

# Theoretical study of the solvation of $\text{HgCl}_2$ , $\text{HgClOH}$ , $\text{Hg}(\text{OH})_2$ and $\text{HgCl}_3^-$ . A Density Functional Theory cluster approach.

Ludovic Castro<sup>1</sup>, Aurélien Dommergue<sup>2</sup>, Alexandre Renard<sup>2</sup>, Christophe Ferrari<sup>2</sup>, Alejandro Ramirez-Solis<sup>3</sup>, Laurent Maron<sup>1</sup>

<sup>1</sup> Université de Toulouse, INSA, UPS, LPCNO, 135 avenue de Rangueil, F-31077 Toulouse, France

<sup>2</sup> Laboratoire de Glaciologie et Géophysique de l'Environnement, CNRS/Université Joseph Fourier Grenoble I, 54 rue Molière 38402 Saint Martin d'Hères, France

<sup>3</sup> Depto. De Fisica, Facultad de Ciencias, Universidad Autonoma del Estado de Morelos Cuernavaca, Morelos 62290, Mexico

---

$\text{HgCl}_2$

E = -183.697817

G = -183.723649

Hg	0.000000	0.009525	-0.000257
Cl	0.000000	-0.000692	2.296746
Cl	0.000000	0.091167	-2.296489

$\text{H}_2\text{O}$

E = -76.391210

G = -76.387923

O	-0.023593	0.000000	-0.016682
H	0.021655	0.000000	0.944399
H	0.897608	0.000000	-0.294380

HgCl<sub>2</sub> with 1 water molecule

E = -260.106155

G = -260.115806

O	-0.755296	0.486146	0.097560
Hg	-0.057554	-2.037953	0.129724
Cl	1.657926	-1.544246	-1.354730
Cl	-1.711573	-2.780155	1.569908
H	-0.334261	0.925532	-0.650618
H	-1.690837	0.713644	0.058110

HgCl<sub>2</sub> with 2 water molecules

E = -336.519143

G = -336.505844

O	-0.716272	0.487434	0.108527
Hg	-0.031643	-1.916158	0.088226
Cl	1.768436	-1.611869	-1.386575
Cl	-1.632029	-2.681235	1.590549
H	-1.182038	0.776432	0.900275
H	0.097965	1.036646	0.015372
O	1.706927	1.560681	-0.376768
H	2.356621	1.515654	0.333501
H	1.946418	0.832414	-0.971520

HgCl<sub>2</sub> with 3 water molecules

E = -412.930792

G = -412.897195

O	-0.305204	1.411946	-0.734723
Hg	-0.943014	-2.069033	-2.529435
O	1.549209	-0.274399	-1.867058
Cl	-1.841731	-1.708903	-4.657933
Cl	0.250350	-2.925181	-0.684770
H	-0.169868	1.368334	0.217749
H	0.469718	0.964301	-1.130002
H	2.326522	-0.237748	-2.433298
H	1.593941	-1.108398	-1.372368
O	-2.246723	-0.236516	-1.498663
H	-1.590665	0.444491	-1.189177
H	-2.747516	0.173948	-2.213701

Alternate structure for HgCl<sub>2</sub> with 3 water molecules

E = -412.930152

G = -412.895713

O	-0.798667	0.586856	-0.121885
Hg	-0.128062	-1.706594	0.152656
Cl	1.832697	-1.688511	-1.151174
Cl	-1.840980	-2.414049	1.605629
O	1.674095	1.605618	-0.640763
H	-1.297690	0.885661	0.670913
H	0.006794	1.138055	-0.237496
H	2.300245	1.660162	0.089373
H	1.931421	0.801353	-1.117937
O	-2.305000	0.863790	2.127026
H	-2.599424	-0.058532	2.074522
H	-1.832756	0.914562	2.965266

HgCl<sub>2</sub> with 4 water molecules

E = -489.347057

G = -489.288983

O	0.331540	1.890423	-0.346235
Hg	-0.297327	-0.055629	-1.746800
Cl	1.834559	-0.935274	-2.202133
Cl	-2.616217	0.473045	-1.837675
O	1.486065	0.236085	1.384474
H	-0.437274	2.338281	0.023437
H	0.787034	1.417842	0.400691
H	0.873666	-0.511442	1.229358
H	2.294527	-0.012713	0.920033
O	-0.416758	-1.571838	0.479615
H	-0.185028	-2.473519	0.231335
H	-1.382763	-1.569145	0.712633
O	-3.039318	-1.347285	0.801791
H	-3.193596	-0.860248	-0.027626
H	-3.322000	-0.746337	1.499845

HgCl<sub>2</sub> with 6 water molecules

E = -642.173960

G = -642.070964

O	0.541667	1.745816	-0.178269
Hg	-0.272059	-0.068325	-1.429274
O	-0.224670	-1.563282	0.599687
Cl	1.491065	-1.129092	-2.661731
Cl	-2.672540	0.443003	-1.423706
O	1.235441	0.299025	1.945171
O	-2.861771	-1.622700	1.070991
H	-0.220803	2.342711	0.013192
H	0.843667	1.342442	0.678576
H	0.765163	-0.500644	1.621970

