Supplementary Materials: Hydrogen Bond versus Halogen Bond in HXO_n (X = F, Cl, Br, and I) Complexes with Lewis Bases

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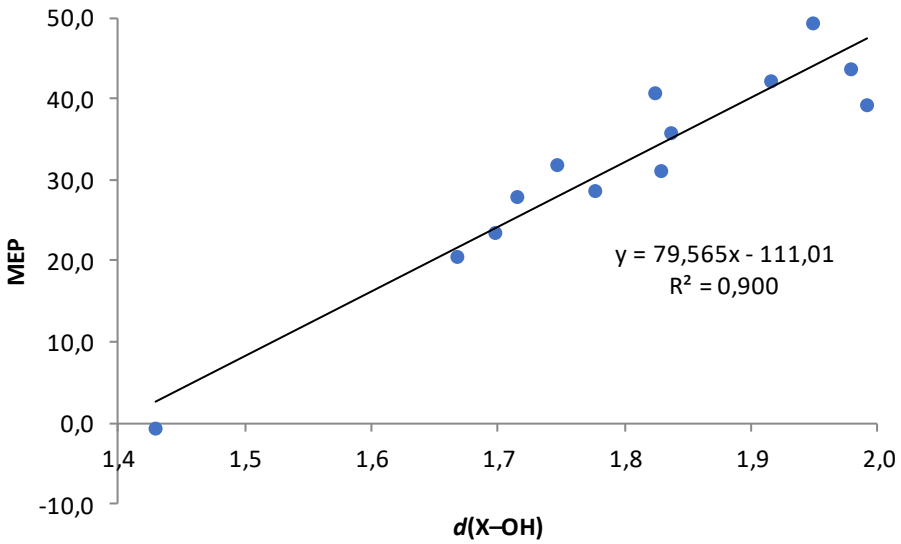

Figure S1. Graphical representation of d(X-OH) (in Å) versus XB MEP (in kcal/mol) in halogen oxoacids.

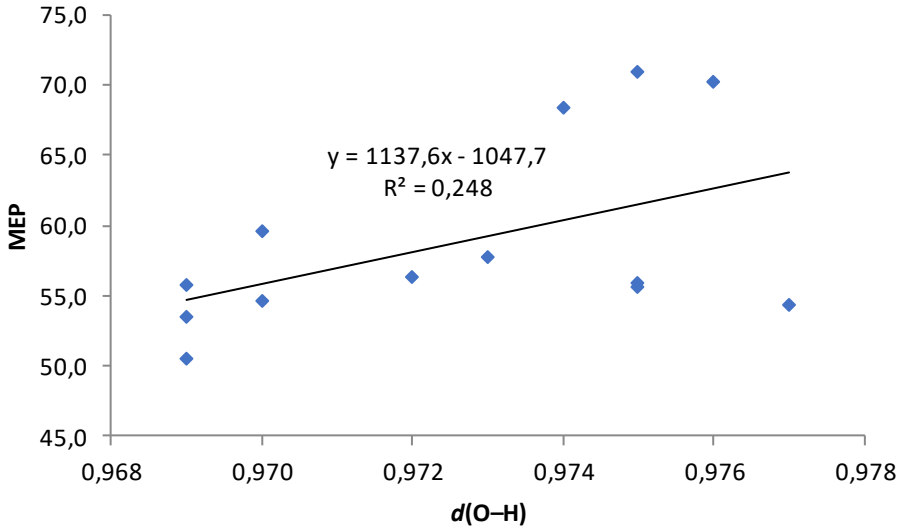

Figure S2. Graphical representation of d(O-H) (in Å) versus HB MEP (in kcal/mol) in halogen oxoacids.

