

# A theoretical study of abiotic methylation reactions of gaseous elemental mercury by halogen containing molecules

## *Supporting Informations*

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Electronic energies, Gibbs free energies and cartesian coordinates

Hg°

E = -153.613110  
G = -153.630617

CH<sub>3</sub>Cl

E = -54.925608  
G = -54.911296

Cl	0.000620	-0.001005	-0.027292
C	0.003503	-0.005739	1.774474
H	1.038431	0.011543	2.112311
H	-0.528907	0.880066	2.117139
H	-0.497741	-0.911333	2.112364

TS Hg° with CH<sub>3</sub>Cl

E = -208.438908  
G = -208.434182

Hg	0.225663	-0.298204	0.224526
C	-0.312485	-0.042552	2.659421

Cl	2.193239	0.397512	2.127110
H	-0.233206	0.998259	2.942302
H	0.198874	-0.759949	3.285793
H	-1.272761	-0.357865	2.264978

### CH<sub>3</sub>HgCl

E = -208.545569

G = -208.537722

Hg	0.029622	0.000000	0.072361
C	0.001726	0.000000	2.154551
Cl	0.061712	0.000000	-2.268633
H	-0.518900	0.893484	2.503727
H	-0.518900	-0.893484	2.503727
H	1.028499	0.000000	2.524730

### CH<sub>3</sub>Br

E = -53.306864

G = -53.294323

Br	0.000381	-0.000681	-0.144517
C	0.003453	-0.005820	1.806757
H	1.039090	0.011452	2.140726
H	-0.529123	0.880786	2.145386
H	-0.497895	-0.912204	2.140645

### TS Hg<sup>o</sup> with CH<sub>3</sub>Br

E = -206.824755

G = -206.821623

Hg	0.189732	-0.339725	0.221417
C	-0.334792	-0.048136	2.657440
Br	2.328846	0.466481	2.126480
H	-0.243965	0.984520	2.965682
H	0.162002	-0.787954	3.270195
H	-1.302499	-0.337986	2.262917

### CH<sub>3</sub>HgBr

E = -206.930322

G = -206.923994

Hg	0.030014	0.000000	0.088363
C	0.001461	0.000000	2.179098
Br	0.062783	0.000000	-2.379667

H	-0.519485	0.893785	2.527031
H	-0.519485	-0.893785	2.527031
H	1.028471	0.000000	2.548607

### CH<sub>3</sub>I

E = -51.342668

G = -51.331446

I	0.000120	-0.000222	-0.316497
C	0.003457	-0.006025	1.857272
H	1.041304	0.011491	2.181209
H	-0.530063	0.882686	2.185896
H	-0.498913	-0.914397	2.181116

### TS Hg° with CH<sub>3</sub>I

E = -204.867741

G = -204.865760

Hg	0.114760	-0.324318	0.194988
C	-0.369929	-0.048451	2.655007
I	2.553273	0.446818	2.156074
H	-0.274560	0.986016	2.957292
H	0.115521	-0.788785	3.276312
H	-1.339741	-0.334079	2.264457

### CH<sub>3</sub>HgI

E = -204.971664

G = -204.966432

Hg	0.029608	-0.000004	0.115337
C	0.000956	0.000000	2.215686
I	0.065043	0.000002	-2.545184
H	-0.520328	0.894486	2.561019
H	-0.520328	-0.894485	2.561022
H	1.028807	0.000001	2.582583

### Cl<sup>-</sup>

E = -15.100269

G = -15.115292

### Br<sup>-</sup>

E = -13.490510

G = -13.506685

I

E = -11.541593

G = -11.558441

CH<sub>3</sub>Hg<sup>+</sup>

E = -193.171718

G = -193.162250

Hg	0.000939	0.001799	0.542936
C	-0.000145	-0.000313	2.704020
H	1.063293	-0.000427	2.940082
H	-0.531983	0.920601	2.939976
H	-0.532105	-0.921660	2.937982

Cl

E = -14.963436

G = -14.979113

Br

E = -13.362368

G = -13.379198

I

E = -11.417508

G = -11.435011

CH<sub>3</sub>Hg

E = -193.443793

G = -193.437791

Hg	-0.000072	-0.000232	0.351614
C	0.000027	0.000180	2.731629
H	1.056024	0.000031	2.994054
H	-0.527976	0.914568	2.994478
H	-0.528003	-0.914548	2.993221

