Unconventional Radical and Radical-Hole Site-Based Interactions in Halogen-Bearing Dimers and Trimers: A Comparative Study

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Cartesian atomic coordinates

For $NH_3\cdots{}^{\bullet}XO_3$ Complexes

$NH_3\cdots{}^{\bullet}ClO_3$

Cl	-0.63948200	2.38881800	0.00000000
O	-0.27859000	3.80379000	0.00000000
O	-0.27827700	1.68141300	1.22535800
O	-0.27827700	1.68141200	-1.22535800
N	-3.44158700	2.38892500	0.00000000
H	-3.81485200	1.44769800	0.00000000
H	-3.81472600	2.85958900	-0.81515500
H	-3.81472600	2.85958900	0.81515500

S**2 value = 0.7516

$NH_3\cdots{}^{\bullet}BrO_3$

Br	-0.79626200	1.33341300	0.00000000
O	-0.36633000	2.10951600	-1.34430600
O	-0.36632900	2.10951600	1.34430700
O	-0.36608700	-0.21935500	0.00000000
N	-3.63583800	1.33340100	0.00000000
H	-4.00763200	2.27562800	0.00000000
H	-4.00763000	0.86228900	0.81599500
H	-4.00763000	0.86228900	-0.81599400

S**2 value = 0.7547

$NH_3\cdots{}^{\bullet}IO_3$

I	-3.85918200	0.94781900	-0.00580000
O	-3.42706700	2.00064400	1.36630500
O	-3.00996700	-0.61929600	0.02359800
O	-5.61981400	0.78270000	-0.23053900
N	-2.88551600	2.32389900	-2.38934700
H	-3.08728600	1.79539700	-3.23026100
H	-1.88250400	2.46437300	-2.35199100
H	-3.31644100	3.23539600	-2.49249500

S**2 value = 0.7589

For $^{\bullet}XO_3\cdots NH_3$ Complexes

$^{\bullet}ClO_3\cdots NH_3$

Cl	-0.43819400	2.39103100	0.00033500
O	-0.09871700	3.81176200	-0.00015600
O	-0.10119000	1.68034400	1.23126500
O	-0.10177400	1.67963900	-1.23034400
N	2.46446900	2.38697500	-0.00029000
H	2.83639300	1.44565800	-0.00008100
H	2.83899500	2.85684800	0.81418000
H	2.83883300	2.85642600	-0.81507800

S**2 value = 0.7521

$^{\bullet}BrO_3\cdots NH_3$

Br	-0.57482700	1.33345700	0.00022400
O	-0.19202300	0.55082200	1.35478900
O	-0.19189300	0.55168200	-1.35483700
O	-0.19299400	2.89808600	0.00073900
N	2.26631300	1.33315200	-0.00014000
H	2.63543300	0.39072300	-0.00075200
H	2.63819000	1.80320600	0.81544100
H	2.63705900	1.80379300	-0.81590400

S**2 value = 0.7553

$^{\bullet}IO_3\cdots NH_3$

I	-3.98923100	0.75933100	0.31912000
O	-3.49109100	1.93165100	1.57233200
O	-3.05093800	-0.75698300	0.20143100
O	-5.73099400	0.67352700	-0.07171900
N	-4.81950300	-0.40934800	2.34249800
H	-5.25603100	-1.28365600	2.07479000
H	-5.49984400	0.17168200	2.81807000
H	-4.04671900	-0.60012900	2.96938100

S**2 value = 0.7560

For $NH_3\cdots{}^{\bullet}XO_3\cdots NH_3$ Complexes

$NH_3\cdots{}^{\bullet}ClO_3\cdots NH_3$

Cl	-0.55306400	2.38890800	0.00015300
O	-0.20428700	3.80808200	0.00084700
O	-0.20454300	1.67878900	1.22896000
O	-0.20430200	1.67984600	-1.22919200
N	2.44013600	2.38868600	-0.00015100
H	2.81396000	1.44821200	-0.00066400
H	2.81439200	2.85835600	0.81443900
H	2.81417700	2.85914600	-0.81438500
N	-3.49127800	2.38894600	-0.00004900
H	-3.86822200	1.44927300	-0.00051700
H	-3.86851900	2.85900400	-0.81355500
H	-3.86860100	2.85823800	0.81386100

S**2 value = 0.7518

$NH_3\cdots{}^{\bullet}BrO_3\cdots NH_3$

Br	-0.68940700	1.33389200	-0.00424700
O	-0.28115900	2.11473200	-1.35344300
O	-0.28800400	2.11279900	1.34814700
O	-0.28490000	-0.22595500	-0.00427700
N	2.25060500	1.33334700	0.00123900
H	2.62118000	2.27502100	0.00105400
H	2.61982200	0.86328300	-0.81533600
H	2.62341400	0.86209000	0.81548800
N	-3.67542200	1.33295300	0.00054900
H	-4.05274900	2.27277300	0.00207200
H	-4.05007100	0.86209500	0.81514800
H	-4.05361900	0.86326000	-0.81308200

S**2 value = 0.7548

$NH_3\cdots{}^{\bullet}IO_3\cdots NH_3$

I	-3.95070400	0.83362200	0.18857500
O	-3.51479000	2.02444800	1.45280100
O	-2.97259900	-0.66494000	0.12867100
O	-5.69163000	0.67207600	-0.19658300
N	-2.93040700	2.24839000	-2.26721400
H	-3.09437800	1.70224400	-3.10433000
H	-1.93369100	2.41828800	-2.20699800
H	-3.38311300	3.14512100	-2.39699200
N	-4.77762900	-0.34676200	2.24961500
H	-5.18600800	-1.23756100	1.99415700
H	-5.47789400	0.22266000	2.70893100
H	-4.00468900	-0.50325300	2.88494500

S**2 value = 0.7555