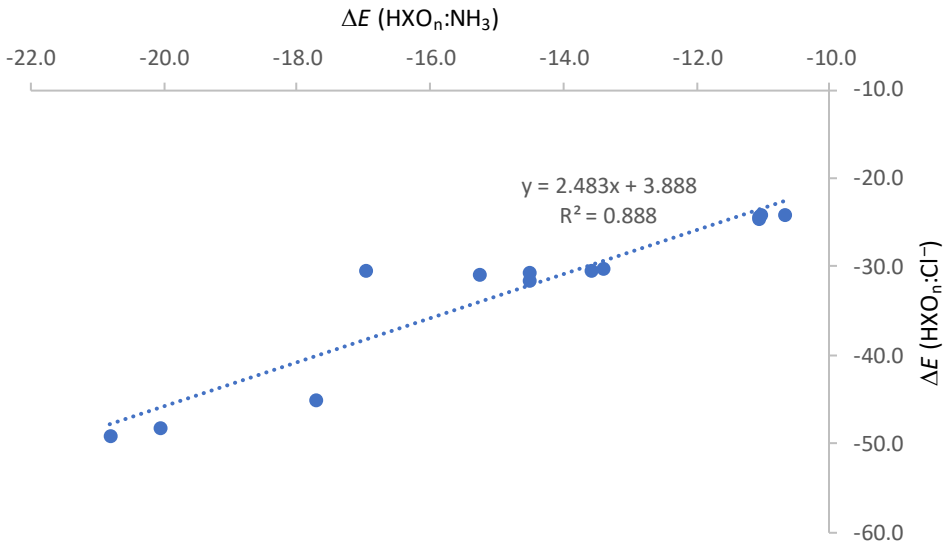

Figure S3. Graphical representation of interaction energies of HB HXO_n:NH_3 versus HB HXO_n:Cl^- (in kcal·mol^{-1}).

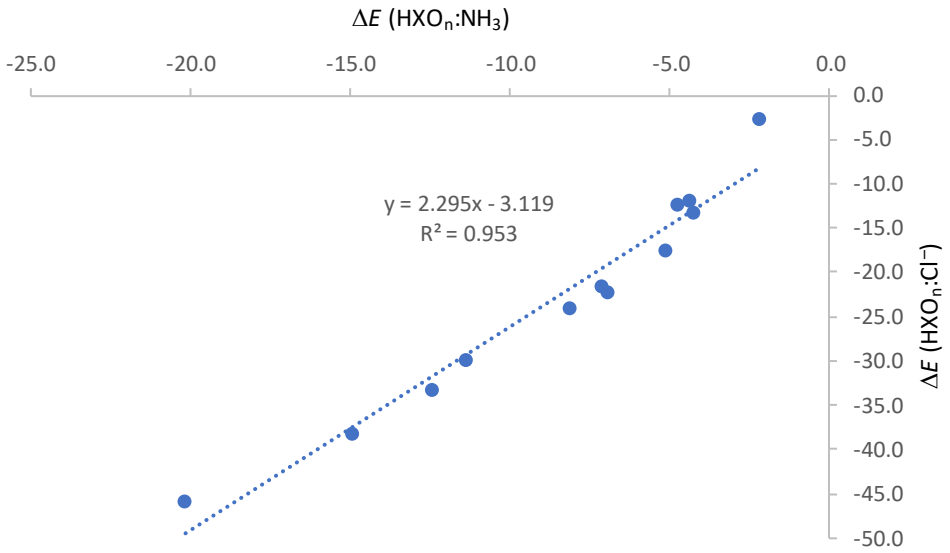

Figure S4. Graphical representation of interaction energies of XB HXO_n:NH_3 versus XB HXO_n:Cl^- (in kcal·mol^{-1}).

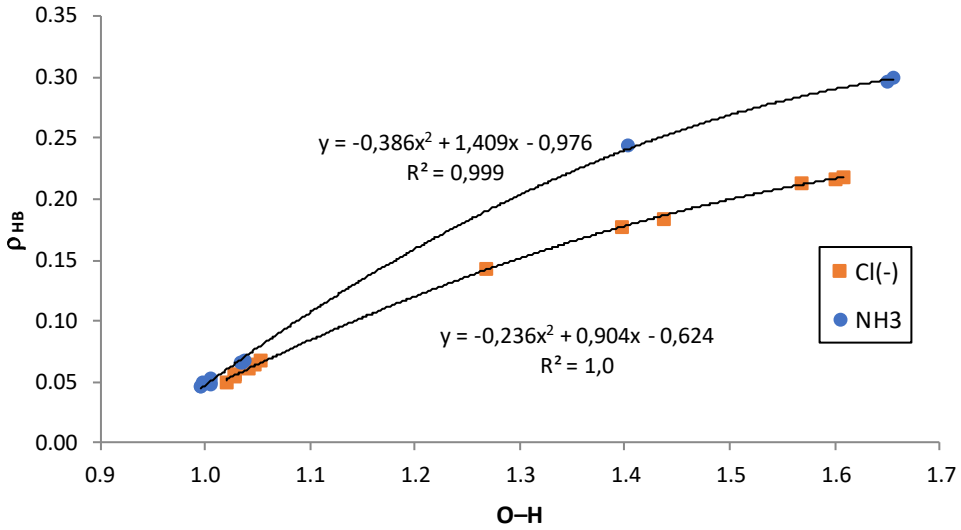

Figure S5. Second-order polynomial relationship between the O–H distance (in Å) and the electron density for HB, ρ_{HB}, complexes.

