

Supplementary Information for:

Cation-Cation and Anion-Anion Complexes Stabilized by Halogen Bonds

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Contents of Supplementary Information:

Table S1. Molecular graph and geometry of the complexes calculated at M06-2x/aug-cc-pVTZ computational level.

Table S2. Difference between the binding energy of hydrogen-bonded (HB) and halogen-bonded cation-cation complexes (E_{rel} in $\text{kJ}\cdot\text{mol}^{-1}$). Negative values indicate that HB is more stable than halogen-bonded systems.

Table S3. Basis set superposition error (BSSE in $\text{kJ}\cdot\text{mol}^{-1}$) for selected ion-ion complexes and their corresponding transition states (TS).

Table S4. Relative binding energies of complexes **1** $[\text{NH}_3^+, \text{N}]:\text{XNH}_3^+$ and **4** $[\text{CO}_2^-, \text{NI}]:\text{Y}^-$ with three explicit water molecules. Complex A shows halogen bond and complex B shows a water molecule linking the two charged systems.

Table S5. Electron density (ρ_{BCP}), Laplacian ($\nabla^2\rho_{\text{BCP}}$) and total electron density energy (H_{BCP}), in a.u., for the intermolecular bond critical point in all complexes in gas phase.

Table S6. DF-DFT-symmetry-adapted perturbation theory (SAPT) electrostatic, exchange, induction, and Hartree-Fock higher-order energy contributions (E_{el} , E_{exch} , E_{i} , and δHF , respectively) of ion-ion complexes. Energies in $\text{kJ}\cdot\text{mol}^{-1}$.

Table S7. CSD reference codes, contact distances (in Å) and type of intermolecular contact.

Figure S1. Energy (kJ/mol) dissociation profile with BSSE and without BSSE correction of **1** $[\text{NH}_3(+), \text{N}]:\text{ClNH}_3(+)$ vs. the $\text{N}\cdots\text{Cl}$ distance (Å) (top) and Energy (kJ/mol) dissociation profile of **1** $[\text{CO}_2(-), \text{Cl}]:\text{F}(-)$ vs. the $\text{I}\cdots\text{F}(-)$ distance (Å) (bottom).

Figure S2. Binding energy along the dissociation path. E_{b} in $\text{kJ}\cdot\text{mol}^{-1}$ and distances in Å.

Figure S3. Corrected binding energy along the dissociation path. E_{corr} in $\text{kJ}\cdot\text{mol}^{-1}$ and distances in Å.

Figure S4. Representation of the binding energy in water ($E_{\text{H}_2\text{O}}$, $\text{kJ}\cdot\text{mol}^{-1}$) versus the binding energy in gas phase (E_{b} , $\text{kJ}\cdot\text{mol}^{-1}$) for cation-cation complexes.

Figure S5. Binding energy along the dissociation path of $\mathbf{3}[\text{CO}_2^-, \text{C-Br}]:\text{F}^-$ in water. $E_{\text{H}_2\text{O}}$ in $\text{kJ}\cdot\text{mol}^{-1}$ and distances in \AA .

Figure S6. Schematic representation of the explicit solvent complexes under study.

