Supporting Information (26 pages)

Disproportionation of Bromous Acid HOBrO by Direct O-Transfer and via Anhydrides $O(BrO)_2$ and $BrO–BrO_2$. Ab Initio Study of the Mechanism of a Key Step of the Belousov-Zhabotinsky Oscillating Reaction

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Table S1. Total Energies and Thermochemical Data at MP2(full)/6-311G*

Molecule	Energy	VZPE	TE	S	ν_1	ν_2	μ
H_2O	-76.253654	13.72	15.50	45.03	1738	3861	2.340
$(H_2O)_2$	-152.520277	29.94	33.54	69.37	93	158	3.061
OH	-75.576720	5.43	6.91	42.55	3796		1.969
HBr	-2573.469652	3.76	5.24	47.43	2632		1.176
HOBr, C_s, **1a**	-2648.498668	8.04	9.92	59.20	619	1225	1.887
HOBr, $C_{\infty h}$, **1b**	-2648.424921	7.04	8.57	54.40	-1591	-1591	0.367
$HBrO_2$, C_1, **2a**	-2723.463590	10.01	12.47	67.05	245	401	3.423
$HBrO_2$, C_s, cis, **2b**	-2723.458784	9.26	11.56	66.44	-353	218	1.718
$HBrO_2$, C_s, trans, **2c**	-2723.450710	9.24	11.52	66.34	-404	240	5.021
$HBrO_3$, C_s, anti, **3a**	-2798.476742	12.08	15.27	74.76	46	315	1.887
$HBrO_3$, C_s, syn, **3b**	-2798.469075	11.93	14.63	70.09	-299	291	5.250
chair-**4a**	-5446.970469	22.36	27.34	92.70	82	98	0.003
boat-**4a**	-5446.965926	22.20	27.37	95.05	45	77	3.804
4b	-5446.941740	20.79	26.76	102.92	28	41	3.887
4c	-5446.941610	20.68	26.68	102.10	30	73	5.351
cis-**4d**	-5446.940358	20.58	26.61	101.65	30	87	4.435
trans-**4d**	-5446.940180	20.60	26.65	102.51	32	78	0.013
TS(**4b**,**4c**)	-5446.935157	20.52	26.16	101.16	-69	39	3.397
4e	-5446.956516	21.66	27.06	95.25	56	100	2.530
4f	-5446.951087	21.39	27.04	98.04	55	76	2.402
TS(**4a**,**4e**)	-5446.951473	21.55	26.63	94.98	-52	47	0.810
4g	-5446.950918	21.74	27.49	100.83	18	54	4.194
4h	-5446.953652	21.73	27.27	99.20	31	59	1.208
$(HBrO_3)$(BrOH), **5a**	-5446.983974	21.03	27.06	103.57	36	54	1.535
5b	-5446.981802	21.72	27.00	109.47	16	27	1.071
cis-5c	-5446.996688	22.54	27.70	96.45	30	61	1.115
trans-5c	-5446.995820	22.50	27.69	97.14	27	51	2.783
5d	-5446.989493	21.82	27.37	100.41	193	43	3.461
cis-5e	-5446.989711	21.64	27.34	101.06	30	48	1.976
trans-5e	-5446.989622	21.65	27.37	102.00	24	36	2.602
5f	-5446.988698	21.49	27.33	105.81	11	27	1.115
6b = TS(**4b**,**5a**)	-5446.900617	19.92	25.36	95.32	-507	59	0.889
6b $(OH_2)_2$	-5599.461122	53.22	61.65	117.45	-552	41	2.361
6c = TS(**4c**,**5a**)	-5446.904980	20.74	25.89	93.02	-606	66	4.400

6e = TS(**4e**,**5d**)	-5446.903097	21.23	26.04	90.65	-642	68	3.584
6f = TS(**4f**,**5a,f**)	-5446.897489	20.56	25.68	92.84	-737	64	3.230
$O(BrO)_2$, C_2, **7a**	-5370.689453	5.03	9.37	88.83	48	67	1.246
$O(BrO)_2$, C_s, **7b**	-5370.687274	5.08	9.40	88.33	50	76	5.811
7c = RTS(**7a**,**7b**)	-5370.679799	4.87	8.77	84.51	-53	74	4.126
BrO–BrO_2, C_s, **8a**	-5370.733842	5.89	9.85	88.02	9	114	1.735
BrO–BrO_2, C_1, **8b**	-5370.732801	5.47	9.09	81.92	-145	92	2.646
BrO, **9**	-2647.841104	1.09	2.63	55.51	764		1.312
BrO_2, C_{2v}, **10**	-2722.849310	2.92	5.03	65.95	319	850	3.194
11b, ^{3}(**9**/**10**)	-5370.696867	4.34	9.10	101.27	6	44	3.467
11c = TS(**8a**,**11a**)	-5370.717788	4.83	8.95	90.20	-103	34	2.177
12a = **7a**·OH_2	-5446.965241	21.33	27.29	99.41	49	105	0.955
12b	-5446.997581	21.03	27.15	101.40	47	65	4.177
13a = **8b**·OH_2	-5447.000057	21.52	27.36	98.87	42	78	5.237
13b = **8b**·OH_2	-5447.006660	21.52	27.50	99.67	56	80	2.031
13c = **8b**·OH_2	-5446.998718	21.26	27.44	103.90	28	52	1.586
13d = **8a**·OH_2	-5446.995820	21.13	27.38	103.71	35	50	4.270
14a = TS(**4f**,**12a**)	-5446.932949	18.25	23.38	94.10	-1197	47	1.233
14b = TS(**12a**,**5e**)	-5446.957951	18.04	23.31	95.08	-1300	61	6.081
14c = TS(**4**,**12b**)	-5446.901990	19.10	24.30	95.55	-688	47	3.449
15a = TS(**13b**,**5**)	-5446.955492	18.60	23.73	94.51	-816	44	1.722
15b = TS(**13b**,**5**)	-5446.957798	20.60	25.43	91.06	-52	86	1.774
15c = TS(**13c**,**5**)	-5446.913388	20.93	25.34	87.02	-811	82	3.818
15d = TS(**13c**,**5**)	-5446.912576	20.74	25.17	87.05	-893	85	5.522
15e = TS(**13d**,**4h**)	-5446.928361	20.46	25.54	93.52	-475	53	5.229
16 = **8b**·$(OH_2)_2$,	-5523.284667	38.14	45.55	109.44	57	73	2.245
17 = TS(**16**, **5**·OH_2)	-5523.228009	34.45	41.46	110.30	-1048	23	1.684
18	-2724.057413	13.21	15.99	72.14	-3264	145	2.263
19	-2799.025851	17.18	20.12	73.50	-1587	141	2.686
20	-2800.330959	34.79	39.20	86.35	-2118	52	2.306