H	2.170684	0.069744	1.945690
H	0.139424	-2.415726	0.249955
H	-1.171353	-1.699061	0.857280
H	-3.102128	-1.083465	0.297261
H	-3.093550	-1.077090	1.831006
O	0.914553	-3.616341	-0.688992
H	0.310868	-4.182458	-1.182775
H	1.319345	-3.041882	-1.364326
O	-1.742653	3.187061	0.018276
H	-2.298816	2.487784	-0.365999
H	-1.729824	3.883810	-0.647602

HgCl<sub>2</sub> with 8 water molecules

E = -794.999580

G = -794.849799

O	0.930523	1.736446	0.245278
Hg	0.580337	-0.047658	-1.503630
Cl	-1.617898	0.537888	-2.413180
O	-0.263710	-1.353276	0.490731
Cl	2.640463	-1.305958	-1.559088
O	1.781905	-0.183078	1.841097
O	-0.020837	-3.557825	-0.959633
O	-2.731216	-0.375669	0.996701
O	-1.844578	2.199138	0.252730
H	0.027977	2.013232	0.489591
H	1.282150	1.135649	0.961863
H	1.065236	-0.781672	1.531753
H	2.576141	-0.529284	1.415557
H	-0.263499	-2.254385	0.066843
H	-1.191893	-1.102145	0.724457
H	-3.286196	-0.595767	0.240015
H	-2.548437	0.577860	0.896904

H	-0.484922	-3.344995	-1.797520
H	0.918056	-3.471879	-1.172380
H	-1.877435	1.935809	-0.687739
H	-2.260137	3.066536	0.308643
O	1.884205	2.083839	-2.297614
H	2.778281	1.738076	-2.407696
H	1.806804	2.312897	-1.353630
O	-1.314903	-2.649719	-3.244892
H	-1.623740	-1.745095	-3.077535
H	-0.820687	-2.594244	-4.069788

HgCl<sub>2</sub> with 12 water molecules

E = -1100.639946

G = -1100.402440

O	0.980417	1.837492	0.601973
Hg	0.473288	0.827176	-1.555201
O	1.951659	3.036794	-1.661852
Cl	-1.653672	1.913566	-2.121002
O	-0.500831	-1.080526	-0.300109
Cl	2.395087	-0.302975	-2.570822
O	1.463155	-0.400719	1.746534
O	0.069114	-3.574284	-0.342816
O	-2.766493	-0.066473	0.738372
O	-0.709754	-4.186650	-2.922797
O	-1.687891	2.562021	0.918605
H	0.117947	2.173178	0.919412
H	1.211801	1.019718	1.160239
H	0.783133	-0.880670	1.241471
H	2.317928	-0.710876	1.371651
H	-0.318519	-2.086895	-0.295845
H	-1.348711	-0.852700	0.157253
H	-3.307873	0.060956	-0.049856

H	-2.488154	0.835094	0.986238
H	-0.488172	-4.006844	-1.017392
H	0.943300	-3.610750	-0.798390
H	-1.785048	2.655540	-0.050806
H	-2.033442	3.370620	1.312081
H	2.807591	2.711684	-1.964251
H	1.935581	2.894590	-0.698667
H	-1.148534	-3.300762	-3.047592
H	-1.219718	-4.828496	-3.424774
O	-0.589894	0.001441	-4.749530
H	0.373032	0.028239	-4.688137
H	-0.892656	0.883496	-4.495196
O	-1.759029	-1.771109	-2.953094
H	-1.455564	-1.428512	-2.096724
H	-1.385974	-1.159651	-3.622525
O	3.751987	-1.050562	0.369314
H	3.461262	-1.025699	-0.556210
H	4.441671	-0.381220	0.428381
O	1.951860	-3.689227	-2.296235
H	2.144310	-2.783058	-2.572377
H	1.148325	-3.940905	-2.792054

HgCl<sub>2</sub> with 24 water molecules (equatorial)

E = -2017.607919

G = -2017.083756

O	0.012099	-0.248917	-5.580104
O	1.179590	2.033464	-4.712322
O	0.755810	-2.786294	-6.063833
O	1.269634	4.648350	-3.920258
O	-2.741806	-0.124987	-5.659232
O	-1.422012	-1.313668	-3.503818
O	-0.853038	-3.822009	-4.000709