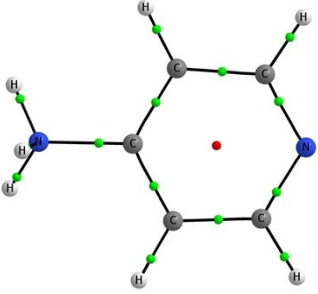
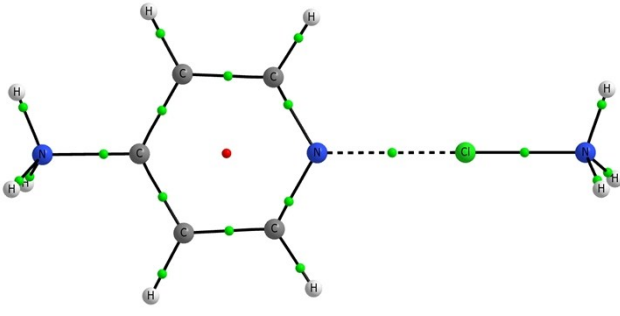
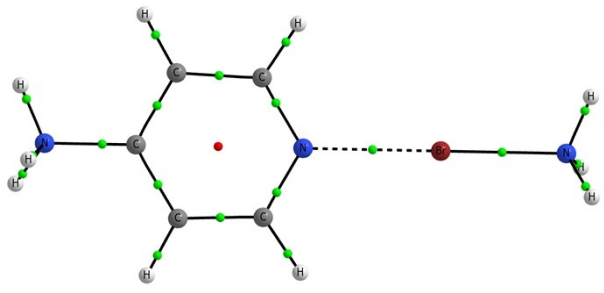
Figure S7. Exponential relationship between $\text{X}\cdots\text{Y}^-$ intermolecular distance and the electron density and laplacian at the BCP (ρ and $\nabla^2\rho$, respectively, in a.u.) for the anion-anion complexes in gas phase.

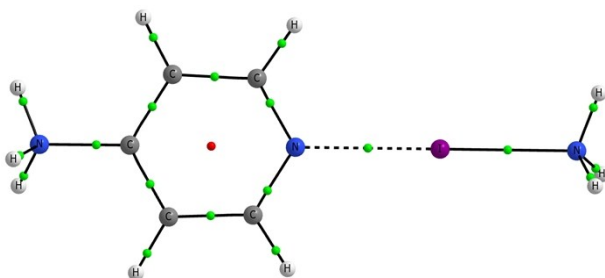
Figure S8. Exponential relationship between $\text{X}\cdots\text{Y}^-$ intermolecular distance and the electron density and laplacian at the BCP (ρ and $\nabla^2\rho$, respectively, in a.u.) for the anion-anion complexes in water.

Figure S9. Corrected binding energy (E_{corr} , $\text{kJ}\cdot\text{mol}^{-1}$) vs the electrostatic contribution (E_{el} , $\text{kJ}\cdot\text{mol}^{-1}$) for anion-anion complexes in gas phase.

Figure S10. Corrected binding energy (E_{corr} , $\text{kJ}\cdot\text{mol}^{-1}$) vs the induction contribution ($E_{\text{i}}+\delta\text{HF}$, $\text{kJ}\cdot\text{mol}^{-1}$) for anion-anion complexes in gas phase.

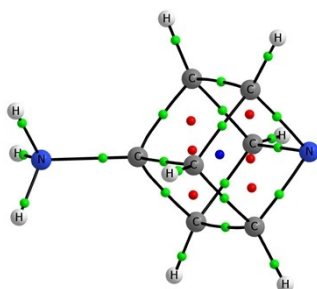
Table S1. Molecular graph and geometry of the complexes calculated at M06-2x/aug-cc-pVTZ computational level.