Table S2. Total Energy and Thermochemical Data at SMD(MP2(full)/6-311G*)

Molecule	Energy	VZPE	TE	S	ν_1	ν_2	μ
H_2O	-76.270007	13.61	15.39	45.06	1707	3853	2.763
HBr	-2573.470980	3.73	5.22	47.44	2612		1.346
1a	-2648.506074	8.02	9.90	59.21	614	1251	2.167
2a	-2723.475670	10.08	12.49	66.78	253	453	4.577
3a	-2798.487046	12.01	15.18	74.09	65	317	2.566
6b	-5446.917076	20.01	25.38	94.42	-499	62	4.805
6c	-5446.920610	20.61	25.81	93.06	-652	74	6.048
6e	-5446.913915	20.82	25.72	91.39	-692	67	4.682
6f	-5446.909592	20.52	25.69	94.16	-740	42	5.142
7a	-5370.696874	4.92	9.28	89.03	44	68	1.653
8a	-5370.738929	5.82	9.79	87.08	14	119	2.044
BrO, **9**	-2647.843158	1.06	2.60	55.53	742		1.539
BrO_2, **10**	-2722.855204	2.87	4.98	66.00	318	840	3.739
12a	-5446.978439	21.03	27.07	100.25	43	107	1.816
12b	-5447.015599	21.28	27.20	99.04	66	74	5.563
14a	-5446.945775	18.29	23.47	94.59	-1129	51	0.927
14b	-5446.969328	18.15	23.35	94.46	-1409	61	8.375
15a	-5446.972188	19.19	24.26	93.44	-983	61	4.588
15b	-5446.967102	20.54	25.35	90.75	-37	88	2.197
15e	-5446.939309	19.65	24.85	95.34	-523	49	8.375

Table S3. $HOBrO_2$ Rotational Energy Profile Energies

∠(O_a-Br-O-H)	E(MP2/6-311G*)	∠(O_a-Br-O-H)	E(MP2/6-311G*)
-57.646	-2798.476742	42.354	-2798.473475
-47.646	-2798.476733	52.354	-2798.472981
-37.646	-2798.476691	62.354	-2798.472407
-27.646	-2798.476568	72.354	-2798.471739
-17.646	-2798.476317	82.354	-2798.471004
-7.646	-2798.475922	92.354	-2798.470271
2.354	-2798.475423	102.354	-2798.469638
12.354	-2798.474893	112.354	-2798.469212
22.354	-2798.47439	122.354	-2798.469076
32.354	-2798.473928		

Technical note: The PES scan was performed as a function of the dihedral angle ∠(H–O–Br–O_a) starting at the minimum **3a**. The plot in Fig. 1 shows the energy as a function of the dihedral angle ∠(H–O–Br–X) where *syn*-**3b** appears at ∠(H–O–Br–X) = 0° and *anti*-**3a** appears at |∠(H–O–Br–X)| = 180°; this is in keeping with the notions of *syn* and *anti* relative to X (the center of the putative Br lone pair. This mapping is an excellent approximation because the ∠(H–O–Br–O_a) + ∠(H–O–Br–O_b) = 243.2±0.5 at every point.

Table S4. $O(BrO)_2$ Rotational Energy Profile Energies

∠(Br-O-Br-O)	E(MP2/6-311G*)	∠(Br-O-Br-O)	E(MP2/6-311G*)
70	-5370.689453	260	-5370.686640
80	-5370.689281	270	-5370.687154
90	-5370.688725	280	-5370.687267
100	-5370.687774	290	-5370.687056
110	-5370.686505	300	-5370.686646
120	-5370.685057	310	-5370.686197
130	-5370.683597	320	-5370.685882
140	-5370.682277	330	-5370.685888
150	-5370.681202	340	-5370.726907
160	-5370.680427	350	-5370.732285
170	-5370.679964	360	-5370.733065
180	-5370.679800	370	-5370.733065
190	-5370.679916	380	-5370.733825
200	-5370.680321	390	-5370.733853
210	-5370.681031	400	-5370.733856
220	-5370.682032	410	-5370.733844
230	-5370.683249	420	-5370.733781
240	-5370.684544	430	-5370.733781
250	-5370.685733		

Gaussian 09, Rev. A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J.; Gaussian, Inc., Wallingford, CT, 2009.

