.298804	-0.456724
H	6.609115	6.061545	0.053714
C	6.432252	0.032740	-5.416991
H	7.173002	-0.762346	-5.316886
C	6.323104	0.746869	-6.614201
H	6.978617	0.510854	-7.454329

Complex $[2\text{-Cl}_2]^-$



Method 1

Hg	-1.954028	0.071533	-0.221871
Sb	1.089892	-0.056423	-0.219456
Cl	-4.660895	0.190922	-0.278491
Cl	0.917517	-0.169540	-2.996917
C	0.879203	2.130266	-0.544437
C	-1.829405	-2.089690	-0.168254
C	-0.357571	2.832334	-0.373691
C	-1.635209	2.210138	-0.153713
C	2.070895	2.790918	-0.816460
H	2.997574	2.228765	-0.964119
C	4.016680	-0.093881	0.931916
H	3.493711	-0.002804	1.890442
C	3.284091	-0.148308	-0.271229
C	0.896007	0.049056	1.979690
C	1.039882	1.280703	2.653159
H	1.242364	2.195681	2.084182
C	0.706069	-2.239475	-0.367841
C	0.542779	-5.049819	-0.414747
H	0.460820	-6.144694	-0.427611
C	0.915460	1.354937	4.051509
H	1.028704	2.321836	4.557359
C	-0.598356	-2.825655	-0.276282
C	0.488084	-1.033313	4.137553
H	0.263450	-1.941458	4.710421

C	-0.652459	-4.284674	-0.283753
C	0.951872	4.938014	-0.710862
H	0.964332	6.034783	-0.762252
C	-3.029609	-2.791427	-0.040627
H	-3.965669	-2.225825	0.032564
C	1.853616	-3.013853	-0.490387
H	2.836787	-2.542656	-0.575733
C	0.617219	-1.105990	2.739253
H	0.485876	-2.071991	2.238406
C	1.774777	-4.432121	-0.522075
H	2.693273	-5.021940	-0.626863
C	-3.076491	-4.211705	-0.028415
H	-4.043642	-4.720544	0.072393
C	-2.753543	3.017760	0.061424
H	-3.728590	2.541090	0.214547
C	2.108706	4.208303	-0.914036
H	3.058206	4.709182	-1.137910
C	5.421665	-0.154003	0.913674
H	5.979279	-0.111578	1.857426
C	3.978031	-0.261607	-1.494237
H	3.405935	-0.302220	-2.429713
C	0.638032	0.197434	4.797087
H	0.533908	0.255489	5.887413
C	-1.909808	-4.943259	-0.157069
H	-1.926067	-6.041361	-0.165717
C	-1.464364	5.058999	-0.209314
H	-1.387653	6.153681	-0.252922
C	-0.286069	4.288819	-0.431328
C	-2.672730	4.436744	0.048570
H	-3.578031	5.032031	0.223182
C	6.107504	-0.267264	-0.306088
H	7.203381	-0.313669	-0.319798
C	5.382774	-0.320342	-1.508319
H	5.910899	-0.408644	-2.465817