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	<p>1[NH₃⁺,N]:ClNH₃⁺ C,0.4470959879,-1.1475898563,0.0325729689 C,1.8334051009,-1.2024665067,0.0354782266 C,2.502039314,0.004438342,-0.0020100317 C,1.8360615951,1.2100116527,-0.040519784 C,0.4471975225,1.1574490246,-0.0400154573 N,-0.2132499385,0.0062912907,-0.0042835378 H,-0.1440371859,-2.0538244551,0.0604979015 H,2.3440474806,-2.1561393171,0.0658367387 H,2.345868522,2.1641795256,-0.0702404352 H,-0.1415642088,2.0652467066,-0.0692049901 Cl,-2.4806933215,0.0024187665,-0.0048321545 N,-4.3142790012,-0.0050319983,-0.0044853307 H,-4.652461084,-0.3992352809,0.8753879252 H,-4.6586103105,0.9517205595,-0.1035313007 H,-4.6518032034,-0.5706934564,-0.7855203111 N,3.9861499977,-0.0034306282,0.0012902565 H,4.3559404918,-0.4322239626,0.8582111022 H,4.3594224632,-0.5330189168,-0.7955177923 H,4.3673437782,0.9466155102,-0.0559389943</p>
	<p>1[NH₃⁺,N]:BrNH₃⁺ C,-0.6928012663,-0.8360207735,-0.0456363405 C,0.6933805304,-0.8341687111,-0.0505528194 C,1.3158911647,0.3971579417,-0.0002684412 C,0.6043431104,1.5763423939,0.0530000432 C,-0.7804884188,1.4747781646,0.0536587265 N,-1.392656464,0.2957589043,0.0052082344 H,-1.2532975893,-1.761005976,-0.0832241343 H,1.2391467454,-1.7678097237,-0.0925213335 H,1.0765959511,2.5493262609,0.0928978032 H,-1.4074536695,2.356045981,0.0936951027 Br,-3.6229067757,0.2136061738,0.0021261617 N,-5.6598998449,0.1396594687,-0.00352141 H,-6.0088948289,0.093479565,0.9530801452 H,-6.0357393584,0.9727492956,-0.4548569157 H,-5.9758292223,-0.6846410399,-0.5130493773 N,2.7985951512,0.4454678902,-0.0039298319 H,3.1915528111,-0.0524619284,0.8043810306 H,3.185332377,0.0121719287,-0.8514990272 H,3.1448998668,1.4101408245,0.0323866434</p>



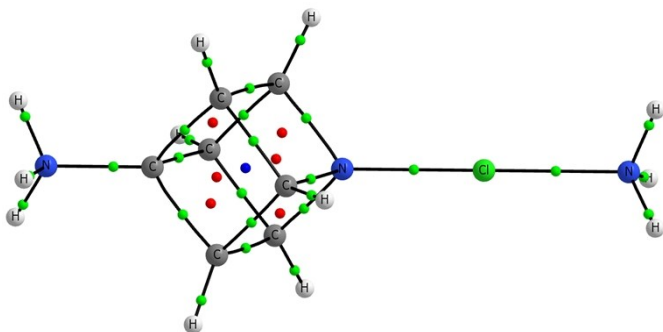
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 N,0.6656463798,0.0053277307,0.0035899602
 H,0.7384249199,-2.058421688,0.0433528991
 H,3.2232254878,-2.1571727265,0.0399768525
 H,3.2227047379,2.1657226613,-0.0433908594
 H,0.7387152115,2.0679113896,-0.0362031665
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 N,-3.9512099722,-0.0031663727,-0.0114150417
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 H,-4.3061856771,-0.7695556913,-0.5808534658
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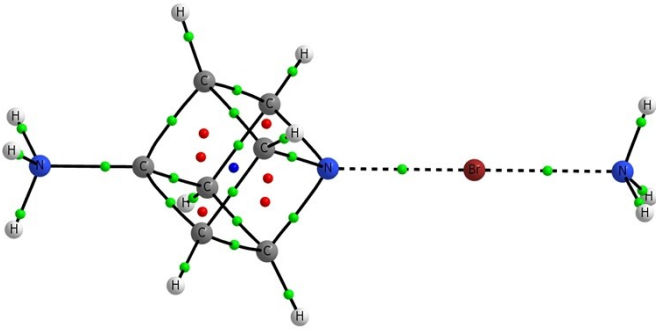
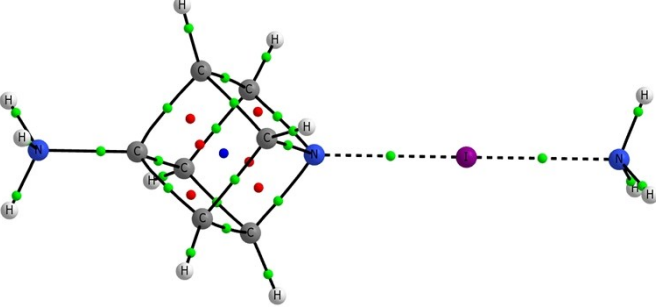
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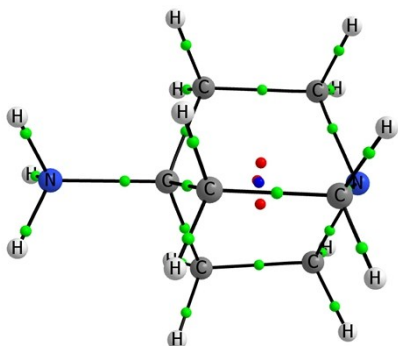
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 N,3.7135561555,-0.0006308258,0.00125272
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2[NH₃⁺,N]:CINH₃⁺