Cartesian Coordinates of Stationary Structures, MP2(full)/6-311G*

HOBr, C_s, **1a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.021318	-0.385154	0.000000
2	8	0	0.021318	1.472060	0.000000
3	1	0	-0.916689	1.703913	0.000000

HOBr, $C_{\infty h}$, **1b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.377957
2	8	0	0.000000	0.000000	-1.364886
3	1	0	0.000000	0.000000	-2.309414

$HBrO_2$, C_1, **2a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.602770	0.448530	-0.116006
2	1	0	-1.782400	0.851737	0.746815
3	35	0	0.114820	-0.310783	0.009366
4	8	0	1.323232	0.804678	-0.018323

$HBrO_2$, C_s, cis, **2b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.374975	-0.960781	0.000000
2	1	0	-0.881604	-1.799046	0.000000
3	35	0	0.000000	0.355150	0.000000
4	8	0	1.485176	-0.368121	0.000000

$HBrO_2$, C_s, trans, **2c**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.236369	-1.118706	0.000000
2	1	0	-2.123385	-0.723017	0.000000
3	35	0	0.000000	0.348471	0.000000
4	8	0	1.501792	-0.315476	0.000000

$HBrO_3$, C_s, anti, **3a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.679440	-1.319285	0.454377
2	35	0	0.132835	0.000430	-0.266359
3	8	0	0.654991	1.331553	0.451957
4	8	0	-1.693488	-0.014026	0.122462
5	1	0	-1.776753	-0.000978	1.092184

$HBrO_3$, C_s, syn, TS, **3b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.398462	0.697553	1.333135
2	35	0	-0.262884	0.121934	0.000000
3	8	0	0.398462	0.697553	-1.333135
4	8	0	0.398462	-1.647290	0.000000
5	1	0	-0.362170	-2.250212	0.000000

$HBrO_2$ Dimer, 6-ring, chair-**4a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.306212	1.504803	0.473865
2	1	0	-0.391157	1.607275	0.075881
3	35	0	-1.912795	-0.066993	-0.155975
4	8	0	-1.110095	-1.329089	0.612609
5	35	0	1.916444	0.059638	0.153366
6	8	0	1.285410	-1.491124	-0.504678
7	1	0	0.387349	-1.601951	-0.077751
8	8	0	1.115412	1.346924	-0.570145

$HBrO_2$ Dimer, 6-ring, boat-**4a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.148276	1.476645	0.211464
2	35	0	1.854282	0.032926	-0.270670
3	8	0	1.449771	-1.289265	0.885833
4	1	0	0.500871	-1.506599	0.691477
5	8	0	-1.147309	-1.476309	0.210961
6	35	0	-1.854938	-0.033097	-0.270125
7	8	0	-1.448097	1.289740	0.885064
8	1	0	-0.499042	1.506088	0.689769

$HBrO_2$ Dimer with 4-ring Formed by $(BrO)_2$, **4b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.541584	0.041892	0.209220
2	1	0	3.681007	0.577597	1.003831
3	35	0	1.681984	-0.177551	0.057948
4	8	0	0.989949	1.260060	-0.385723
5	35	0	-1.895527	0.069574	-0.329066
6	8	0	-0.803185	-1.166731	-0.188154
7	1	0	-3.452824	-0.416549	1.324447
8	8	0	-2.822620	0.317048	1.259766

$HBrO_2$ Dimer with 4-ring Formed by(HOBr)(BrO), **4c**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.375880	-0.402880	-0.540491
2	1	0	3.883277	-0.552472	0.271258
3	35	0	1.714883	0.234976	-0.008816
4	8	0	0.852861	-1.004740	0.680139
5	35	0	-1.798619	-0.267784	-0.002478
6	8	0	-0.840167	1.414660	0.180036
7	1	0	-1.135198	1.776925	1.029398
8	8	0	-3.365742	-0.016560	-0.432853

$HBrO_2$ Dimer, cis-**4d**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.364940	0.211575	-0.469730
2	35	0	1.844585	-0.238038	-0.039368
3	8	0	0.771475	1.282333	0.474505
4	1	0	1.119564	1.563461	1.334030
5	8	0	-3.364567	-0.212897	-0.470259
6	35	0	-1.844825	0.238056	-0.039231
7	8	0	-0.771151	-1.281505	0.475500
8	1	0	-1.116762	-1.560146	1.336823

$HBrO_2$ Dimer, trans-**4d**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.502278	-0.197193	0.129033
2	35	0	-1.924274	0.224431	-0.050856
3	8	0	-0.758702	-1.304796	0.071767
4	1	0	-0.927393	-1.813137	-0.736323
5	8	0	3.501915	0.195643	-0.135186
6	35	0	1.924229	-0.224295	0.051301
7	8	0	0.758947	1.305703	-0.068010
8	1	0	0.929891	1.813520	0.739909

$HBrO_2$ Dimer with$(BrOH)_2$ Ring, TS(**4b,4c**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.337866	1.530328	-0.374732
2	1	0	-1.800930	1.775951	-1.190317
3	35	0	-2.073716	-0.109865	0.166092
4	8	0	-1.422691	-1.325815	-0.733514
5	35	0	1.625661	0.079796	-0.153306
6	8	0	0.995693	-0.019316	1.365702
7	1	0	3.648888	-1.084986	-0.015986
8	8	0	3.494112	-0.140015	-0.162607

