

**Supplementary Materials**  
**for**  
**Thermodynamics of reactions of ClHg• and BrHg• radicals**  
**with atmospherically abundant free radicals**

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<u>Species</u>	<u>B3LYP</u>	<u>B3LYP ZPE</u>	<u>CCSD</u>	<u>CCSD(T)</u>	<u>T1 Diag</u>
BrHg•	-570.47347	0.9	-568.98573	-569.02146	0.019
Br	-416.87989	0.0	-415.74309	-415.75140	0.004
NO	-129.94325	11.8	-129.70673	-129.72598	0.025
NO <sub>2</sub>	-205.16046	23.0	-204.77953	-204.81699	0.031
O <sub>2</sub> ( <sup>3</sup> S <sub>g</sub> )	-150.38462	9.7	-150.12201	-150.14094	0.018
OOH	-150.97335	37.0	-150.70799	-150.72659	0.030
ClO	-535.37180	5.1	-534.72945	-534.74826	0.036
BrO	-492.06934	4.4	-490.79932	-490.82055	0.0284
Br-Hg-Br	-987.46115	3.7	-984.84532	-984.89380	0.012
Br-Hg-NO	-700.43233	16.5	-698.70088	-698.76761	0.024
Br-Hg-ONO	-775.67761	26.3	-773.82564	-773.90050	0.018
Br-Hg-NO <sub>2</sub>	-775.68039	30.4	-773.82067	-773.89764	0.020
Br-Hg-OO•	-720.86581	13.4	-719.11403	-719.17410	0.025
Br-Hg-OOH	-721.50155	44.7	-719.75748	-719.81827	0.017
ClHg	-613.77696	1.5	-612.91753	-612.95128	0.023
Cl	-460.17533	0.0	-459.67005	-459.67622	0.007
Cl-Hg-Cl	-1074.07376	5.4	-1072.71282	-1072.75733	0.016
Cl-Hg-NO	-743.73873	17.2	-742.63520	-742.69947	0.028
Cl-Hg-ONO	-818.98408	27.3	-817.75929	-817.83217	0.021
Cl-Hg-NO <sub>2</sub>	-818.98666	31.5	-817.75439	-817.82935	0.023
Cl-Hg-OO•	-764.17173	14.4	-763.04816	-763.10599	0.029
Cl-Hg-OOH	-764.80831	45.7	-763.69164	-763.75037	0.020
Hg	-153.56632	0.0	-153.21769	-153.24311	0.014
BrHgOBr	-1062.6146	10.0	-1059.86961	-1059.93238	0.015
BrHgOCl	-1105.9149	11.2	-1103.79559	-1103.85576	0.016
ClHgOBr	-1105.9210	11.1	-1103.80334	-1103.86409	0.016
ClHgOCl	-1149.2213	12.2	-1147.72928	-1147.78742	0.019
HgOBr	-645.6378	5.0	-644.01581	-644.06474	0.024
HgOCl	-688.9396	5.8	-687.94528	-687.99134	0.026
HgOOH	-304.53963	37.3	-303.92643	-303.97062	0.023
HgONO <sub>2</sub>	-433.91187	37.5	-433.04961	-433.12401	0.030
NO <sub>3</sub>	-280.33633	27.3	-279.81145	-279.86909	0.023

**Table S2.** Absolute Energies (Hartree), zero point energies (ZPE, in kJ/mol at B3LYP/aVTZ), and values of the  $T_1$  diagnostic for all anionic species. See manuscript for definition of aVTZ basis set. 1 Hartree = 2625.5 kJ/mol.