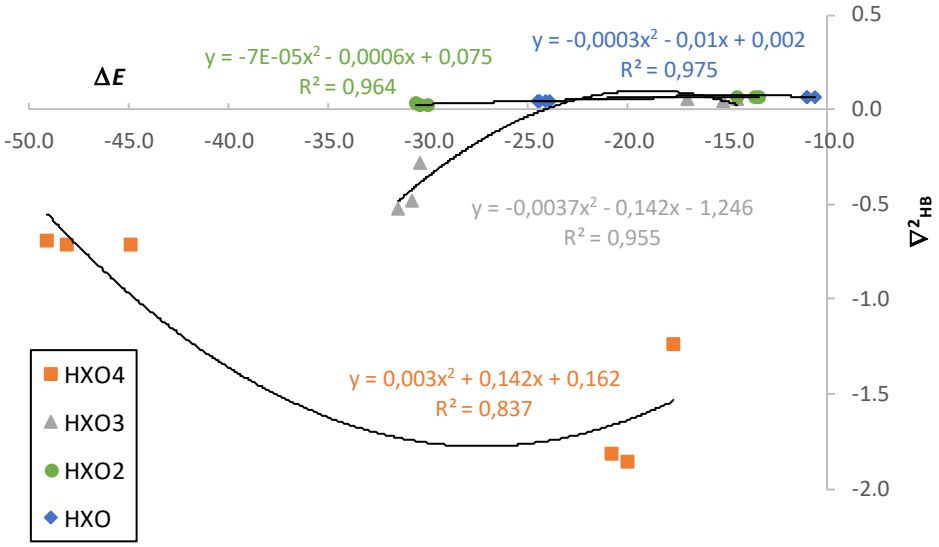

Figure S6. Second-order polynomial relationship between the interaction energy, ΔE, (in kcal·mol^{-1}) and the Laplacian of the electron density for HB, $\nabla^2\rho_{HB}$, complexes.

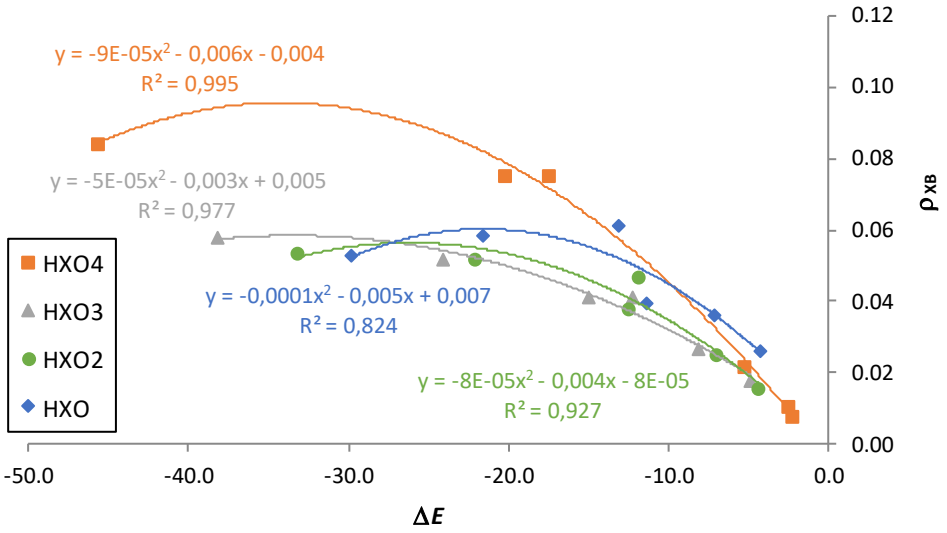

Figure S7. Second-order polynomial relationship between the interaction energy, ΔE, (in kcal·mol^{-1}) and the electron density for HB, ρ_{HB}, complexes.