$HBrO_2$ Dimer, **4e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.279119	0.257161	-0.243956
2	1	0	3.662686	0.301701	0.644439
3	35	0	1.513585	-0.254844	-0.022101
4	8	0	0.746939	1.063415	0.677657
5	35	0	-1.974107	-0.135312	0.136018
6	8	0	-0.844267	-1.289634	-0.305340
7	1	0	-0.670920	1.645588	-0.256395
8	8	0	-1.540979	1.432581	-0.675253

$HBrO_2$ Dimer, TS(**4a,4e**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.035190	0.630379	1.286330
2	1	0	1.949136	0.977564	-1.697151
3	35	0	1.729875	-0.372700	0.154378
4	8	0	2.632460	0.629888	-1.101660
5	35	0	-2.085190	-0.005218	0.002746
6	8	0	-1.020001	1.480643	-0.254741
7	8	0	-1.294668	-1.385408	-0.461822
8	1	0	-0.336960	1.405561	0.452979

$HBrO_2$ Dimer, **4f**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.200901	-0.101453	-0.474392
2	1	0	-1.113892	1.967075	0.913205
3	35	0	-1.652364	-0.220000	0.061680

4	8	0	-0.787156	1.552392	0.100908
5	35	0	1.918917	-0.309234	-0.222788
6	8	0	0.876914	-1.085075	0.818157
7	1	0	1.024499	1.753909	-0.010788
8	8	0	1.956145	1.484414	0.147374

$HBrO_2$ Dimer, **4g**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.511309	-1.125164	0.862916
2	1	0	-0.611035	1.224489	-0.620649
3	35	0	-2.398438	-0.036414	-0.041517
4	8	0	-1.444567	1.518151	-0.196924
5	35	0	2.368851	-0.204141	-0.146965
6	8	0	0.579134	-0.370337	-0.721353
7	8	0	2.570866	0.989841	0.963906
8	1	0	0.093619	-0.904995	-0.050827

$HBrO_2$ Dimer, **4h**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.434754	-1.466486	0.279598
2	1	0	-0.173893	1.356940	-0.474004
3	35	0	-2.050037	0.022205	-0.077506
4	8	0	-0.789658	1.347146	0.298937
5	35	0	1.845676	-0.334957	-0.131470
6	8	0	1.716498	0.490316	1.497840
7	1	0	0.761434	0.679142	1.586690
8	8	0	1.328548	0.742803	-1.301193

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Product Aggregate,(HOBr)($HBrO_3$), **5a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.308825	1.614101	-0.521465
2	1	0	-0.358092	1.669750	-0.312417
3	35	0	-1.875531	-0.086018	-0.060576
4	8	0	-0.771267	-1.028728	-0.755924
5	35	0	1.861260	-0.202716	-0.101199
6	8	0	-1.767190	-0.133525	1.532061
7	1	0	3.770183	0.103438	1.134195
8	8	0	3.483207	0.589711	0.350374

Product Aggregate,(HOBr)($HBrO_3$), **5b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-2.654712	1.408454	-0.261391
2	1	0	-2.861238	1.630266	0.664040
3	35	0	-1.620644	-0.134338	-0.220484
4	8	0	-0.645729	0.167622	1.024082
5	35	0	2.078993	0.054411	0.145614
6	8	0	-2.648555	-1.308303	0.115715
7	1	0	4.339465	-0.331293	0.085492
8	8	0	3.758939	-0.080463	-0.644540

Product Aggregate,$(HOBr)(HBrO_3)$, Cis-**5c**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.227578	-1.037967	-1.227399
2	1	0	0.265237	-1.134410	-1.030741
3	35	0	1.894483	0.087511	0.039642
4	8	0	1.343916	1.536071	-0.347035
5	35	0	-2.474482	0.211658	-0.024009
6	8	0	1.185223	-0.457585	1.389677
7	1	0	-0.674752	-0.886333	0.942784
8	8	0	-1.168035	-1.096787	0.127359

Product Aggregate,$(HOBr)(HBrO_3)$, Trans-**5c**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.913332	1.407648	-0.355906
2	1	0	0.094355	1.166754	0.139815
3	35	0	2.024908	-0.033442	-0.252619
4	8	0	2.665273	0.022293	1.207800
5	35	0	-2.788302	-0.006602	-0.056720
6	8	0	0.984009	-1.268205	-0.385599
7	1	0	-0.695073	-0.832800	0.490688
8	8	0	-1.147676	-0.028288	0.808250

Product Aggregate,$(HOBr)(HBrO_3)$, **5d**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.062486	-1.006167	-1.300896
2	1	0	-0.105725	-1.061425	-1.111120
3	35	0	-1.814560	0.071381	-0.013761
4	8	0	-1.579757	-0.703328	1.361005
5	35	0	2.165040	-0.351972	0.088516
6	8	0	-0.914417	1.408633	-0.097876
7	1	0	0.956034	1.581125	-0.036042
8	8	0	1.917023	1.463487	-0.145892

Product Aggregate, (HOBr)($HBrO_3$), Cis-**5e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.947351	-0.698942	-0.502272
2	1	0	-1.537896	-1.185420	1.793026
3	35	0	-1.606164	0.125141	-0.211249
4	8	0	-0.815138	-0.908442	1.202779
5	35	0	2.630510	0.187129	-0.015293
6	8	0	-1.903283	1.532216	0.483087
7	1	0	0.899698	-1.278022	0.387499
8	8	0	1.264033	-0.983081	-0.465038

Product Aggregate, (HOBr)($HBrO_3$), Trans-**5e**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.345114	-1.381410	0.135539
2	1	0	-1.428811	0.105566	2.157261
3	35	0	-1.451947	-0.100632	-0.223979
4	8	0	-0.742315	0.334575	1.508835
5	35	0	2.418275	-0.239999	-0.105219
6	8	0	-2.342548	1.168838	-0.597177
7	1	0	0.900374	1.153277	0.908876
8	8	0	1.268346	1.210905	0.009778