<u>Species</u>	<u>SCF</u>	<u>ZPE</u>	<u>CCSD</u>	<u>CCSD(T)</u>	<u><math>T_1</math></u>
Br-Hg-Br <sup>-</sup>	-987.53609	1.5	-984.90310	-984.95260	0.016
Br-Hg-NO <sup>-</sup>	-700.53459	13.0	-698.80093	-698.86040	0.016
Br-Hg-ONO <sup>-</sup>	-775.76137	23.5	-773.89065	-773.96595	0.023
Br-Hg-NO <sub>2</sub> <sup>-</sup>	-775.76939	24.2	-773.88860	-773.96588	0.027
Br-Hg-OO <sup>-</sup>	-720.93793	11.2	-719.16581	-719.24058	0.022
Br-Hg-OOH <sup>-</sup>	-721.56845	40.3	-719.80169	-719.86383	0.025
Br-Hg <sup>-</sup>	-570.58640	0.4	-569.09488	-569.13287	0.013
Hg-NO <sup>-</sup>	-283.50239	10.2	-282.90082	-282.95603	0.053
Hg-ONO <sup>-</sup>	-358.81860	21.8	-358.09087	-358.15473	0.022
Hg-NO <sub>2</sub> <sup>-</sup>	-358.81819	22.3	-358.08937	-358.15325	0.022
Hg-OO <sup>-</sup>	-303.98962	7.9	-303.36931	-303.41840	0.024
Hg-OOH <sup>-</sup>	-304.60278	37.4	-303.98408	-304.03478	0.022
Br <sup>-</sup>	-417.00817	0.0	-415.86314	-415.87443	0.004
NO <sup>-</sup> (triplet)	-129.95523	8.4	-129.70606	-129.72569	0.032
NO <sub>2</sub> <sup>-</sup>	-205.24209	20.4	-204.86124	-204.89858	0.025
O <sub>2</sub> <sup>-</sup>	-150.40429	7.0	-150.13180	-150.15394	0.025
HO <sub>2</sub> <sup>-</sup>	-151.01030	34.1	-150.73969	-150.76337	0.023
Cl-Hg-Cl-	-1074.14502	2.3	-1072.76169	-1072.81458	0.019
Cl-Hg-NO <sup>-</sup>	-743.83945	12.4	-742.73355	-742.79137	0.019
Cl-Hg-ONO <sup>-</sup>	-819.06598	22.1	-817.82397	-817.89711	0.027
Cl-Hg-NO <sub>2</sub> <sup>-</sup>	-819.07401	22.6	-817.82124	-817.89661	0.032
Cl-Hg-OO* <sup>-</sup>	-764.24290	10.8	-763.09909	-763.17196	0.028
Cl-Hg-OOH <sup>-</sup>	-764.87261	40.4	-763.73345	-763.79380	0.025
Cl-Hg <sup>-</sup>	-613.89099	0.7	-613.02804	-613.06423	0.017
Cl <sup>-</sup>	-460.31052	0.0	-459.79555	-459.80504	0.006
Hg-	-153.55647	0.0	-153.21769	-153.24311	0.014

**Table S3.** Cartesian coordinates (Ångstroms) of all Hg-containing species at B3LYP/aVTZ (integers refer to the atomic number of the atom). See manuscript for definition of aVTZ basis set.

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 Neutrals  
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HgBr<sub>2</sub>

80	0.000000	0.000000	0.000000
35	0.000000	0.000000	2.424902
35	0.000000	0.000000	-2.424902

HgCl<sub>2</sub>

80	0.000000	0.000000	0.000000
17	0.000000	0.000000	2.286253
17	0.000000	0.000000	-2.286253

BrHgNO

80	0.000000	0.378806	0.000000
35	-0.313829	-2.113207	0.000000
7	0.160879	2.678926	0.000000
8	1.232231	3.113156	0.000000

BrHgNO<sub>2</sub>

80	0.000000	0.000000	0.194133
35	0.000000	0.000000	-2.231132
7	0.000000	0.000000	2.337214
8	0.000000	1.082255	2.887403
8	0.000000	-1.082255	2.887403

BrHgONO

80	0.121880	-0.141817	-0.000038
35	-2.254227	0.213371	0.000044
8	2.113946	-0.523065	0.000179
7	2.870124	0.663345	-0.000039
8	4.018144	0.427311	0.000049

BrHgOO•

80	0.000000	0.367496	0.000000
8	0.395760	2.432719	0.000000
8	1.656335	2.728721	0.000000