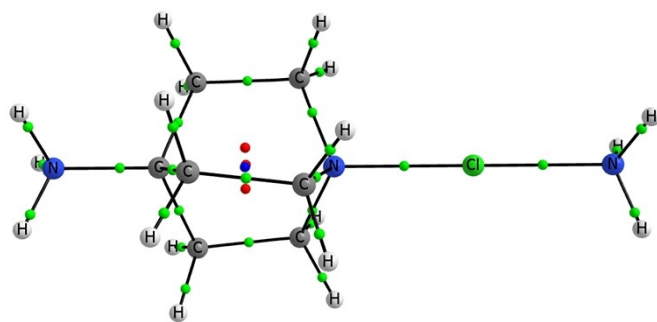
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 C,-1.6444310637,0.660179109,-0.5725461663
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 H,-2.3042737674,1.0643876372,-1.3318920019
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	<p>2[NH₃⁺,N]:BrNH₃⁺ N,-0.3777008414,-0.0017722903,0.0008369337 C,0.4988434918,0.8845266395,0.8783185999 C,0.4995000043,0.3165879437,-1.2045967557 C,1.3953848821,1.2405219763,-0.3376203062 C,0.5005651632,-1.2039097753,0.3288400919 C,1.396568336,-0.9135092891,-0.9047794734 C,1.3964723107,-0.3274640515,1.2440454504 C,2.2775518089,0.0002303735,0.0005765602 H,0.0282940185,1.5774051688,1.5662672465 H,0.0296063421,0.5645720939,-2.1491378708 H,1.7391682037,2.2324352756,-0.6080462119 H,0.0314883038,-2.1463959902,0.586055327 H,1.7413288422,-1.6430033411,-1.6287472235 H,1.7419511044,-0.5886100145,2.237864256 N,3.7635145737,0.0008779576,0.0004723955 H,4.1402378551,-0.9198447684,0.2528015857 H,4.1395236912,0.6801943465,0.6716864385 H,4.1391351715,0.2431450742,-0.9234750907 Br,-2.4842140751,-0.0011382102,0.0002353311 N,-4.6157355442,-0.0002429799,-0.0012922013 H,-4.9657598734,-0.5650026891,-0.7715327789 H,-4.9669862223,-0.3845008145,0.872661865 H,-4.9651075468,0.9493643643,-0.105804169</p>
	<p>2[NH₃⁺,N]:INH₃⁺ C,1.3292910366,-1.1519571007,0.0247275912 C,2.714079731,-1.2023172362,0.0227441661 C,3.3833482327,0.0047452408,-0.0022281271 C,2.7154955401,1.2098725548,-0.0237733358 C,1.3282372168,1.1604445889,-0.019852361 N,0.6656463798,0.0053277307,0.0035899602 H,0.7384249199,-2.058421688,0.0433528991 H,3.2232254878,-2.1571727265,0.0399768525 H,3.2227047379,2.1657226613,-0.0433908594 H,0.7387152115,2.0679113896,-0.0362031665 I,-1.7089591328,0.0024262438,-0.0009719057 N,-3.9512099722,-0.0031663727,-0.0114150417 H,-4.3172727179,-0.112613492,0.9328557593 H,-4.3118252831,0.8695862964,-0.3931883688 H,-4.3061856771,-0.7695556913,-0.5808534658 N,4.8666635694,-0.0028832096,-0.0059157403 H,5.2408813723,-0.4639484876,0.8326276006 H,5.2365081286,-0.5024159101,-0.8241006918 H,5.2489992187,0.9485132084,-0.029059765</p>