Product Aggregate,(HOBr)($HBrO_3$), **5f**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.566254	0.143863	-1.213854
2	1	0	1.234076	2.136505	0.225831
3	35	0	1.533029	-0.234805	-0.054584
4	8	0	0.579525	1.419116	0.185110
5	35	0	-2.267515	-0.440752	-0.070830
6	8	0	2.254616	-0.460066	1.350753
7	1	0	-1.228397	1.562182	0.209339
8	8	0	-2.187728	1.390314	0.172283

O-Transfer TS, **6b =** TS(**4b,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.291548	-0.264486	0.549231
2	1	0	-3.191021	0.078344	1.453049
3	35	0	-1.588560	-0.112065	-0.279808

4	8	0	-1.170082	1.444849	-0.028578
5	35	0	1.717628	0.040162	0.197162
6	8	0	0.190847	-0.867360	-0.043063
7	1	0	4.017245	-0.660818	0.160129
8	8	0	3.602835	0.074383	-0.317658

O-Transfer TS, **6c =** TS(**4c,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.257256	-1.354794	0.702898
2	1	0	-1.108419	1.795043	0.636834
3	35	0	-1.780327	-0.149007	-0.228754
4	8	0	-2.000988	1.401056	0.697667
5	35	0	1.629794	-0.089661	0.006024
6	8	0	0.029366	0.544498	-0.673596
7	1	0	3.927055	0.039492	-0.620060
8	8	0	3.535134	0.224095	0.245377

O-Transfer TS, **6e =** TS(**4e,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.902540	-1.186423	1.050674
2	1	0	0.987983	-1.525385	1.090083
3	35	0	1.744814	0.033506	-0.291618
4	8	0	1.253952	1.484237	0.283049
5	35	0	-2.081782	-0.279819	-0.048809
6	8	0	-0.145978	-0.592691	-0.499615
7	1	0	-0.598584	1.388229	0.346322
8	8	0	-1.584953	1.389642	0.475708

O-Transfer TS, **6f =** TS(**4f,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.054585	0.216342	0.442883
2	1	0	-1.431106	2.093531	-0.395993
3	35	0	-1.597229	-0.319561	-0.115297
4	8	0	-0.701034	1.454520	-0.402360
5	35	0	2.023067	-0.311122	-0.074025
6	8	0	0.166217	-0.781854	0.389394
7	1	0	0.847168	1.585337	0.177912
8	8	0	1.799352	1.410371	0.425628

Dibromotrioxide, Br_2O_3, **7a**

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	-2.117958	-1.028043	-0.750971
2	35	0	-1.592602	0.312576	0.043168
3	35	0	1.592659	-0.312637	0.042745
4	8	0	0.000291	-0.000764	1.125035
5	8	0	2.117415	1.029075	-0.749933

Dibromotrioxide, Br_2O_3, **7b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.108670	1.334623	0.134502
2	35	0	-1.644109	-0.219973	-0.121908
3	35	0	1.644009	-0.219881	-0.122137
4	8	0	0.000640	-0.744875	0.798167
5	8	0	2.108470	1.334617	0.135028

Dibromotrioxide, Br_2O_3, **7c**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.941978	-0.298168	0.447023
2	35	0	-1.523892	0.248823	-0.185142
3	35	0	1.665526	-0.227206	-0.176473
4	8	0	0.055691	-0.893649	0.545486
5	8	0	2.266636	1.097243	0.589557

Dibromotrioxide, BrO-BrO_2, **8a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.450991	-1.404485	1.329460
2	35	0	-1.093097	-0.791092	0.000000
3	35	0	1.402348	1.176647	0.000000
4	8	0	-0.450991	-1.404485	-1.329460
5	8	0	-0.450991	1.122168	0.000000

Dibromotrioxide, BrO-BrO_2, **8b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.057247	-0.664628	1.017687
2	35	0	1.356308	0.037815	-0.252620
3	35	0	-1.822687	0.046295	0.119200
4	8	0	0.584652	1.425221	0.079983

5	8	0	-0.601490	-1.128573	-0.513959

Brominemonoxide, BrO, **9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	-1.422277
2	35	0	0.000000	0.000000	0.325092

Brominedioxide, BrO_2, **10**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.415282	-0.589584	0.000000
2	35	0	0.000000	0.269861	0.000000
3	8	0	-1.415282	-0.591056	0.000000

Triplet Radical Pair **11b**, ^{3}(**9**/**10**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.344878	-0.132860	-0.008171
2	35	0	-1.687853	-0.133662	0.000730
3	35	0	2.397413	0.114379	-0.002360
4	8	0	-0.947776	1.352567	0.007192
5	8	0	1.188325	-1.135344	0.008108

Triplet Radical Pair **11c**, TS(**8a**,**11a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.585947	-0.689266	0.991382
2	35	0	1.718577	-0.040971	-0.249186
3	35	0	-2.249939	0.157204	0.130046
4	8	0	1.148258	1.521904	-0.028404
5	8	0	-1.409495	-1.341156	-0.441743

Dibromotrioxide Hydrate, Br_2O_3•OH_2, **12a** = **7a**•OH_2,

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.540267	-1.214177	-0.337317
2	1	0	-0.088985	2.824402	0.857477
3	35	0	-1.564269	0.090886	-0.035781
4	8	0	-0.183553	2.369408	0.020544