35 -0.469050 -2.019749 0.000000

BrHgOOH

80 -0.330678 -0.129999 0.003467  
35 2.064815 0.170645 -0.001557  
8 -2.329062 -0.432290 -0.021349  
8 -2.968392 0.873654 -0.099881  
1 -3.434662 0.896491 0.746929

ClHgNO

80 0.000000 0.056359 0.000000  
17 -2.297427 -0.562127 0.000000  
7 2.172275 0.777265 0.000000  
8 2.981292 -0.049177 0.000000

ClHgNO<sub>2</sub>

80 0.000000 0.000000 0.155787  
17 0.000000 0.000000 2.451900  
7 0.000000 0.000000 -1.971810  
8 0.000000 1.082412 -2.521410  
8 0.000000 -1.082412 -2.521410

ClHgONO

80 -0.236973 -0.097108 -0.000022  
8 1.726195 -0.556717 0.000010  
7 2.539164 0.597914 -0.000329  
8 3.672801 0.306801 0.000308  
17 -2.471076 0.328385 0.000089

ClHgOO•

80 0.000000 0.083202 0.000000  
17 -2.269878 -0.284381 0.000000  
8 2.054827 0.428072 0.000000  
8 2.768664 -0.655780 0.000000

BrHgOBr

O -1.776200 -0.566246 0.000000  
Hg 0.000000 0.387678 0.000000  
Br -1.640549 -2.408891 0.000000  
Br 2.046537 1.652198 0.000000

BrHgOCl

O 1.442091 1.648975 0.000000  
Hg 0.000000 0.226020 0.000000  
Cl 3.019927 0.989095 0.000000

Br -1.796443 -1.373944 0.000000

ClHgOBr

O -1.222936 -0.927031 0.000000

Hg 0.000000 0.664825 0.000000

Br -0.336789 -2.548627 0.000000

Cl 1.268888 2.554836 0.000000

ClHgOCl

O -1.487870 -1.080269 0.000000

Cl -0.914447 -2.692332 0.000000

Hg 0.000000 0.279101 0.000000

Cl 1.614621 1.887276 0.000000

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Anions

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ClHgOOH<sup>-</sup>

80 0.017844 -0.101759 0.003087

17 2.267697 0.297264 -0.002278

8 -1.953879 -0.493495 -0.020178

8 -2.651815 0.782642 -0.098413

1 -3.132848 0.774047 0.740471

HgBr<sub>2</sub><sup>-</sup>

80 0.000000 0.000000 0.273257

35 0.000000 2.742626 -0.312293

35 0.000000 -2.742626 -0.312293

HgCl<sub>2</sub><sup>-</sup>

80 0.000000 0.000000 0.234238

17 0.000000 2.524427 -0.551148

17 0.000000 -2.524427 -0.551148

BrHgNO<sup>-</sup>

80 0.422377 -0.004599 -0.000330

35 -2.594336 -0.005256 0.000400

7 3.431752 0.536282 0.000749

8 4.123670 -0.400267 0.000894

BrHgNO<sub>2</sub><sup>-</sup>

80 0.200604 -0.000045 -0.000045

35 -2.650860 0.000050 0.000054

7	2.933483	0.000062	0.000061
8	3.512384	-1.077724	0.000080
8	3.512288	1.077900	0.000080

BrHgONO<sup>-</sup>

80	-0.157736	-0.172038	-0.047136
35	2.597543	0.198863	0.073256
8	-2.430603	0.686036	-0.239167
7	-3.309876	-0.130080	0.249823
8	-4.460149	0.278141	0.171441

BrHgOO<sup>-</sup>

80	0.000000	0.415477	0.000000
8	0.029064	2.734578	0.000000
8	1.161719	3.378851	0.000000
35	-0.272179	-2.347016	0.000000

BrHgOOH<sup>-</sup>

80	0.422170	-0.410357	-0.036752
35	-2.350636	0.445809	0.032454
8	2.676888	0.377067	0.504087
8	3.059960	1.497592	-0.296317
1	2.603919	2.227978	0.142097