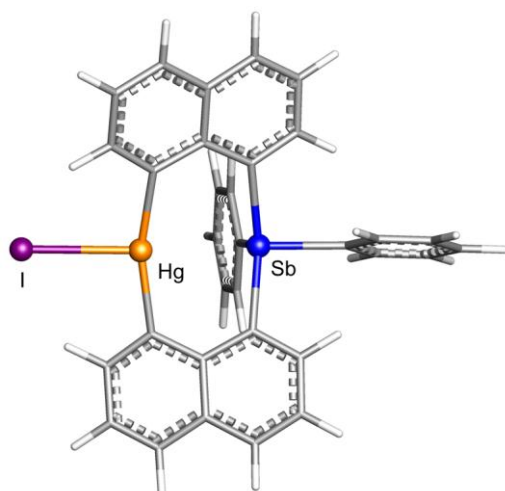
Method 2

Hg	1.333899	0.043206	1.448324
Sb	-0.683752	0.294600	-0.813833

Cl	3.114192	-0.337901	3.485387
Cl	-0.059137	2.875277	-0.731111
C	1.154969	0.082778	-2.043082
C	-0.325711	0.476743	2.734456
C	2.447834	-0.194878	-1.507869
C	2.760833	-0.299767	-0.114110
C	0.932422	0.187685	-3.402461
H	-0.063971	0.406744	-3.785537
C	-2.842239	-0.440806	-2.985639
H	-2.700941	-1.446617	-2.587171
C	-2.116729	0.636424	-2.456180
C	-1.031448	-1.905478	-0.688650
C	-0.354499	-2.785924	-1.547466
H	0.368006	-2.400190	-2.269020
C	-2.039818	0.765999	0.884429
C	-4.006609	1.353803	2.791711
H	-4.761598	1.584398	3.547402
C	-0.590259	-4.164372	-1.488055
H	-0.051641	-4.834331	-2.161442
C	-1.644556	0.763808	2.254916
C	-2.171211	-3.814568	0.307039
H	-2.873320	-4.209731	1.044002
C	-2.682989	1.072702	3.223277
C	3.253363	-0.272188	-3.866167
H	4.082090	-0.413734	-4.564359
C	-0.077983	0.506856	4.099796
H	0.932183	0.286381	4.451337
C	-3.336345	1.043391	0.496673
H	-3.612697	1.040025	-0.557375
C	-1.936469	-2.435841	0.243328
H	-2.463911	-1.773350	0.931859
C	-4.333922	1.339083	1.455856
H	-5.350770	1.555148	1.124778
C	-1.090905	0.815520	5.037582
H	-0.850969	0.833706	6.102777
C	4.063229	-0.587721	0.269881
H	4.288974	-0.659263	1.335904
C	1.988919	0.010800	-4.327562

H	1.788284	0.099373	-5.396325
C	-3.753965	-0.237184	-4.028421
H	-4.311814	-1.085183	-4.430718
C	-2.316546	1.921602	-2.980748
H	-1.751669	2.757635	-2.563575
C	-1.500636	-4.682058	-0.560927
H	-1.678044	-5.758458	-0.507176
C	-2.368744	1.092174	4.607426
H	-3.163112	1.332640	5.318466
C	4.829829	-0.672893	-2.021882
H	5.619428	-0.807303	-2.765584
C	3.516363	-0.382147	-2.474666
C	5.097532	-0.777115	-0.675851
H	6.109407	-0.998597	-0.329974
C	-3.948821	1.045190	-4.550915
H	-4.659700	1.203497	-5.364968
C	-3.228392	2.122684	-4.023679
H	-3.375426	3.127689	-4.424785

Complex 2-I



Method 1

Hg	-1.438940	-0.011581	-0.402754
Sb	1.584636	0.029977	-0.033910
I	-4.180415	-0.041887	0.648415
C	3.732460	0.033862	0.380725
C	-1.070474	-2.130759	-0.713119
C	-1.142812	2.115833	-0.736210
C	0.189657	4.116490	-1.400038
C	0.218044	-2.658910	-1.066511
C	4.155142	-0.042378	1.722251
H	3.418256	-0.097988	2.530994
C	0.840083	-0.051948	1.984571
C	6.487322	0.021148	1.020074
H	7.554324	0.016153	1.268573
C	-0.039393	1.078370	3.947236
H	-0.360294	1.999310	4.445991
C	0.749235	-1.292361	2.647236
H	1.033000	-2.221956	2.140603
C	4.708852	0.105243	-0.639969
H	4.412822	0.171363	-1.694544
C	0.137845	2.718746	-0.982320
C	1.409143	2.066461	-0.828397
C	1.461374	-1.943952	-0.979898
C	2.615791	2.716107	-1.077114
H	3.569804	2.207102	-0.923772

C	1.439386	4.746856	-1.664850
H	1.433777	5.795107	-1.988363
C	-2.291820	2.896919	-0.876662
H	-3.270079	2.446303	-0.671485
C	-0.863280	-4.844237	-1.580655
H	-0.771453	-5.880067	-1.929808
C	6.077308	0.098394	-0.320933
H	6.821435	0.154438	-1.123428
C	0.310901	-4.037983	-1.533864
C	1.564234	-4.579825	-1.940119
H	1.589139	-5.614263	-2.304639
C	0.440881	1.135905	2.628317
H	0.480522	2.097574	2.104440
C	2.633475	4.067050	-1.510341
H	3.592424	4.559116	-1.705370
C	2.674740	-2.507832	-1.365687
H	3.610351	-1.953637	-1.263446
C	2.726288	-3.833042	-1.870311
H	3.688205	-4.256677	-2.178528
C	-1.020859	4.855323	-1.538014
H	-0.958702	5.904559	-1.851831
C	-2.240543	4.260335	-1.272618
H	-3.171240	4.831496	-1.369227
C	-2.180902	-2.974893	-0.767070
H	-3.163507	-2.580880	-0.481170
C	-0.125591	-0.154263	4.614436
H	-0.511799	-0.195244	5.638660
C	5.525410	-0.048627	2.038783
H	5.837897	-0.107758	3.087474
C	0.267020	-1.336732	3.965735
H	0.187849	-2.300665	4.480283
C	-2.084974	-4.328983	-1.187444
H	-2.985602	-4.953597	-1.210983