5	35	0	1.625821	-0.590349	-0.067312
6	8	0	0.146887	-0.527451	1.024059
7	1	0	0.709126	2.131156	-0.265338
8	8	0	2.230127	0.937924	-0.330273

Dibromotrioxide Hydrate, $Br_2O_3 \cdot OH_2$, **12b** = **7a**$\cdot OH_2$,

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.012486	-1.737462	-0.108249
2	1	0	2.983939	2.310238	-0.578698
3	35	0	1.437259	-0.679311	0.061841
4	8	0	2.645060	1.921801	0.228041
5	35	0	-1.597201	0.188469	-0.260125
6	8	0	-0.213300	1.132158	-0.410275
7	1	0	1.733066	2.207144	0.313163
8	8	0	-2.309151	0.266263	1.191168

Dibromotrioxide Hydrate, $BrO\text{-}BrO_2 \cdot OH_2$, **13a** = **8b**$\cdot OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.084720	0.862265	-0.407843
2	1	0	0.683891	2.643251	-0.585892
3	35	0	1.395778	-0.471966	0.204393
4	8	0	-0.194691	2.897500	-0.301395
5	35	0	-1.773441	-0.308435	-0.107451
6	8	0	0.442015	-1.328478	-0.866024
7	1	0	-0.427145	2.284249	0.399377
8	8	0	-0.711862	0.367031	1.174455

Dibromotrioxide Hydrate, $BrO\text{-}BrO_2 \cdot OH_2$, **13b** = **8b**$\cdot OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.750404	-0.508486	1.298028
2	1	0	-2.378016	2.468566	0.454294
3	35	0	-1.138710	-0.472037	-0.186212
4	8	0	-1.942343	2.139905	-0.333062
5	35	0	2.031876	0.129538	0.076553
6	8	0	-0.217137	-1.756075	-0.508698
7	1	0	-1.032582	2.451187	-0.305574
8	8	0	0.428609	1.008120	0.004901

Dibromotrioxide Hydrate, $BrO\text{-}BrO_2 \cdot OH_2$, **13c** = **8b**$\cdot OH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-1.508424	0.862122	-1.325057
2	1	0	3.793624	1.427968	-0.772870
3	35	0	-1.728387	-0.006278	-0.000031
4	8	0	3.719392	0.866810	0.000122
5	35	0	1.406139	-0.378749	-0.000009
6	8	0	-1.508552	0.861669	1.325312
7	1	0	3.793178	1.428601	0.772702
8	8	0	-0.240932	-1.263179	-0.000180

Dibromotrioxide Hydrate, $BrO–BrO_2•OH_2$, **13d** = **8b**•OH_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.470787	-1.419118	-0.000421
2	1	0	-0.354544	2.537259	0.763001
3	35	0	1.818565	-0.143822	-0.000035
4	8	0	-0.023064	3.011295	0.000097
5	35	0	-1.310213	-0.533589	0.000044
6	8	0	-1.292033	0.368720	-1.321939
7	1	0	-0.354358	2.538649	-0.763764
8	8	0	-1.291116	0.368286	1.322319

Transition State Structure for 1,4-Water Addition to Dibromotrioxide **7**, **14a =** TS(**4f,12a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.102833	-0.436616	-0.448319
2	1	0	-0.757208	2.386082	0.803178
3	35	0	-1.449939	-0.138052	0.069501
4	8	0	-0.501483	1.979281	-0.035423
5	35	0	1.744133	-0.403958	-0.198093
6	8	0	0.489360	-0.994667	0.829795
7	1	0	0.718439	1.707332	-0.005224
8	8	0	1.832699	1.311617	0.116789

Transition State Structure for 1,4-Water Addition to Dibromotrioxide **7**, **14b =** TS(**5,12a**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.426188	0.018931	1.214100
2	1	0	0.576106	2.404999	0.309709
3	35	0	1.732561	-0.090297	-0.250584
4	8	0	0.193360	1.701039	-0.235021
5	35	0	-1.944301	-0.448134	0.102685
6	8	0	0.509898	-1.199511	-0.349498
7	1	0	-1.048038	1.651658	-0.123630
8	8	0	-2.144092	1.328093	-0.005785

Transition State Structure for 1,2-Water Addition to Dibromotrioxide **7a, 14c =** TS(**4,12b**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.235896	-1.766334	-0.381596
2	1	0	1.931761	2.396065	-0.450583
3	35	0	1.710285	-0.236394	0.131435
4	8	0	1.407054	1.992741	0.255309
5	35	0	-1.878705	-0.028740	-0.218124
6	8	0	-0.228829	0.677274	-0.809088
7	1	0	0.164636	1.537154	-0.309926
8	8	0	-1.939333	-0.235374	1.409701

Transition State Structure for 1,2-Water Addition to Mixed Anhydride **8, 15a =** TS(**13b,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.387545	0.520135	0.950726
2	1	0	-0.981927	2.648378	-0.502975
3	35	0	-1.390924	-0.153505	-0.135912
4	8	0	-0.559083	1.816668	-0.739850
5	35	0	2.299412	-0.218634	-0.009572
6	8	0	-1.790992	-1.822952	-0.251823
7	1	0	0.438777	1.382316	0.048370
8	8	0	0.830880	0.610421	0.734267

Transition State Structure for 1,2-Water Addition to Mixed Anhydride **8, 15b =** TS(**13b,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.840636	-0.371770	1.414039
2	1	0	-0.298885	2.402371	0.916134
3	35	0	-1.443159	0.015820	-0.039179
4	8	0	-0.559637	2.006623	0.076330
5	35	0	2.108355	-0.284014	0.073098
6	8	0	-2.410880	-1.321413	-0.561482
7	1	0	0.539265	1.285053	-0.681534
8	8	0	0.870871	0.398980	-1.106609

