Supplementary Information to:

Benchmark Thermochemistry of Chloramines, Bromamines, and Bromochloramines: Halogen Oxidants Stabilized by Electron Correlation

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Supplementary Information

Optimized Geometries, with coordinates in Bohr. The model chemistry is indicated in parentheses.

H_2 (AE-CCSD(T)/aug-cc-pVQZ)

H	0.00000000	0.00000000	0.70108673
H	0.00000000	0.00000000	-0.70108673

N_2 (AE-CCSD(T)/aug-cc-pVQZ)

N	0.00000000	0.00000000	1.03764068
N	0.00000000	0.00000000	-1.03764068

O_2 (AE-CCSD(T)/aug-cc-pVQZ)

O	0.00000000	0.00000000	1.13922333
O	0.00000000	0.00000000	-1.13922333

Cl_2 (AE-CCSD(T)/aug-cc-pVQZ)

Cl	0.00000000	0.00000000	1.88919509
Cl	0.00000000	0.00000000	-1.88919509

Br_2 (AE-CCSD(T)/aug-cc-pVQZ)

Br	0.00000000	0.00000000	2.15289952
Br	0.00000000	0.00000000	-2.15289952

HCl (AE-CCSD(T)/aug-cc-pVQZ)

Cl	0.00000000	0.00000000	0.06754727
H	0.00000000	0.00000000	-2.34371101

HBr (AE-CCSD(T)/aug-cc-pVQZ)

Br	0.00000000	0.00000000	0.03352007
H	0.00000000	0.00000000	-2.62480873

NH_3 (AE-CCSD(T)/aug-cc-pVQZ)

N	0.00000000	-0.00000007	-0.12755526
H	0.52290825	-0.90130902	0.59076593
H	0.01910294	1.76953179	0.59076553
H	-1.54201116	-0.86822179	0.59076594

H_2O (AE-CCSD(T)/aug-cc-pVQZ)

H	0.00000000	-1.43048941	0.98402826
O	0.00000000	0.00000000	-0.12400545
H	0.00000000	1.43048941	0.98402826

HOCl (AE-CCSD(T)/aug-cc-pVQZ)

H	-2.61817495	1.63840308	0.00000000
O	-2.14218076	-0.11860230	0.00000000
Cl	1.05530087	0.00702940	0.00000000

HOBr (AE-CCSD(T)/aug-cc-pVQZ)

H	-3.30726752	1.63594240	0.00000000
O	-2.82221738	-0.11762873	0.00000000
Br	0.61423334	0.00294884	0.00000000

NH_2Cl (AE-CCSD(T)/aug-cc-pVQZ)

N	2.23834626	0.00035926	-0.14938635
H	2.75235390	-1.52668576	0.88990901
H	2.77931371	1.51166594	0.89918960
Cl	-1.05575901	0.00028902	0.00825791

$NHCl_2$ (AE-CCSD(T)/aug-cc-pVQZ)

N	0.00029142	-1.60102491	-0.16108085
H	-0.09791735	-2.55978615	1.50251967
Cl	2.65526471	0.35593995	0.01139714
Cl	-2.65255937	0.35895588	0.00980316

NCl_3 (AE-CCSD(T)/aug-cc-pVQZ)

N	-1.07140387	0.00000003	0.00000000
Cl	0.14301248	-1.54542252	2.67675026
Cl	0.14301249	3.09084503	0.00000000
Cl	0.14301248	-1.54542252	-2.67675026

NH_2Br (AE-CCSD(T)/aug-cc-pVQZ)

N	-0.14731129	2.94534561	0.00000000
H	0.89705829	3.44615957	-1.52710267
H	0.89705820	3.44615930	1.52710281
Br	0.00322682	-0.61063305	0.00000000

$NHBr_2$ (AE-CCSD(T)/aug-cc-pVQZ)

N	0.00018299	-1.91523168	-0.15770407
H	-0.11697966	-2.87207630	1.50607992
Br	2.88430786	0.18747499	0.00476453
Br	-2.88284644	0.18903676	0.00398472

NBr_3 (AE-CCSD(T)/aug-cc-pVTZ)

N	-0.00000010	-0.00000011	-1.19775081
Br	2.42495000	-2.35936212	0.07084198
Br	0.83079273	3.27974917	0.07084197
Br	-3.25574271	-0.92038704	0.07084198

NHBrCl (AE-CCSD(T)/aug-cc-pVQZ)

N	1.18723587	-1.66610171	-0.16159297
Br	-1.88948559	0.14883771	0.00416660
Cl	3.75319661	0.40413037	0.01043165
H	1.23545984	-2.52767504	1.55701050

$NBrCl_2$ (AE-CCSD(T)/aug-cc-pVTZ)

N	-1.13390506	-1.02781227	0.00000000
Cl	0.15793366	-2.54348239	-2.69794123
Br	0.06123594	2.43641543	-0.00000001
Cl	0.15793366	-2.54348234	2.69794126

NBr_2Cl (AE-CCSD(T)/aug-cc-pVTZ)

N	-0.80436316	-1.15422838	0.00000000
Cl	-3.86482701	0.16703972	0.00000003
Br	0.92761792	0.06539392	2.93260742
Br	0.92761790	0.06539392	-2.93260743

Computed anharmonic Frequencies for the halamines and the hypohalous acids (in cm^{-1}).
Method: B2PLYPD/aug-cc-pVQZ

NH_2Cl	**$NHCl_2$**	**NCl_3**	**NH_2Br**	**$NHBr_2$**	**NBr_3**
3383.152	3286.672	629.059	3383.555	3284.393	556.153
3305.095	1298.063	628.631	3304.355	1227.111	555.744
1542.489	995.449	535.755	1502.408	914.956	435.482
1168.339	662.361	350.747	1097.598	589.874	210.506
1023.194	609.434	254.907	973.414	504.101	147.706
675.861	283.474	255.15	581.284	170.185	148.08

NHBrCl	**$NBrCl_2$**	**NBr_2Cl**	**HOCl**	**HOBr**
3281.558	618.085	607.051	3601.349	3606.984
1268.015	609.766	570.176	1231.855	1156.92
951.899	489.797	459.125	733.624	634.538
647.164	317.832	267.812		
538.323	211.697	193.103		
226.097	209.423	160.666		