CH<sub>3</sub>

E = -39.826896

G = -39.816883

C	0.105970	0.165308	0.026538
H	-0.081832	-0.033659	1.073671
H	1.066520	-0.079377	-0.408008
H	-0.668347	0.607690	-0.586730

HgCl

E = -168.614408

G = -168.639844

Hg	-0.030921	-0.061842	-0.463819
Cl	0.130921	0.261842	1.963819

HgBr

E = -167.003824

G = -167.030652

Hg	-0.035889	-0.071777	-0.538330
Br	0.135889	0.271777	2.038330

HgI

E = -165.050834

G = -165.078654

Hg	-0.043384	-0.086767	-0.650756
I	0.143384	0.286767	2.150756

TS CH<sub>3</sub>HgCl with CH<sub>3</sub>Cl

E = -263.352138

G = -263.317677

C	0.511050	0.162585	-1.973645
Cl	2.446315	-0.375549	-0.791541
Hg	0.351204	-0.019559	0.560922
Cl	4.609604	-0.925931	-0.033944
H	-0.228901	0.233805	3.127751
C	-0.873278	0.108758	2.256898
H	-1.446836	-0.815769	2.333747
H	0.163430	1.192060	-1.876257
H	-0.289668	-0.578637	-2.002251
H	1.163919	0.053913	-2.833285
H	-1.539705	0.964321	2.143597

Adduct of CH<sub>3</sub>Cl with CH<sub>3</sub>HgCl

E = -263.475278

G = -263.441617

C	0.667235	0.062756	-2.664146
Cl	-0.603372	0.159219	-1.381206
Hg	1.289895	-0.099074	1.527645
Cl	3.217127	-0.198653	0.178876
H	-0.053260	-0.112518	3.814709
C	-0.375204	-0.022987	2.775923
H	-1.042696	-0.847092	2.518246
H	0.625410	0.985410	-3.240257
H	0.440565	-0.799218	-3.289135
H	1.629926	-0.049807	-2.167425
H	-0.885016	0.929739	2.622758

Adduct of Cl<sub>2</sub> with CH<sub>3</sub>HgCH<sub>3</sub>

E = -263.377487

G = -263.346270

C	0.151546	0.335997	-1.922182
Cl	2.898671	-0.781002	-0.337022
Hg	-0.278899	0.235132	0.151252
Cl	4.743317	-1.459988	0.217785
H	0.123973	0.363170	2.809316
C	-0.762176	0.155037	2.202753
H	-1.138238	-0.837701	2.466820
H	-0.739498	0.713460	-2.434996
H	0.391904	-0.648406	-2.333078
H	0.980533	1.017875	-2.130598
H	-1.531576	0.893700	2.445699

CH<sub>3</sub>HgCH<sub>3</sub>

E = -233.368655

G = -233.328217

Hg	0.010091	0.000764	0.000033
C	0.002285	-0.000009	2.110741
C	0.019686	0.000015	-2.110649
H	-1.002962	-0.000850	-2.499644
H	0.533168	0.887522	-2.492492
H	0.534439	-0.887023	-2.491869
H	-1.023534	0.000612	2.491299
H	0.512600	-0.887791	2.496168
H	0.513870	0.886759	2.496825