O	-0.710874	-0.827059	-0.938486
Hg	0.926415	1.048630	-1.268171
O	0.924019	1.337547	0.984848
O	2.147886	3.117107	-1.754096
Cl	-1.147905	2.131589	-2.392022
Cl	2.446240	-0.627122	-2.352824
O	2.015480	-0.845070	1.516402
O	3.851933	2.443584	-3.592818
O	-2.764641	0.021176	0.482234
O	-1.480100	2.580930	0.823959
O	4.308277	0.456738	1.048942
O	3.218461	2.674926	2.114542
O	0.770244	-2.857660	-0.021587
O	1.150232	-4.327277	-2.155551
O	-0.311987	5.064147	0.555758
O	-0.791626	5.342626	-2.070039
O	2.590510	4.795436	0.483430
O	-4.070150	0.713124	-1.852664
H	-0.897669	-0.139585	-5.926899
H	0.339431	-1.137842	-5.881275
H	0.901542	1.268938	-5.268707
H	0.512284	1.996829	-4.007076
H	-1.460922	-0.553325	-0.332924
H	-3.363300	0.262303	-0.258385
H	-0.237239	-1.605497	-0.545506
H	0.395745	-3.474707	0.615706
H	0.991544	-3.402118	-0.838352
H	-1.220441	-1.100738	-2.558494
H	0.370774	-4.247401	-2.745645
H	-0.732359	-0.867815	-4.050930
H	1.888921	-4.070110	-2.733884
H	-1.151764	-2.896165	-3.762962
H	-1.644537	-4.364885	-4.068354
H	-2.543859	0.860158	0.915239
H	1.793223	-1.576619	0.909939



H	2.929834	-0.516246	1.296946
H	-1.145115	3.500971	0.933876
H	-1.534823	2.491758	-0.143027
H	-0.000310	1.604152	1.191285
H	1.211863	0.397089	1.306716
H	4.051437	1.327569	1.450650
H	4.631213	0.669331	0.161184
H	2.918474	2.868044	-2.352171
H	1.629668	3.699604	-2.349394
H	2.578276	4.250462	-0.323575
H	1.644739	4.927537	0.670408
H	-0.619651	5.860117	1.001890
H	-0.438043	5.232819	-0.416600
H	-1.226944	4.498286	-2.265152
H	-0.068818	5.360885	-2.722497
H	1.183760	3.852854	-4.489040
H	2.128145	5.027857	-4.138384
H	4.441268	1.785613	-3.177379
H	3.157456	1.962027	-4.076920
H	-3.267617	0.951487	-2.342913
H	-4.604468	1.514411	-1.861469
H	2.333114	2.305326	1.972894
H	3.170638	3.511979	1.600255
H	-2.622564	-0.513822	-4.772318
H	-3.262798	-0.767863	-6.150461
H	1.598978	-2.936547	-5.601456
H	0.121804	-3.284391	-5.512333
O	2.834229	-3.159267	-4.152186
H	2.749232	-2.289987	-3.717422
H	3.777637	-3.296295	-4.288604
O	5.165448	0.696772	-1.819255
H	4.435862	0.052210	-1.902748
H	5.984721	0.192442	-1.865753

HgCl<sub>2</sub> with 24 water molecules (apical)

E = -2017.617607

G = -2017.088672

O	0.639246	2.075238	1.877741
O	1.429773	2.370562	-0.565386
Hg	0.157191	0.638883	-1.550188
O	-0.275871	-0.168881	-3.792349
Cl	1.970987	-1.108354	-1.446588
Cl	-1.713288	2.259258	-1.550246
O	-1.059665	-1.238824	-0.138390
O	3.846501	2.083960	-1.632373
O	-3.368032	-0.307115	0.695277
O	-0.597180	-3.881595	-0.109174
O	-1.233136	1.756836	-5.095897
O	0.866537	-0.604849	2.104318
O	3.022247	1.889791	-4.165830
O	0.801572	3.515933	-4.439165
O	1.233520	4.684950	-2.181862
O	1.270055	-4.082332	-2.338579
O	5.366548	-0.130808	-0.775210
O	-4.039655	0.254901	-2.143616
O	2.262306	-0.788458	-4.519001
O	-2.136127	-1.736541	-2.685193
O	-1.488929	-4.325884	-2.700382
O	3.648686	-1.276325	1.075583
O	-2.228255	2.202297	1.511986
H	-0.324244	2.216208	1.901769
H	0.748553	1.114839	2.081034
H	0.301554	-0.908582	1.373086
H	1.776881	-0.842365	1.870789
H	-0.886193	-2.216051	-0.030367
H	-1.933602	-0.985874	0.283439
H	-3.825811	-0.102646	-0.140535

H	-3.134798	0.552555	1.093732
H	-1.187020	-4.229500	-0.803463
H	0.274623	-4.070479	-0.495406
H	-2.088014	2.424938	0.569721
H	-2.727098	2.937459	1.885450
H	2.389323	2.218992	-0.768126
H	1.222167	2.305701	0.423633
H	-1.841160	-3.409439	-2.831367
H	-2.030709	-4.922395	-3.225129
H	0.574328	-0.468436	-4.204006
H	-0.663043	0.608721	-4.356917
H	-1.781261	-1.588535	-1.778625
H	-1.487291	-1.251557	-3.256497
H	3.076297	-1.357087	0.283442
H	3.862957	-2.181866	1.330521
H	1.303110	-3.131992	-2.140550
H	0.368010	-4.238698	-2.685340
H	0.897425	4.010672	-3.556573
H	0.894223	4.182927	-5.127711
H	2.203995	4.849754	-2.136657
H	1.082859	3.997780	-1.505875
H	2.455536	-0.749667	-3.566411
H	2.515886	-1.736402	-4.711866
H	4.425115	1.346905	-1.353413
H	3.563764	1.914046	-2.572420
H	-3.345807	0.917676	-1.961241
H	-3.526265	-0.528763	-2.434035
H	6.260622	0.054721	-0.469105
H	4.879200	-0.498147	-0.004632
H	-0.705651	2.527175	-4.798734
H	-2.177013	1.889567	-4.848041
H	2.236684	2.460037	-4.329764
H	2.815167	1.026227	-4.564779
O	5.155241	-1.726759	-3.174199
H	5.208771	-1.276584	-2.311870