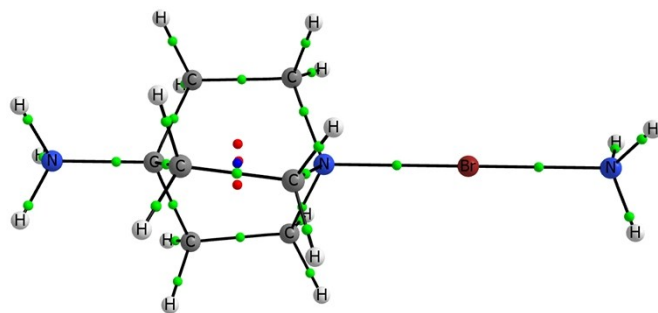
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 H,-2.4165351886,0.7640460918,2.0213861057
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 H,-0.0174666698,-1.6844021725,1.218113789
 H,-0.0914894087,-2.0072985903,-0.5085559165
 C,-2.0121101049,-1.3975875676,0.3558958379
 H,-2.3460410112,-1.6686470847,1.3600525482
 H,-2.414429796,-2.1323904435,-0.3449965327
 N,-4.0224229269,-0.0021061296,0.0001601474
 H,-4.3830202182,-0.6585028664,-0.6971911349
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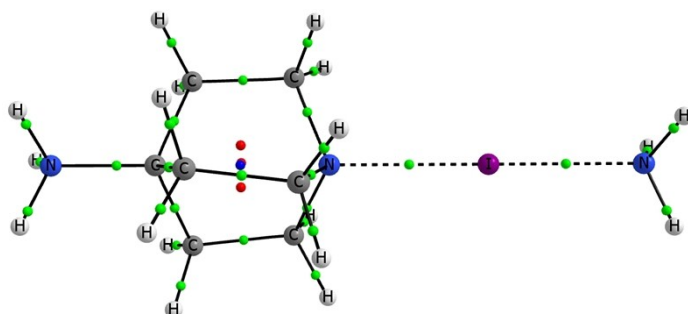
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 H,-2.2598113353,-0.4649817096,-2.097339969
 H,-0.1670320094,1.5464362188,-1.3862269987
 H,0.0440328595,-0.0566751717,-2.0909852149
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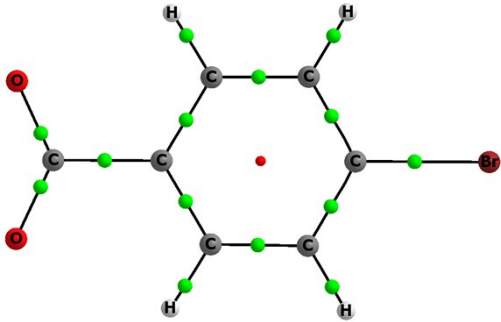
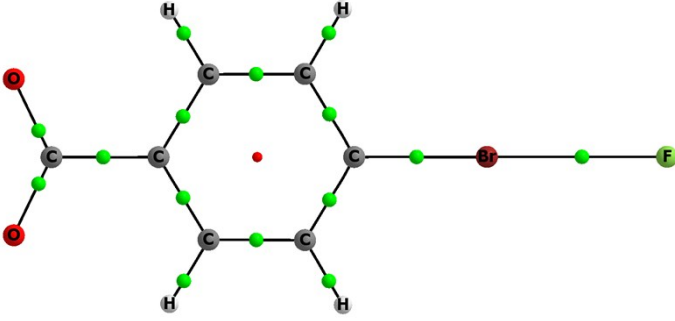
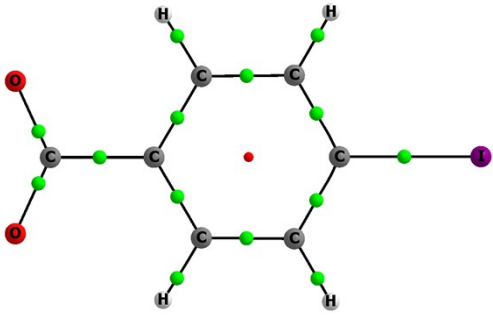
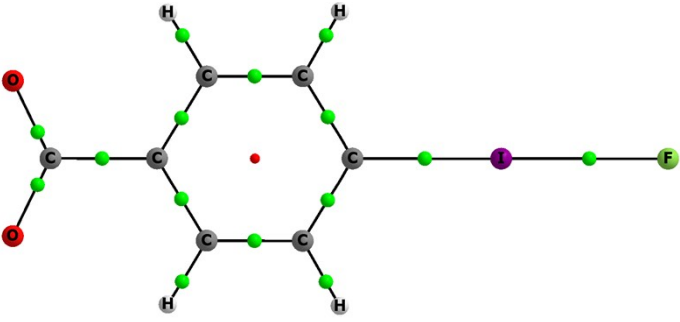
3[NH₃⁺, N]:BrNH₃⁺