Cl<sub>2</sub>

E = -30.007120

G = -30.027706

Cl 0.000000 -0.042108 -0.298967

Cl 0.000000 0.242108 1.718967

TS CH<sub>3</sub>HgBr with CH<sub>3</sub>Br

E = -260.138793

G = -260.106767

C 0.463715 0.162062 -1.974820

Br 2.542653 -0.376211 -0.818802

Hg 0.353051 -0.020115 0.591986

Br 4.966145 -0.958352 -0.026797

H -0.296848 0.211798 3.147565

C -0.918983 0.116123 2.257115

H -1.518436 -0.793897 2.303644

H 0.085172 1.177543 -1.848991

H -0.315856 -0.601475 -1.980064

H 1.065521 0.091692 -2.876199

H -1.559002 0.990828 2.137354

Adduct of CH<sub>3</sub>Br with CH<sub>3</sub>HgBr

E = -260.237651

G = -260.209661

C 0.263014 0.302693 -2.731143

Br 1.799667 -0.157418 -1.621574

Hg 1.614772 -0.407709 2.192120

Br 4.044649 -0.829880 2.032312

H -0.701620 -0.020215 3.436856

C -0.438244 -0.057138 2.378310

H -0.980603 -0.867434 1.887770

H 0.210235 1.387647 -2.800255

H -0.630950 -0.101678 -2.259895

H 0.417612 -0.141556 -3.712788

H -0.678559 0.894547 1.901067

Adduct of Br<sub>2</sub> with CH<sub>3</sub>HgCH<sub>3</sub>

E = -260.162661

G = -260.134658

C	0.076984	0.241154	-1.928893
Br	3.064247	-0.483031	-0.437303
Hg	-0.340905	0.150743	0.149038
Br	5.198165	-0.975279	0.349668
H	-0.281522	0.852570	2.746335
C	-0.825105	0.076801	2.199446
H	-0.555297	-0.896720	2.618744
H	0.808243	1.017913	-2.169494
H	-0.858199	0.487524	-2.443517
H	0.434562	-0.715944	-2.318747
H	-1.897613	0.233933	2.346421

Br<sub>2</sub>

E = -26.793654

G = -26.817093

Br	0.000000	-0.095993	-0.307179
Br	0.000000	0.595993	1.907179

TS CH<sub>3</sub>HgI with CH<sub>3</sub>I

E = -256.229892

G = -256.200362

C	0.378777	0.254995	-1.986031
I	2.661900	-0.464054	-0.878204
Hg	0.360057	-0.041242	0.638350
I	5.491690	-1.301471	0.016811
H	-0.470226	0.638490	3.061522
C	-0.983652	0.120771	2.250682
H	-1.262918	-0.888448	2.555635
H	0.050524	1.273400	-1.776395
H	-0.421253	-0.485773	-1.967834
H	0.921348	0.210929	-2.926494
H	-1.859115	0.682400	1.923949

Adduct of CH<sub>3</sub>I with CH<sub>3</sub>HgI

E = -256.315226

G = -256.288807

C	0.254948	0.278850	-2.949579
I	1.883102	-0.214172	-1.598119
Hg	1.553581	-0.437091	2.295388
I	4.141301	-1.043660	2.062473
H	-0.757378	-0.139983	3.587545
C	-0.478670	0.033426	2.546748
H	-1.069569	-0.604785	1.887683



H	0.000244	1.324346	-2.791581
H	-0.581173	-0.375062	-2.712429
H	0.613898	0.108196	-3.962089
H	-0.629860	1.082672	2.287369

Adduct of I<sub>2</sub> with CH<sub>3</sub>HgCH<sub>3</sub>

E = -256.254475

G = -256.226680

C	0.003768	0.309257	-1.942853
I	3.024074	-0.482361	-0.411896
Hg	-0.354570	0.158171	0.150306
I	5.649074	-1.123537	0.409978
H	-0.272166	0.786106	2.763834
C	-0.835650	0.038346	2.198854
H	-0.587032	-0.952641	2.588694
H	0.724516	1.090865	-2.195115
H	-0.961043	0.579879	-2.387280
H	0.328954	-0.636173	-2.383749
H	-1.903964	0.216493	2.351131

I<sub>2</sub>

E = -22.884756

G = -22.910204

I	0.000000	-0.039518	-0.395177
I	0.000000	0.239518	2.395177

TS MeHgCl with MeHgCl

E = -417.035142

G = -417.005006

Hg	-0.122628	1.055754	0.221439
Cl	1.662606	1.370386	2.407268
C	0.613720	-0.203961	-1.291926
Hg	-0.840460	1.668325	2.980897
Cl	-1.744659	1.186348	5.100430
C	-1.625027	2.791150	1.054453
H	0.785338	0.392030	-2.189170
H	1.548014	-0.629199	-0.924899
H	-0.120612	-0.985582	-1.488607
H	-2.534584	2.399887	0.599612
H	-1.036787	3.381980	0.343640
H	-1.923143	3.514234	1.825260