H	5.014267	-1.016085	-3.808851
O	-3.925649	1.762224	-4.551511
H	-4.366861	1.332212	-5.290598
H	-4.147321	1.223441	-3.765955
O	3.990414	4.788866	-2.085985
H	4.129192	3.859921	-1.806461
H	4.331155	4.818369	-2.986068
O	3.134929	-3.282398	-4.400439
H	2.548166	-3.739423	-3.768722
H	3.902824	-2.990807	-3.871800

### Optimized clathrate

E = -1833.801575

G = -1833.277814

O	0.166223	1.848823	0.940406
H	-0.447022	1.542747	0.198435
H	-0.190752	1.323453	1.675916
O	3.715424	-0.808833	-3.238236
H	3.910368	0.017891	-2.731287
H	3.616448	-1.543249	-2.590016
O	2.416923	0.554143	0.409486
H	1.633714	1.134572	0.621762
H	3.073875	0.723348	1.093613
O	3.727614	1.558156	-1.931573
H	3.091197	2.028744	-2.499038
H	3.221821	1.287957	-1.143929
O	-0.756092	4.455559	0.476519
H	-1.305897	4.730818	1.216944
H	-0.327815	3.626920	0.771538
H	1.378994	1.328351	-3.619606
O	1.546687	2.290263	-3.740206
H	1.829838	2.326036	-4.687247

H	-0.002131	2.941517	-3.757700
O	-0.954998	3.211376	-3.880489
H	-0.933141	4.073116	-4.308720
O	1.993625	1.987758	-6.418893
H	1.499289	1.153427	-6.565419
H	1.601047	2.622924	-7.025000
O	-2.407123	3.321616	-1.450555
H	-1.929851	3.338358	-2.303859
H	-1.855213	3.850271	-0.834683
H	-1.612169	1.746452	-4.868801
O	-1.802906	0.836794	-5.171092
H	-1.802467	0.325796	-4.333488
O	-1.710573	0.949512	-0.608147
H	-2.140513	1.805723	-0.912056
H	-1.534306	0.418639	-1.426582
O	-1.233455	-0.477430	-2.809202
H	-1.461339	-1.437858	-2.747559
H	-0.273955	-0.460577	-3.023488
O	-2.564338	-3.865962	-5.114066
H	-3.245966	-3.234647	-5.367334
H	-1.771784	-3.598362	-5.628963
O	-1.504012	-3.134573	-2.770504
H	-1.549484	-3.597272	-1.902221
O	-0.941161	-3.884921	-0.280482
H	-1.500764	-3.702164	0.498237
H	-0.292483	-3.162672	-0.267801
O	-1.849704	-3.036731	2.210263
H	-2.589746	-3.183453	2.806139
H	-1.772434	-2.055075	2.055488
O	0.952491	-3.190542	-3.853493
H	1.110453	-2.220165	-3.784129
H	0.091465	-3.305375	-3.378510
H	0.780202	-4.455687	1.640471
O	0.846466	-3.717138	2.259032
H	-0.089014	-3.534782	2.484281

H	1.214260	-2.420543	1.156998
O	1.055950	-1.821995	0.383482
H	1.668682	-1.050712	0.427767
O	2.881802	-2.940806	-1.707693
H	2.249293	-2.618498	-1.044562
H	2.326268	-3.305187	-2.419590
O	-1.187511	-0.588022	1.539624
H	-1.668347	-0.126527	0.814007
H	-0.398328	-0.963249	1.087241
O	-0.160330	-3.008576	-6.254651
H	0.227235	-3.600510	-6.908479
H	0.355421	-3.160862	-5.410121
H	-2.047420	-3.554855	-3.479452
O	0.347984	-0.196256	-6.295008
H	-0.512833	0.197488	-5.962286
H	0.163459	-1.126061	-6.528681
O	1.298630	-0.463900	-3.805539
H	1.106679	-0.387328	-4.775539
H	2.321129	-0.588198	-3.639068

HgClOH with 24 water molecules (equatorial)

E = -2078.353974

G = -2077.809715

O	-0.523982	-0.375863	-6.081609
O	1.293288	-2.239869	-5.781290
O	1.253044	1.382504	-5.028205
O	2.219337	2.811934	-7.016835
Hg	0.720866	2.318727	-9.136733
O	-0.868458	3.371222	-8.082096
Cl	1.869536	0.108848	-9.479011
O	1.939259	4.009414	-10.160006
O	-0.656916	1.876990	-11.177397

