Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for: Intermolecular Interactions and Proton Transfer in the Hydrogen Halide–Superoxide Anion Complexes

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Table S1: The CCSD(T)/aug-cc-pVQZ optimized geometries for HOX ($\tilde{X}\ ^1A'$) for X = F, Cl, Br, I.

X	R_{OX}	R_{OH}	θ_{HOX}
F	1.436	0.977	97.9
Cl	1.694	0.965	102.9
Br	1.834	0.965	103.0
I	1.996	0.964	104.9

Table S2: The CCSD(T)/aug-cc-pVQZ optimized geometries for XO ($\tilde{X}\ ^2\Pi$) for X = F, Cl, Br, I.

X	R_{OX}
F	1.354
Cl	1.574
Br	1.725
I	1.890

Table S3: The CCSD(T)/aug-cc-pVQZ optimized geometries for XO^{-1} ($\tilde{X}\ ^1\Sigma$) for X = F, Cl, Br, I.

X	R_{OX}
F	1.517
Cl	1.686
Br	1.817
I	1.949

Table S4: The CCSD(T)/aug-cc-pVQZ optimized geometries for OH ($\tilde{X}\ ^2\Pi$) and OH^{-1} ($\tilde{X}\ ^1\Sigma$) .

Species	R_{OH}
OH	0.971
OH^{-1}	0.965