ClHgNO<sup>-</sup>

80	0.019902	-0.011073	-0.000326
17	2.850151	0.005094	0.000840
7	-2.962431	0.549946	0.000636
8	-3.663467	-0.381299	0.000921

ClHgNO<sub>2</sub><sup>-</sup>

80	0.000000	0.220813	0.000000
17	-0.000009	2.917327	0.000000
7	0.000006	-2.522264	0.000000
8	-1.077827	-3.100234	0.000000
8	1.077840	-3.100231	0.000000

ClHgONO<sup>-</sup>

80	0.262059	-0.195713	-0.000034
8	-1.971878	0.743817	-0.000270
7	-2.908992	-0.151837	0.000255
8	-4.038210	0.317165	0.000130
17	2.792878	0.484240	0.000123

ClHgOO<sup>-</sup>

80	0.012750	-0.028912	-0.000001
17	-2.605692	0.106521	0.000002
8	2.271594	-0.457687	0.000003
8	3.137998	0.520454	0.000001

ClHgOOH<sup>-</sup>

80	0.017364	-0.135157	-0.006392
17	2.733051	0.277437	0.016401
8	-2.230703	0.860382	0.013091
8	-3.321220	-0.056754	-0.087837
1	-3.435647	-0.332875	0.830517



**Table S4.** Harmonic vibrational frequencies ( $\text{cm}^{-1}$ ) and mode assignments for all species at B3LYP/aVTZ. See manuscript for definition of aVTZ basis set.

<u>Compound</u>	<u>Frequency (<math>\text{cm}^{-1}</math>)</u>	<u>Mode Description</u>
Cl-Hg-NO <sub>2</sub>	70	Cl-Hg-NO <sub>2</sub> bend in plane
	77	Cl-Hg-NO <sub>2</sub> bend out of plane
	248	NO <sub>2</sub> rotation in plane
	253	Symmetric Cl-Hg-NO <sub>2</sub> stretch
	360	Antisymmetric Cl-Hg-NO <sub>2</sub> stretch
	508	Nitrogen wagging
	828	NO bend
	1357	Symmetric O=N=O stretch
	1566	Antisymmetric O=N=O stretch
HgCl <sub>2</sub>	91	Cl-Hg-Cl bend1
	91	Cl-Hg-Cl bend2
	332	Symmetric stretch
	386	Antisymmetric stretch
Cl-Hg-NO	60	Cl-Hg-N Bend (in plane)
	71	Cl-Hg-N Bend (out of plane)
	190	Symmetric Cl-Hg-NO stretch
	308	Antisymmetric Cl-Hg-NO stretch
	501	Hg-N=O bend/Hg-N stretch
	1753	N=O stretch
Cl-Hg-OO	79	Cl-Hg-OO bend (in plane)
	97	Cl-Hg-OO bend (out of plane)
	227	Symmetric Cl-Hg-OO stretch
	352	Antisymmetric Cl-Hg-OO stretch
	497	Hg-O-O bend/Hg-O stretch
	1149	O-O stretch
Cl-Hg-OOH	89	Cl-Hg-OOH bend (in plane)
	103	Cl-Hg-OOH bend (out of plane)
	232	Symmetric Cl-Hg-OOH stretch
	286	H-atom rock
	362	Antisymmetric Cl-Hg-OOH stretch
	557	Hg-O stretch
	911	O-O stretch
	1349	H-atom wag
	3749	O-H stretch