O	3.184981	-2.175510	-7.856361
O	4.385979	3.399877	-10.086653
O	2.817144	0.000991	-12.489631
O	4.120483	2.597497	-12.610001
O	3.006681	-0.494187	-4.450759
O	1.809826	5.394457	-6.588397
O	2.173194	4.419342	-12.967984
O	0.332587	5.764664	-8.951528
O	0.062235	-0.466052	-12.323562
O	-0.014334	3.114547	-3.409389
O	-0.579432	4.572048	-5.529636
O	-2.312497	1.097994	-7.764690
O	-3.137382	1.535524	-10.191318
O	-2.933295	4.303662	-9.595966
O	-1.420702	5.890963	-11.047555
O	4.704664	1.989804	-7.649586
O	4.892908	-0.366249	-6.495492
O	-0.547009	4.018140	-13.070033
H	-1.192673	-0.594989	-5.422891
H	0.119401	-1.149084	-6.075953
H	-1.677911	0.446982	-7.418543
H	-1.826062	1.959717	-7.758844
H	2.161962	3.802761	-6.880254
H	0.966850	5.281140	-6.101290
H	3.155850	2.574243	-7.237914
H	5.437790	2.503706	-7.295030
H	4.795237	1.070422	-7.258952
H	1.627424	1.939633	-5.773391
H	4.338125	-0.368281	-5.688992
H	0.547424	0.818408	-5.436282
H	4.506011	-1.079432	-7.033153
H	2.388580	0.277859	-4.596918
H	3.226785	-0.506849	-3.514188
H	1.527183	5.816355	-7.418498
H	4.549195	2.688204	-9.444645

H	4.401601	3.015811	-11.009555
H	-0.198864	6.055604	-9.727591
H	-0.184438	5.003035	-8.606116
H	1.578886	4.811612	-9.710378
H	2.943973	3.862411	-10.015349
H	3.437347	3.257722	-12.898268
H	3.677033	1.741845	-12.713945
H	-0.383581	1.046013	-11.643709
H	-1.596260	1.734955	-10.907311
H	-0.613047	3.242526	-12.483953
H	-0.811485	4.756851	-12.492903
H	-1.919761	6.663754	-11.330140
H	-2.074035	5.290715	-10.580098
H	-2.261064	4.030502	-8.931275
H	-3.222293	3.451728	-9.968775
H	-2.905762	1.211874	-9.272132
H	-3.807538	0.949459	-10.554125
H	0.985427	-0.333588	-12.617436
H	0.159053	-0.979396	-11.512211
H	-1.387180	5.084670	-5.428791
H	-0.448140	4.060998	-4.683549
H	2.083386	4.483415	-12.002524
H	1.247171	4.223487	-13.233583
H	0.478515	2.420617	-3.916253
H	0.652185	3.569101	-2.883793
H	1.857710	-2.404087	-6.559407
H	1.900819	-1.781291	-5.165901
H	2.763882	-1.454885	-8.368171
H	3.384353	-2.871733	-8.491014
H	2.783428	0.083572	-11.517827
H	3.489283	-0.661949	-12.681150
H	-0.638387	3.614787	-7.162976

HgClOH with 24 water molecules (apical)



E = -2078.354883

G = -2077.812145

O	0.529695	2.156214	1.707434
O	1.325157	2.460996	-0.735116
Hg	0.086587	0.495692	-1.450361
O	-1.131161	-1.437027	-0.072929
O	-0.313453	-0.231521	-3.801280
Cl	1.945053	-1.112225	-1.409467
O	-1.682839	1.684042	-1.301718
O	-1.221091	1.816853	-5.007683
O	-3.413345	-0.425040	0.738930
O	3.793565	2.148108	-1.716584
O	3.109972	1.857384	-4.274523
O	-2.154767	-1.823944	-2.681087
O	-1.467230	-4.393718	-2.765630
O	-0.652940	-4.087392	-0.123351
O	0.765780	-0.537815	2.067596
O	2.267258	-0.798197	-4.497553
O	3.173761	-3.277176	-4.324072
O	4.003376	4.845505	-2.170010
O	-3.700447	2.299965	-3.973059
O	1.260732	4.730785	-2.322437
O	0.910970	3.524103	-4.563713
O	1.262957	-4.100016	-2.320191
O	-3.857599	0.362754	-2.025107
O	5.314710	-0.020855	-0.727868
O	3.626956	-1.206149	1.126305
O	5.151570	-1.670663	-3.086640
O	-2.235836	2.104048	1.214987
H	-0.442884	2.259081	1.683345
H	0.657376	1.208899	1.945615
H	0.194534	-0.940774	1.389563
H	1.674660	-0.804229	1.867705