Transition State Structure for 1,4-Water Addition to Mixed Anhydride **8, 15c =** TS(**13c,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.492421	1.327061	-0.708679

2	1	0	0.892326	1.618372	-0.282751
3	35	0	-1.443884	0.021342	-0.157138
4	8	0	1.930611	1.512627	0.021071
5	35	0	1.530545	-0.492648	0.062084
6	8	0	-1.571009	0.217142	1.435616
7	1	0	2.017738	1.817742	0.937110
8	8	0	-0.610080	-1.424378	-0.413944

Transition State Structure for 1,4-Water Addition to Mixed Anhydride **8**, **15d =** TS(**13c,5**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.456496	1.383634	-0.571624
2	1	0	0.892849	1.626608	-0.065248
3	35	0	-1.446914	0.043057	-0.176903
4	8	0	1.950173	1.492447	0.189873
5	35	0	1.530056	-0.504897	0.075267
6	8	0	-1.680476	0.106106	1.410375
7	1	0	2.487107	1.741415	-0.577183
8	8	0	-0.599442	-1.382640	-0.503663

Transition State Structure **15e =** TS(**13d,4h**)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.882325	-1.250736	-0.464969
2	1	0	0.239678	1.589347	1.221478
3	35	0	1.949071	-0.059050	0.009259
4	8	0	0.533684	1.755884	0.305938
5	35	0	-1.521523	-0.378936	-0.141578
6	8	0	-1.686423	1.266356	-0.851342
7	1	0	-0.805746	1.691349	-0.549323
8	8	0	-1.529347	-0.265404	1.505253

Dibromotrioxide Hydrate, $BrO–BrO_2(OH_2)_2$, **16** = **8b•**$(OH_2)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.496696	-0.594549	1.340272
2	1	0	-2.492710	1.442909	-0.499260
3	35	0	-0.819766	-0.954544	-0.090347
4	8	0	-2.635994	0.718063	-1.131118
5	35	0	2.088248	0.366276	-0.028092
6	8	0	0.619548	-1.783028	0.103494
7	1	0	-2.618847	1.094701	-2.010413
8	8	0	0.502504	1.040518	-0.533429
9	8	0	-1.594208	2.374832	0.793659
10	1	0	-0.699195	2.165341	0.496505
11	1	0	-1.747354	1.839759	1.575490

Transition State Structure for 1,2-Water Addition to Mixed Anhydride **8** with extra water, **17**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.980047	0.697298	0.263527
2	1	0	-0.583631	2.436161	0.944264
3	35	0	-1.628871	0.016301	-0.324825
4	8	0	-0.414304	1.791798	0.252562
5	35	0	2.811003	-0.063484	-0.211593
6	8	0	-2.069901	-1.400686	-1.115015
7	1	0	0.549173	1.113190	0.370868
8	8	0	1.089299	0.023092	0.410923
9	8	0	-0.720852	-1.007010	1.912933
10	1	0	0.188265	-0.776241	1.622827
11	1	0	-0.762020	-1.957649	2.037229

H-Transfer Transition State between BrO and water, **18** = TS(**9**•OH_2, **1a**•OH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.654540	0.949996	0.004458
2	35	0	-0.818809	-0.121004	0.004280
3	8	0	2.401105	-0.435652	-0.081070
4	1	0	2.691310	-0.219858	0.813897
5	1	0	1.521866	0.340249	-0.350806

H-Transfer Transition State between BrO_2 and water, **19** = TS(**10**•OH_2, **2a**•OH)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.830316	-1.168357	0.526740
2	35	0	0.323227	-0.132013	-0.291902
3	8	0	-1.489670	0.909977	-0.070199
4	1	0	-1.529719	1.788664	0.313233
5	1	0	-1.550660	-0.348162	0.572141
6	8	0	1.290914	0.655873	0.709858

H-Transfer Transition State between BrO and water in the presence of a second water molecule, **20** = TS(**9**•$(OH_2)_2$, **1a**•OH•OH_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.236874	0.109132	0.899718
2	35	0	-1.259367	-0.131308	-0.118530
3	8	0	1.560448	1.513021	-0.221301
4	1	0	2.165939	0.780715	-0.447264

5	1	0	0.763967	1.052251	0.499349
6	8	0	2.677681	-0.975965	-0.236239
7	1	0	3.449577	-1.226169	0.270541
8	1	0	1.898332	-1.180528	0.288513

Cartesian Coordinates of Stationary Structures, SMD(MP2(full)/6-311G*)

H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.116030
2	1	0	0.000000	0.762476	-0.464118
3	1	0	0.000000	-0.762476	-0.464118

HBr

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.039732
2	1	0	0.000000	0.000000	-1.390622

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.021263	-0.386189	0.000000
2	8	0	0.021263	1.473817	0.000000
3	1	0	-0.914323	1.726091	0.000000

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-0.107252	-0.315768	0.007518
2	8	0	1.565807	0.475196	-0.118276
3	1	0	1.817117	0.783080	0.768581
4	8	0	-1.323718	0.808405	-0.010690

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.675468	1.321798	0.452665
2	35	0	-0.124355	0.000049	-0.268562

3	8	0	-0.678576	-1.320224	0.452883
4	8	0	1.674392	-0.001655	0.131691
5	1	0	1.789628	-0.001082	1.101744