Cl-Hg-ONO	74	Cl-Hg-ONO bend (in plane)
	88	Cl-Hg-ONO bend (out of plane)
	162	Hg-ON=O bend
	192	Hg-O-NO bend
	353	Symmetric Cl-Hg-ONO stretch
	408	Antisymmetric Cl-Hg-ONO stretch
	690	Antisymmetric Hg-O-NO stretch
	890	O-N=O bend
	1715	N=O stretch
	Br-Hg-NO <sub>2</sub>	57
62		Br-Hg-NO <sub>2</sub> bend (out of plane)
210		Symmetric Br-Hg-NO <sub>2</sub> stretch
238		Hg-NO <sub>2</sub> rock
284		Antisymmetric Br-Hg-NO <sub>2</sub> stretch
495		HgNO <sub>2</sub> pyramidal
825		NO bend
1355		Symmetric O=N=O stretch/Hg-N stretch
1564		Antisymmetric O=N=O stretch
HgBr <sub>2</sub>		66
	66	Br-Hg-Br bend2
	206	Symmetric Br-Hg-Br stretch
	274	Antisymmetric Br-Hg-Br stretch
Br-Hg-NO	50	Br-Hg-NO bend (in plane)
	56	Br-Hg-NO bend (out of plane)
	173	Symmetric Br-Hg-NO stretch
	236	Antisymmetric Br-Hg-NO stretch
	489	Hg-N=O bend/Hg-N stretch
	1756	N=O stretch
Br-Hg-OO	63	Br-Hg-OO bend (in plane)
	86	Br-Hg-OO bend (out of plane)
	191	Symmetric Br-Hg-OO stretch
	261	Antisymmetric Br-Hg-OO stretch
	480	Hg-O-O bend/Hg-O stretch
	1153	O-O stretch
Br-Hg-OOH	78	Br-Hg-OOH bend (in plane)
	79	Br-Hg-OOH bend (out of plane)
	214	Symmetric Br-Hg-OOH stretch

	257	Antisymmetric Br-Hg-OOH stretch
	296	H-atom rock
	547	Hg-O stretch
	909	O-O stretch
	1347	H-atom wag
	3750	O-H stretch
Br-Hg-ONO	58	Br-Hg-ONO bend (in plane)
	65	Br-Hg-ONO bend (out of plane)
	156	Hg-ON=O bend (out of plane)
	185	Hg-O-NO bend
	246	Symmetric Br-Hg-ONO stretch
	392	Antisymmetric Br-Hg-ONO stretch
	695	Antisymmetric Hg-O-N stretch
	893	O-N=O bend
	1708	N=O stretch
HgBr <sub>2</sub> <sup>-</sup>	14	Br-Hg-Br in plane bend
	112	Symmetric Br-Hg-Br stretch
	131	Asymmetric Br-Hg-Br stretch
BrHgNO-	11	Br-Hg-NO bend, in plane
	21	Br-Hg-NO bend, out of plane
	58	Symmetric Br-Hg-NO stretch
	92	Asymmetric Br-Hg-NO stretch
	223	Hg-N=O bend
	1770	N=O stretch
BrHgNO <sub>2</sub> <sup>-</sup>	15	Br-Hg-NO <sub>2</sub> bend out of plane
	17	Br-Hg-NO <sub>2</sub> bend in plane
	88	Symmetric Br-Hg-NO <sub>2</sub> stretch
	114	Asymmetric Br-Hg-NO <sub>2</sub> stretch
	121	Hg-N-O bend in plane
	158	N pyramidal stretch
	772	Symmetric Hg-N-O stretch
	1292	Asymmetric Hg-N-O stretch
	1474	Asymmetric O-N-O stretch
BrHgONO-	10	Br, NO wag
	26	wag
	103	NO <sub>2</sub> rock