H	-0.975105	-2.415546	0.023667
H	-2.007602	-1.170158	0.338333
H	-3.828290	-0.198733	-0.115215
H	-3.126771	0.435455	1.105154
H	-1.221168	-4.401590	-0.850488
H	0.229679	-4.229036	-0.504774
H	-2.047158	2.072985	0.233464
H	-2.789013	2.876943	1.368334
H	2.285752	2.300986	-0.919017
H	1.121469	2.410370	0.255634
H	-1.831623	-3.476072	-2.864875
H	-1.972816	-4.969883	-3.346196
H	0.539985	-0.512099	-4.210782
H	-0.677298	0.565294	-4.327868
H	-1.818933	-1.698025	-1.764730
H	-1.507822	-1.320207	-3.237311
H	3.057582	-1.329981	0.339814
H	3.877032	-2.094891	1.406046
H	1.269500	-3.155640	-2.096279
H	0.371969	-4.265201	-2.693491
H	1.007184	4.039887	-3.689893
H	0.992611	4.173961	-5.269673
H	2.224518	4.932104	-2.268530
H	1.141159	4.029335	-1.648781
H	2.435333	-0.736943	-3.542337
H	2.542667	-1.744631	-4.666251
H	4.366683	1.430123	-1.383225
H	3.564101	1.943498	-2.665691
H	-3.041678	0.861906	-1.749437
H	-3.493943	-0.463152	-2.399582
H	6.199817	0.191364	-0.413236
H	4.827310	-0.388456	0.042752
H	-0.584975	2.541608	-4.833776
H	-2.106172	2.069754	-4.655919
H	2.336662	2.437073	-4.454161

H	2.868181	0.976780	-4.615249
H	5.202879	-1.197549	-2.236385
H	5.012422	-0.977166	-3.740434
H	-4.384621	2.286541	-4.648971
H	-3.925736	1.572498	-3.348867
H	4.107768	3.909793	-1.894062
H	4.386130	4.877266	-3.052851
H	2.575085	-3.734845	-3.703612
H	3.925405	-2.972329	-3.780608
H	-1.549662	2.445281	-1.881128

Hg(OH)<sub>2</sub> with 24 water molecules (equatorial)

E = -2139.089029

G = -2138.527932

O	-0.493702	-0.123876	-5.612375
O	1.201760	-2.039348	-5.971373
O	-0.308990	2.578131	-4.866499
O	1.359180	4.430096	-4.150192
O	-1.782234	-1.695199	-3.791600
O	-0.390724	-3.824995	-4.515516
O	-0.969571	-1.044892	-1.374551
Hg	0.835490	1.018434	-1.776423
O	2.301475	-0.532541	-1.825360
O	0.939460	1.267690	0.661808
O	2.513777	2.887388	-2.247483
O	-0.837888	2.244307	-2.196781
O	1.861256	-0.924879	1.708699
O	4.992771	2.031439	-2.869289
O	-2.755115	0.187374	0.155385
O	0.954374	-2.777931	-0.489867
O	1.609719	-4.096478	-2.616908
O	4.222740	0.262910	1.703267

O	3.043782	2.646794	1.990824
O	-1.368111	2.636588	0.538192
O	2.814918	4.580546	0.055222
O	-0.023787	5.038132	0.378527
O	-0.604184	4.993378	-2.188895
O	-4.313087	-0.765859	-3.725211
O	-3.485342	1.273181	-2.259578
O	4.778600	-0.024207	-1.122555
O	2.938522	-1.985133	-3.848770
H	-1.030308	-0.057682	-6.410103
H	0.225917	-0.807624	-5.814046
H	-0.173203	1.669173	-5.192883
H	-0.608860	2.460644	-3.935609
H	-1.609771	-0.656978	-0.712315
H	-3.213564	0.608771	-0.600374
H	-0.406797	-1.717788	-0.933631
H	0.777830	-3.373479	0.246114
H	1.197839	-3.355346	-1.285583
H	-1.490275	-1.451685	-2.864402
H	0.851758	-4.146723	-3.235760
H	-1.353273	-1.042419	-4.399744
H	2.236503	-3.499110	-3.073764
H	-1.002391	-3.096819	-4.211316
H	-0.942696	-4.539232	-4.848383
H	-2.365701	0.944512	0.626108
H	1.874082	-1.583945	1.003299
H	2.795796	-0.556936	1.760708
H	-1.002740	3.525007	0.744370
H	-1.255081	2.581883	-0.435298
H	0.054533	1.635587	0.881415
H	1.126944	0.396130	1.123537
H	3.930579	1.198417	1.873522
H	4.532735	0.279799	0.782611
H	3.429193	2.601292	-2.493071
H	2.206486	3.496535	-2.956688