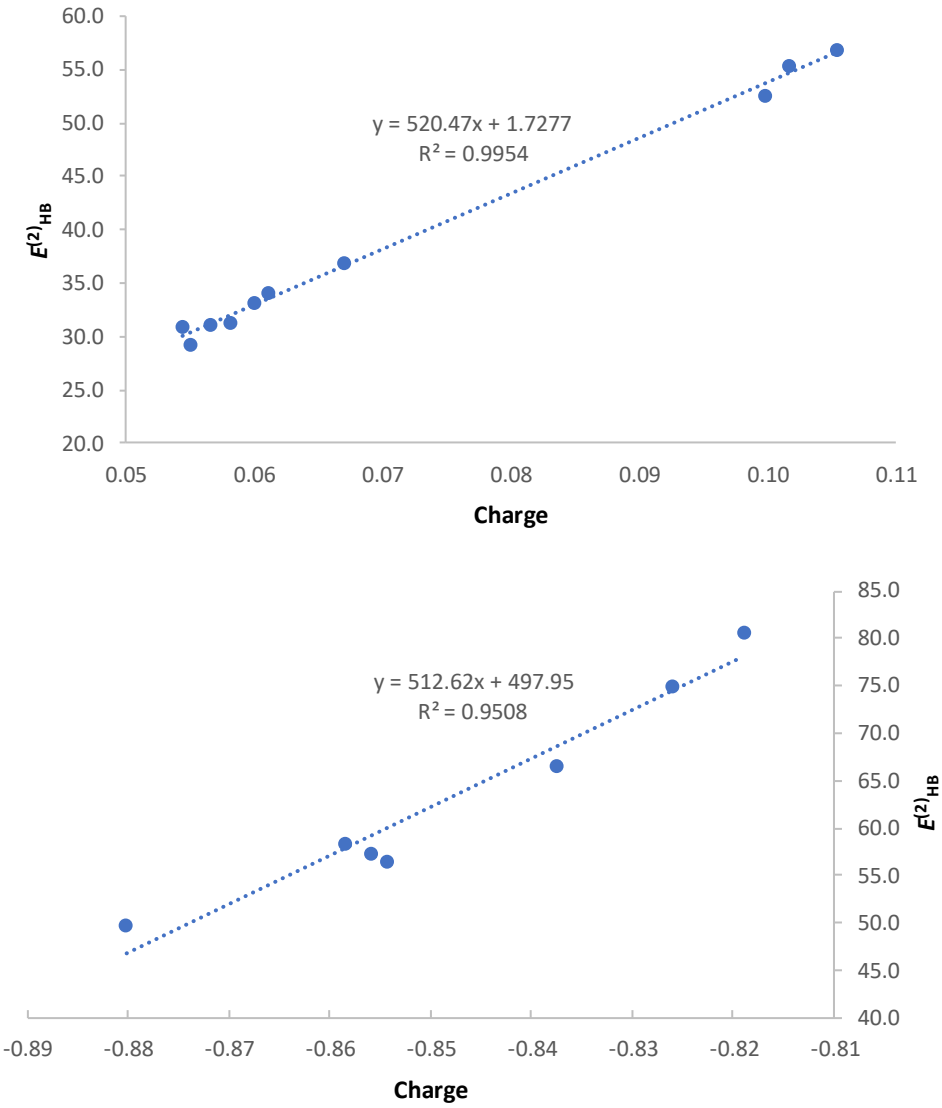

Figure S8. Value of the charge of the Lewis base, in *e*, (NH_3, up, Cl^-, down) vs. $E^{(2)}_{HB}$, in kcal·mol^{-1}, for all HB complexes with no proton transfer.

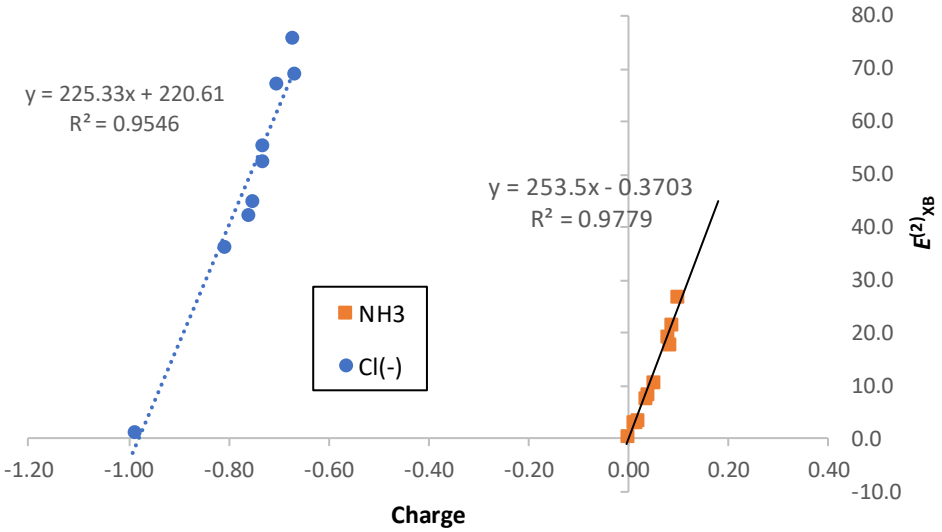

Figure S9. Value of the charge of the Lewis base, in *e*, vs. $E^{(2)}_{XB}$, in kcal·mol^{-1}, for all XB complexes.