	120	NO2 twist
	129	Asymmetric Br-Hg-ONO stretch
	196	Hg-O-NO in plane bend
	780	ONO in plane bend
	1096	N-O stretch/Asymmetric O=N-O stretch
	1471	Asymmetric O-N=O stretch (mostly N=O stretch)
BrHgOO-	40	Br-Hg-OO in plane bend
	66	Br-Hg-OO out of plane bend
	99	Symmetric Br-Hg-OO stretch
	166	Asymmetric Br-Hg-OO stretch
	370	Hg-O-O bend
	1132	O-O stretch
BrHgOOH-	16	Br, OH wag
	44	HO2 rock
	88	HO2-Hg-Br symmetric stretch
	118	HO2-Hg-Br Asymmetric stretch
	223	HO2 twist
	333	H wag
	869	OO stretch
	1314	OOH bend
	3724	OH stretch
HgCl <sub>2</sub> <sup>-</sup>	30	In-plane bend
	179	Symmetric stretch
	183	Asymmetric stretch
ClHgNO-	20	Cl-Hg-NO bend in plane
	26	Cl-Hg-NO bend out of plane
	60	Symmetric Cl-Hg-NO stretch
	135	Asymmetric Cl-Hg-NO stretch
	230	Hg-N=O bend
	1767	N=O stretch
ClHgNO <sub>2</sub> <sup>-</sup>	24	Cl-Hg-NO2 bend, out of plane
	27	Cl-Hg-NO2 bend, in plane
	92	Symmetric Cl-Hg-NO2 stretch
	122	Hg-N-O bend, in plane
	149	N pyramidal stretch

	166	Asymmetric Cl-Hg-NO <sub>2</sub> stretch
	772	Hg-N-O stretch/Hg-N stretch
	1293	Asymmetric Hg-N-O stretch
	1476	Asymmetric O-N-O stretch
ClHgONO-	18	Cl, NO <sub>2</sub> rock
	29	Cl-Hg-ONO bend, in plane
	107	Hg-O-N bend
	117	NO <sub>2</sub> twist
	190	Cl-Hg stretch
	200	Hg-O stretch
	782	O-N=O bend
	1095	Asymmetric O-N=O stretch (mostly O-N stretch)
	1473	Asymmetric O-N=O stretch (mostly N=O stretch)
ClHgOO-	23	Cl-Hg-OO bend in plane
	55	Cl-Hg-OO bend out of plane
	115	Symmetric Cl-Hg-OO stretch
	203	Asymmetric Cl-Hg-OO stretch
	372	Hg-O-O bend
	1117	O-O stretch
ClHgOOH-	10	Cl, OH wag
	16	Cl, HO <sub>2</sub> wag
	99	HO <sub>2</sub> -Hg-Cl symmetric stretch
	153	HO <sub>2</sub> -Hg-Cl Asymmetric stretch
	224	HO <sub>2</sub> twist
	320	H wag
	871	OO stretch
	1313	OOH bend
	3727	OH stretch

**Table S5.** Inputs for thermodynamic analysis of BrHg• molecule (cited errors are 1 s.d.)

$D_e = 5525 \pm 100 \text{ cm}^{-1 \text{ a}}$	(bond dissociation energy at the minimum of the potential well)
$\omega_e (^{79}\text{Br}^{200}\text{Hg}) = 188.7 \pm 0.26 \text{ cm}^{-1 \text{ a}}$	(harmonic vibrational frequency)
$\omega_e x_e = 1.04 \pm 0.1 \text{ cm}^{-1 \text{ a}}$	(anharmonic term)
$R(\text{Br-Hg}) = 2.494 \text{ \AA}^{\text{ b}}$	(Br-Hg internuclear bond distance in HgBr•)
$g_e(\text{Br}) = 2^{\text{ c}}$	(electronic state degeneracy of Br)
$g_e(\text{BrHg}\bullet) = 4^{\text{ c}}$	(electronic state degeneracy of HgBr•)

a) Tellinghuisen and Ashmore (1983)

b) Shepler et al (2007). Note that Goodsite et al. (2004) cited  $R(\text{Br-Hg}) = 2.62 \text{ \AA}$  from Lipson et al (1992), who were citing Tellinghuisen and Ashmore, (1982), who in turn were citing an value from Cheung and Cool (1979), who were citing a conference presentation by Wadt and Hay (1978). Later, Wadt (1979) published a value of 2.61 Å.

c) Chase, et al., 1998

The value of  $\omega_e$  was calculated separately for each isotopologue using the force constant calculated from  $\omega_e$  of  $^{79}\text{Br}^{200}\text{Hg}$ . Then, for each isotopologue,  $D_0$  was calculated as  $D_e - 1/2 \omega_e + 1/4 \omega_e x_e$ .

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