H	2.766577	4.025774	-0.744814
H	1.883172	4.778927	0.259647
H	-0.255269	5.880108	0.782945
H	-0.209230	5.135185	-0.600295
H	-0.834292	4.041630	-2.232023
H	0.126048	5.065947	-2.831035
H	0.791562	3.734687	-4.594639
H	1.758578	4.972946	-4.835441
H	5.096986	1.304002	-2.214479
H	5.027402	1.603675	-3.730179
H	-4.015845	2.060201	-2.417823
H	-3.850093	0.555114	-2.847248
H	2.210628	2.266650	1.661572
H	3.184019	3.386517	1.358387
H	-3.438985	-1.219553	-3.818608
H	-4.846958	-1.349445	-3.175990
H	1.917055	-1.951460	-5.305039
H	0.681117	-2.799628	-5.644726
H	2.674748	-1.343997	-3.107393
H	3.890075	-1.906006	-3.965298
H	3.820561	-0.232892	-1.331712
H	5.256956	-0.858866	-1.103502
H	-1.661752	1.718335	-2.267137
H	1.928634	-1.198985	-1.222375

Hg(OH)<sub>2</sub> with 24 water molecules (apical)

E = -2139.097849

G = -2138.535485

O	0.371234	2.156290	1.722085
O	1.251399	2.802109	-0.649141
Hg	-0.098198	0.695906	-1.487242
O	-1.236440	-1.488905	-0.057656

O	-0.553941	-0.256982	-3.943656
O	1.719816	-0.293162	-1.626122
O	-1.922192	1.615708	-1.226634
O	-1.288260	1.940080	-5.133153
O	-3.544552	-0.568205	0.850908
O	3.638760	1.701159	-1.719045
O	3.202916	1.789889	-4.280639
O	-2.163906	-1.929091	-2.648935
O	-0.814535	-4.212668	-2.687390
O	-0.421336	-4.035173	0.064089
O	0.736818	-0.536653	1.831916
O	2.106264	-0.704539	-4.316664
O	3.424900	-2.990200	-4.094605
O	4.204349	4.366204	-2.547685
O	-3.474756	2.400081	-3.455093
O	1.465967	4.829750	-2.496637
O	1.001054	3.450965	-4.617531
O	1.613972	-3.234370	-1.865022
O	-4.020682	0.146204	-1.975852
O	5.176562	-0.443329	-0.815072
O	2.999192	-1.570180	0.270555
O	5.801280	-2.137028	-2.960879
O	-2.434328	1.997199	1.309729
H	-0.604263	2.190605	1.738826
H	0.579001	1.200735	1.850397
H	0.044816	-0.908553	1.253410
H	1.568855	-0.934425	1.529687
H	-1.038717	-2.449545	0.107843
H	-2.104533	-1.244570	0.376173
H	-4.013170	-0.390300	0.016825
H	-3.285924	0.313037	1.187225
H	-0.817713	-4.420209	-0.737291
H	0.482140	-3.853122	-0.242747
H	-2.267976	2.011233	0.327696
H	-2.971955	2.769203	1.513525

H	2.167429	2.487678	-0.740433
H	0.962134	2.651294	0.303224
H	-1.419081	-3.426961	-2.789945
H	-0.981371	-4.802002	-3.429101
H	0.328191	-0.521171	-4.289769
H	-0.857105	0.540305	-4.474480
H	-1.847534	-1.740238	-1.734068
H	-1.608756	-1.344322	-3.229778
H	2.418218	-1.106393	-0.399351
H	2.917267	-2.504984	0.037351
H	1.521503	-2.270000	-1.939714
H	0.816725	-3.606345	-2.310048
H	1.112639	4.028178	-3.785989
H	1.113801	4.044025	-5.368292
H	2.448821	4.844389	-2.489622
H	1.239859	4.255940	-1.734209
H	2.039853	-0.600466	-3.342182
H	2.605725	-1.563411	-4.419234
H	4.350179	1.077729	-1.464586
H	3.532617	1.700293	-2.726041
H	-3.219972	0.598291	-1.608063
H	-3.651295	-0.670929	-2.363195
H	5.883407	-0.307568	-0.174884
H	4.447094	-0.909917	-0.323220
H	-0.564338	2.562101	-4.911708
H	-2.085779	2.229761	-4.650995
H	2.422995	2.366123	-4.449660
H	2.900191	0.882330	-4.517805
H	5.624330	-1.533573	-2.211649
H	6.267224	-1.603724	-3.612349
H	-4.203202	3.017278	-3.570417
H	-3.869940	1.557881	-3.130777
H	4.177286	3.534698	-2.040442
H	4.375424	4.065367	-3.448055
H	2.919055	-3.329032	-3.335298

H	4.301286	-2.750210	-3.721023
H	2.379620	0.440459	-1.611974
H	-2.103600	2.238627	-1.951745

$\text{HgCl}_3^-$

E = -198.864847

G = -198.897980

Hg	-0.378983	0.000000	-0.026596
Cl	0.724530	0.000000	2.172291
Cl	0.981475	0.000000	-2.074880
Cl	-2.836249	0.000000	-0.140193

$\text{HgCl}_3^-$  with 3 water molecules

E = -428.088753

G = -428.063109

Hg	0.099539	0.002445	0.034402
Cl	2.474451	-0.764644	-0.418012
Cl	-0.541587	2.226593	-0.807559
Cl	-1.287840	-1.573525	1.338774
O	-3.591482	0.490350	-0.279607
H	-2.910920	1.133062	-0.517737
H	-3.126454	-0.123429	0.304501
O	-0.256173	-2.032277	-1.842384
H	0.692179	-2.094893	-1.652054
H	-0.686327	-2.428824	-1.071263
O	1.768100	1.752965	1.640691
H	2.372301	1.192228	1.130619
H	1.367135	2.334728	0.979699