6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.253887	-0.295510	0.582722
2	1	0	-3.117328	-0.244265	1.546587
3	35	0	-1.597520	-0.089121	-0.289449
4	8	0	-1.163079	1.456127	0.019566
5	35	0	1.715188	0.027040	0.191561
6	8	0	0.173933	-0.856837	-0.110012
7	1	0	4.029201	-0.654700	0.198252
8	8	0	3.614253	0.080194	-0.282123

6c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.157770	-1.336991	0.698585
2	1	0	-1.254709	1.829106	0.725194
3	35	0	-1.757815	-0.165091	-0.233430
4	8	0	-2.095789	1.328987	0.717708
5	35	0	1.605770	-0.063906	0.005678
6	8	0	0.036512	0.588208	-0.692700
7	1	0	3.940156	-0.050372	-0.592738
8	8	0	3.546562	0.199316	0.256265

6e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.985065	-1.140467	1.052966
2	1	0	1.109904	-1.559148	1.168371
3	35	0	1.734727	0.033835	-0.301667
4	8	0	1.223046	1.480173	0.287379
5	35	0	-2.085787	-0.287625	-0.039354
6	8	0	-0.156095	-0.600546	-0.497043
7	1	0	-0.590099	1.378912	0.352628
8	8	0	-1.581106	1.393704	0.458538

6f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.085720	-0.119756	0.591242

2	1	0	-1.401501	2.058622	-0.775229
3	35	0	-1.637544	-0.252114	-0.179295
4	8	0	-0.920694	1.509287	-0.132327
5	35	0	2.116341	-0.327103	-0.029977
6	8	0	0.190044	-0.746174	0.260659
7	1	0	0.819413	1.526201	0.125598
8	8	0	1.794393	1.442614	0.277196

7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.104964	-1.039191	-0.741967
2	35	0	-1.588922	0.314803	0.042728
3	35	0	1.589006	-0.314846	0.042237
4	8	0	0.000071	-0.001087	1.110787
5	8	0	2.104525	1.040465	-0.740542

8a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.445345	-1.389393	1.324995
2	35	0	-1.103584	-0.783556	0.000000
3	35	0	1.408963	1.159386	0.000000
4	8	0	-0.445345	-1.389393	-1.324995
5	8	0	-0.445345	1.134528	0.000000

BrO, **9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	-1.420835
2	35	0	0.000000	0.000000	0.324762

BrO_2, **10**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.404759	-0.602688	0.000000
2	35	0	0.000000	0.275746	0.000000
3	8	0	-1.404759	-0.603699	0.000000

12a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-2.493063	-1.262566	-0.327202
2	1	0	-0.270207	2.865541	0.851822
3	35	0	-1.554399	0.069717	-0.041096
4	8	0	-0.262359	2.419436	0.001570
5	35	0	1.631062	-0.584186	-0.057917
6	8	0	0.125175	-0.478725	1.016234
7	1	0	0.663663	2.228365	-0.188405
8	8	0	2.245662	0.935919	-0.340351

12b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.065924	-1.651825	-0.112968
2	1	0	3.605035	1.563855	-0.661213
3	35	0	1.366277	-0.559125	0.031211
4	8	0	3.384033	1.272688	0.226534
5	35	0	-1.693710	0.218855	-0.250901
6	8	0	-0.348511	1.204789	-0.380964
7	1	0	3.003710	2.039486	0.661812
8	8	0	-2.363172	0.212614	1.228466

14a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.097237	-0.139134	-0.499145
2	1	0	-0.839839	2.157023	0.999815
3	35	0	-1.502991	-0.256392	0.056610
4	8	0	-0.645817	1.823267	0.108582
5	35	0	1.831399	-0.337432	-0.191946
6	8	0	0.594048	-0.967328	0.827448
7	1	0	0.503757	1.674069	0.033801
8	8	0	1.754227	1.402290	0.026012

14b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.366694	-0.010180	1.253124
2	1	0	0.563818	2.412217	0.297215
3	35	0	1.734813	-0.085864	-0.243571
4	8	0	0.198524	1.714727	-0.270815
5	35	0	-1.942327	-0.451488	0.097459
6	8	0	0.525696	-1.194544	-0.395474
7	1	0	-0.972592	1.646512	-0.108272
8	8	0	-2.131943	1.333572	0.028790

15a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.024680	-0.015055	-0.028812
2	1	0	1.132879	2.507317	0.371054
3	35	0	1.432708	-0.221480	-0.229594
4	8	0	0.690860	1.707785	0.698867
5	35	0	-2.306899	-0.144712	0.034003
6	8	0	0.823858	-1.214370	0.872679
7	1	0	-0.220124	1.452203	0.094492
8	8	0	-0.828905	0.628790	-0.745216

15b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.737133	-0.394983	1.366472
2	1	0	-0.287598	2.319216	0.987185
3	35	0	-1.438247	0.018731	-0.036039
4	8	0	-0.568886	2.026921	0.109739
5	35	0	2.079480	-0.291140	0.065452
6	8	0	-2.401348	-1.345948	-0.538354
7	1	0	0.523812	1.320446	-0.650280
8	8	0	0.872447	0.450843	-1.108650

15e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.821648	-1.232299	-0.381916
2	1	0	0.698874	1.896326	1.282845
3	35	0	2.020231	-0.133161	0.016677
4	8	0	0.718281	1.811620	0.312909
5	35	0	-1.574973	-0.295358	-0.230343
6	8	0	-1.607282	1.469691	-0.495389
7	1	0	-0.650898	1.771520	-0.180846
8	8	0	-1.886646	-0.632722	1.361435