HgCl<sub>2</sub>

E = -183.697867

G = -183.719997

Hg	0.333057	0.299786	0.000360
Cl	0.906408	1.016719	2.105214
Cl	-0.239465	-0.416505	-2.105575

TS MeHgBr with MeHgBr

E = -413.807267

G = -413.780241

Hg	-0.148714	0.917444	0.278854
Br	0.167292	-0.643111	2.769014
C	0.934283	0.166944	-1.366145
Hg	-0.611945	1.948339	2.952100
Br	-0.167520	3.292529	4.998647
C	-1.968347	2.411040	1.073389
H	1.499533	0.982786	-1.817406
H	1.600197	-0.606691	-0.984019
H	0.226302	-0.250343	-2.083363
H	-2.542733	1.693915	0.478355
H	-1.668970	3.276675	0.483506
H	-2.657600	2.751823	1.855466

HgBr<sub>2</sub>

E = -180.472101

G = -180.496547

Hg	-0.000001	-0.033028	-0.000026
Br	0.109705	0.240718	2.413519
Br	-0.109704	-0.307690	-2.413493

TS MeHgI with MeHgI

E = -409.894756

G = -409.869730

Hg	-0.050034	0.885312	0.317626
I	1.158621	-0.467758	2.923068
C	0.722275	0.038821	-1.457051
Hg	-0.733843	1.671318	2.974257
I	-1.538828	2.646612	5.360296
C	-1.694463	2.687341	1.045529
H	0.261997	0.519243	-2.320384
H	1.801098	0.197727	-1.449930

H	0.494282	-1.027284	-1.434359
H	-2.423943	2.143618	0.443573
H	-1.096712	3.373875	0.444549
H	-2.238672	3.272525	1.791224

HgI<sub>2</sub>

E = -176.559674

G = -176.590881

Hg	0.033557	0.000000	0.001441
I	-0.000818	0.000000	2.633746
I	0.228728	0.000000	-2.623771

CH<sub>3</sub>ClCH<sub>3</sub><sup>+</sup>

E = -94.499278

G = -94.450369

Cl	-0.056030	0.000000	-0.039443
C	0.018148	0.000000	1.803956
C	1.706837	0.000000	-0.584128
H	1.626195	0.000000	-1.671384
H	2.152759	0.915165	-0.199216
H	2.152759	-0.915165	-0.199216
H	-1.033808	0.000000	2.090412
H	0.529762	-0.915172	2.095843
H	0.529762	0.915172	2.095843

TS CH<sub>3</sub>ClCH<sub>3</sub><sup>+</sup> with Hg<sup>0</sup>

E = -248.107999

G = -248.068373

Hg	-0.661513	-0.410711	2.668573
C	0.113008	0.172882	5.018099
Cl	0.908971	0.794582	7.128878
C	-0.009430	-0.151310	8.386594
H	0.388552	0.194859	9.339788
H	-1.064604	0.093383	8.285374
H	0.199189	-1.207353	8.229472
H	0.400470	-0.860860	5.165716
H	-0.891001	0.505105	5.252063
H	0.820663	0.869425	4.583537

Adduct of CH<sub>3</sub>ClCH<sub>3</sub><sup>+</sup> with Hg<sup>0</sup>

E = -248.114769

G = -248.075300

Hg	-0.942713	-0.662661	2.236825
C	0.274925	0.299288	5.435122
Cl	0.929226	0.823827	7.103740
C	-0.036446	-0.169193	8.317802
H	0.362776	0.156237	9.278450
H	-1.081373	0.105553	8.187619
H	0.180142	-1.215415	8.110780
H	0.487084	-0.763887	5.347754
H	-0.782052	0.555749	5.431037
H	0.862576	0.907916	4.748809

Adduct of CH<sub>3</sub>Cl with HgCH<sub>3</sub><sup>+</sup>

E = -248.109542

G = -248.072507

Hg	-0.415679	-0.344431	2.487681
C	-0.036209	0.141043	4.648758
Cl	0.500936	0.964945	7.243727
C	0.084085	-0.185291	8.585793
H	0.334872	0.332649	9.510165
H	-0.981918	-0.395871	8.531561
H	0.688413	-1.081354	8.461644
H	-0.302056	-0.812568	5.095379
H	-0.738057	0.961436	4.766345
H	1.020453	0.384838	4.587287