HgCl<sub>3</sub><sup>-</sup> with 6 water molecules

E = -657.343371

G = -657.242121

O	-3.068885	-1.183378	-0.999923
Cl	-1.452721	-1.604203	1.865195
Hg	-0.071696	-0.068077	0.295891
Cl	-1.170432	1.707734	-1.087455
Cl	2.405681	-0.666578	0.459126
O	-0.399535	-1.773155	-1.546061
O	2.556183	2.257042	1.846451
H	-2.876437	-0.242310	-1.133334
H	-2.922304	-1.315722	-0.047652
H	-0.100474	-2.555264	-1.032570
H	-1.378412	-1.755979	-1.491508
H	2.850704	1.355436	1.634820
H	2.357214	2.617957	0.953955
O	0.652745	-3.551808	0.307325
H	1.418749	-2.964371	0.410011
H	0.034246	-3.221199	0.982521
O	1.895014	2.826375	-0.809681
H	2.229086	2.002796	-1.187084
H	0.928544	2.726414	-0.886025
O	0.037100	1.457834	2.344322
H	0.968823	1.797501	2.298697
H	0.024493	0.759116	3.008777

HgCl<sub>3</sub><sup>-</sup> with 9 water molecules

E = -886.593284

G = -886.421265

O	-2.769127	-1.512860	-1.483306
O	-0.033225	-1.658732	-1.729180
Hg	-0.126408	-0.166198	0.457076
O	0.244228	1.443216	2.288034
Cl	-1.461429	-2.035762	1.629861
Cl	-1.476730	1.445904	-0.894609
Cl	2.307130	-1.011742	0.856281
O	2.506463	2.327219	1.188560
O	0.717492	-3.734515	-0.102482
O	1.635603	2.500432	-1.378451
H	-2.736758	-0.542816	-1.436911
H	-2.762453	-1.782134	-0.550809
H	0.226851	-2.504502	-1.293944
H	-1.012538	-1.685773	-1.825315
H	2.924721	1.455045	1.155716
H	2.229396	2.478901	0.247643
H	1.456710	-3.209567	0.245275
H	0.003894	-3.531827	0.527951
H	1.836650	1.642437	-1.820794
H	0.668432	2.498235	-1.315919
H	1.090726	1.873240	1.979712
H	0.474064	0.798187	2.995416
O	2.157156	-0.037241	-2.344205
H	1.329362	-0.557985	-2.362946
H	2.587223	-0.375227	-1.544919
O	-2.475764	2.386765	2.286448
H	-2.595525	2.213775	1.345297
H	-1.526530	2.219121	2.402510
O	0.767255	-0.788104	3.809528
H	1.433264	-1.098319	3.175244
H	-0.037156	-1.250544	3.522299

HgCl<sub>3</sub><sup>-</sup> with 12 water molecules

E = -1115.845414

G = -1115.599281

O	-3.227826	-1.187799	-1.051748
O	-0.690979	-1.941832	-1.444941
Hg	-0.069535	-0.291292	0.384752
Cl	2.475653	-0.929383	0.091017
O	0.426683	1.189210	2.331158
Cl	-0.621840	-2.037293	2.204002
Cl	-1.203829	1.399831	-1.065613
O	1.363557	3.403333	1.136877
O	2.746189	2.276642	-0.752446
O	0.624665	-3.909178	-0.061941
O	2.130658	-0.666429	3.330071
O	1.398348	-0.947635	-3.056964
O	-2.337463	1.745725	2.637159
H	-3.022098	-0.318577	-1.424233
H	-3.379982	-0.973839	-0.095243
H	-0.386668	-2.786952	-1.043358
H	-1.673572	-1.839467	-1.318983
H	1.988124	3.979069	1.587852
H	1.864887	3.012834	0.349282
H	1.443545	-3.392462	-0.094273
H	0.229812	-3.623055	0.781366
H	2.887832	1.365144	-0.449183
H	2.280155	2.159859	-1.626957
H	0.846554	2.013670	1.983843
H	1.109423	0.652800	2.802584
H	0.547928	-1.266551	-2.694610
H	1.998967	-1.074992	-2.307296
H	-2.192087	2.548343	2.093719
H	-1.425480	1.442385	2.788994
H	2.542386	-0.841085	2.466015
H	1.387877	-1.293767	3.336964
O	1.363529	1.804412	-2.999550

H	0.478245	1.920736	-2.620334
H	1.403452	0.827015	-3.134760
O	-3.486146	-0.521648	1.581171
H	-2.873856	-1.140394	2.005069
H	-3.159912	0.360938	1.886236
O	-1.493504	3.878719	0.969567
H	-1.637221	3.323427	0.187673
H	-0.523293	3.849993	1.060343

**Fig 1. Optimized clathrate structure**