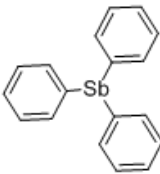
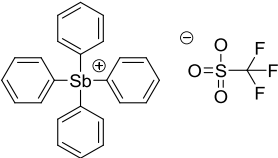
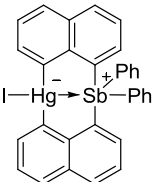
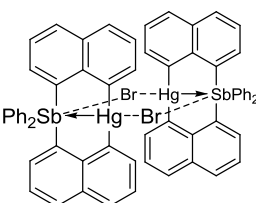
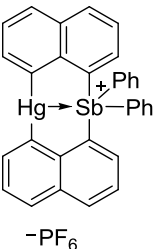
Method 2

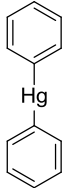
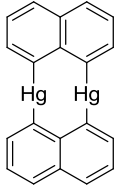
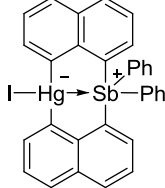
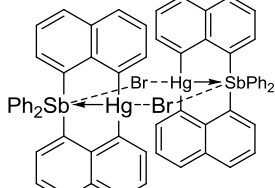
Hg	-1.444816	-0.044034	-0.368586
Sb	1.543588	0.031824	0.107986
I	-4.388080	-0.216298	-0.116702

C	3.727146	0.131395	-0.035901
C	-1.087514	-2.044115	-1.075410
C	-1.240500	2.064829	0.021557
C	-0.037814	4.182350	-0.453386
C	0.196652	-2.670088	-1.020236
C	4.492280	0.424964	1.100516
H	4.011179	0.565450	2.069863
C	1.270298	0.037221	2.242934
C	6.519539	0.350682	-0.228841
H	7.604895	0.434907	-0.303028
C	1.051376	1.239653	4.327832
H	0.994831	2.183893	4.870579
C	1.165960	-1.183444	2.922484
H	1.195251	-2.129041	2.378837
C	4.369267	-0.055610	-1.271265
H	3.793282	-0.299587	-2.165440
C	-0.029275	2.736848	-0.331406
C	1.226257	2.101598	-0.567267
C	1.402092	-2.066012	-0.551447
C	2.342048	2.789220	-1.006090
H	3.289097	2.278273	-1.167626
C	1.117777	4.864911	-0.917734
H	1.067655	5.949276	-1.033460
C	-2.355323	2.819053	0.352131
H	-3.284526	2.309185	0.609333
C	-0.815287	-4.715469	-1.998749
H	-0.701604	-5.748315	-2.332996
C	5.759588	0.057048	-1.366818
H	6.249355	-0.087916	-2.330672
C	0.315900	-4.051038	-1.457949
C	1.550462	-4.740574	-1.335109
H	1.596398	-5.781164	-1.661881
C	1.204298	1.252283	2.937682
H	1.259446	2.203858	2.407261
C	2.277867	4.187044	-1.215499
H	3.159090	4.715207	-1.578919
C	2.591665	-2.764691	-0.436852
H	3.490395	-2.279564	-0.061117

C	2.664634	-4.125462	-0.813558
H	3.605737	-4.663611	-0.702468
C	-1.213730	4.900419	-0.113379
H	-1.204798	5.988409	-0.201722
C	-2.340038	4.233040	0.312691
H	-3.240007	4.786933	0.582863
C	-2.158736	-2.746809	-1.607634
H	-3.141636	-2.274985	-1.637622
C	0.956197	0.024267	5.014481
H	0.827974	0.019869	6.098063
C	5.885197	0.532056	1.003027
H	6.472474	0.756752	1.894574
C	1.010963	-1.184618	4.312857
H	0.923564	-2.133349	4.843810
C	-2.026956	-4.070466	-2.086655
H	-2.896550	-4.579895	-2.503363

Table S1 X-ray Absorption Spectra Fits.

Sb and Hg XANES and EXAFS Fits							
Sample	XANES Edge	Oxidation State	Scatter	N	R, Å	$\Delta\sigma^2$ (x 10^3)	Eo, eV
Sb K-edge							
	30,492.0	Sb ⁺³	Sb-C	3.1	2.14	0.0	-1.5
	30,493.3	Sb ⁺⁵	Sb-C	4.1	2.09	0.0	-2.0
	30,493.3	Sb ⁺⁵	Sb-C	4.2	2.11	0.0	-3.1
	30,493.3	Sb ⁺⁵	Sb-C	3.8	2.13	0.0	-1.5
	30,493.2	Sb ⁺⁵	Sb-C	4.1	2.08	0.0	-1.3
Hg L ₃ Edge							

	12,284.6	Hg ⁺²	Hg-C	2.0	2.09	0.0	-0.1
	12,285.7	Hg ⁺²	Hg-C	2.0	2.10	1.5	-0.5
	12,285.5	Hg ⁺²	Hg-C	1.9	2.06	1.5	-3.5
	12,285.7	Hg ⁺²	Hg-C	1.9	2.06	1.5	-2.8