Table S1. SAPT electrostatic, exchange, dispersion, and induction energy contributions (E_{el}, E_{ex}, E_d, and E_i, respectively) of HB complexes. Energies in kcal·mol^{-1}.

HB	E_{el}	E_{ex}	E_D	E_i
HFO:NH$_3$	-19,4	21,4	-4,3	-8,1
HClO:NH3	-19,9	22,9	-4,9	-8,6
HBrO:NH3	-19,3	22,4	-5,0	-8,3
HIO:NH3	-18,8	22,3	-5,1	-8,0
HClO$_2$:NH3	-25,1	29,3	-6,6	-10,9
HBrO$_2$:NH3	-25,1	29,4	-6,9	-10,6
HIO$_2$:NH3	-25,7	30,4	-7,4	-10,6
HClO$_3$:NH3	-29,1	37,1	-7,5	-15,5
HBrO$_3$:NH3	-30,4	38,7	-7,9	-16,3
HIO$_3$:NH3	-29,4	37,0	-7,7	-15,7
HClO$_4$:NH$_3$	-95,8	176,3	-27,4	-196,6
HBrO$_4$:NH$_3$	-76,2	140,4	-21,8	-151,4
HIO$_4$:NH$_3$	-121,9	50,2	-9,6	-29,0
HFO:Cl-	-30,9	26,8	-5,5	-14,6
HClO:Cl-	-31,2	30,4	-6,5	-17,4
HBrO:Cl-	-30,5	30,8	-6,7	-17,9
HIO:Cl-	-30,1	31,6	-7,2	-19,2
HClO$_2$:Cl-	-40,1	38,4	-7,7	-23,7
HBrO$_2$:Cl-	-39,4	37,5	-7,7	-22,9
HIO$_2$:Cl-	-39,4	36,6	-8,1	-22,7
HClO$_3$:Cl$^-$	-60,1	92,9	-15,3	-107,9
HBrO$_3$:Cl$^-$	-57,5	88,7	-14,7	-100,7
HIO$_3$:Cl$^-$	-51,8	75,7	-12,7	-73,3
HClO$_4$:Cl$^-$	-66,6	87,3	-15,4	-135,6
HBrO$_4$:Cl$^-$	-66,3	86,6	-15,3	-138,3
HIO$_4$:Cl$^-$	-66,1	87,6	-15,3	-135,2

Table S2. SAPT electrostatic, exchange, dispersion, and induction energy contributions (E_{el}, E_{ex}, E_d, and E_i, respectively) of XB complexes. Energies in kcal·mol^{-1}.

XB	E_{el}	E_{ex}	E_D	E_i
HClO:NH3	-11,9	18,3	-4,2	-4,9
HBrO:NH3	-22,0	31,8	-5,9	-9,5
HIO:NH3	-30,4	33,5	-7,2	-8,9
$HClO_2$:NH3	-8,6	10,3	-3,2	-2,1
$HBrO_2$:NH3	-16,6	21,0	-4,9	-5,5
HIO_2:NH3	-32,5	37,3	-7,7	-10,4
$HClO_3$:NH3	-10,6	12,2	-3,7	-2,5
$HBrO_3$:NH3	-18,9	22,9	-5,3	-6,0
HIO_3:NH3	-37,4	42,6	-8,4	-13,0
$HClO_4$:NH3	-4,2	5,7	-2,8	-0,6
$HBrO_4$:NH3	-16,3	21,0	-5,4	-4,0
HIO_4:NH3	-76,4	96,3	-13,6	-34,2
HClO:Cl-	-39,7	69,8	-9,9	-34,4
HBrO:Cl-	-49,3	73,8	-10,3	-37,0
HIO:Cl-	-57,7	59,0	-10,6	-27,7
$HClO_2$:Cl-	-38,2	53,2	-8,3	-24,1
$HBrO_2$:Cl-	-51,2	67,1	-9,7	-31,9
HIO_2:Cl-	-66,2	65,4	-11,0	-30,4
$HClO_3$:Cl$^-$	-38,8	46,3	-7,9	-19,7
$HBrO_3$:Cl-	-56,1	68,4	-10,1	-32,0
HIO_3:Cl$^-$	-77,3	75,6	-12,0	-35,8
$HClO_4$:Cl-	-9,4	14,2	-4,4	-4,5
$HBrO_4$:Cl-	-80,8	114,2	-14,9	-56,3
HIO_4:Cl-	-110,5	123,5	-16,7	-66,9