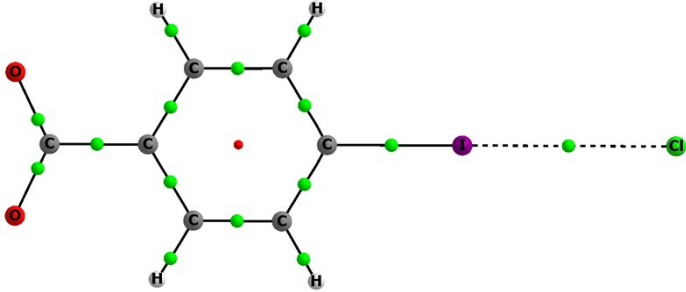
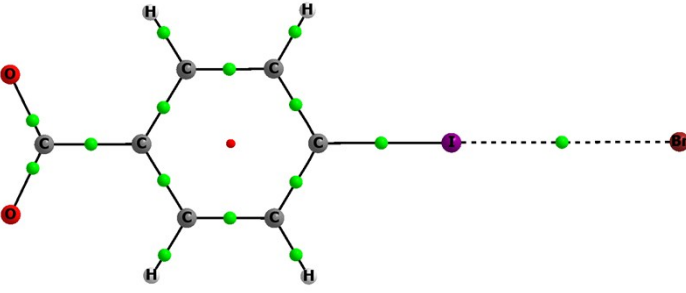
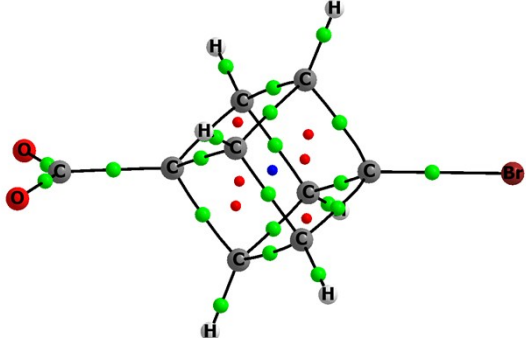
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 C,0,-2.0427203002,-1.3338722,0.5460495736
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 H,0,-2.3043735625,-1.432221864,1.6007811074
 C,0,-0.5048124142,-1.3557200448,0.3606145167
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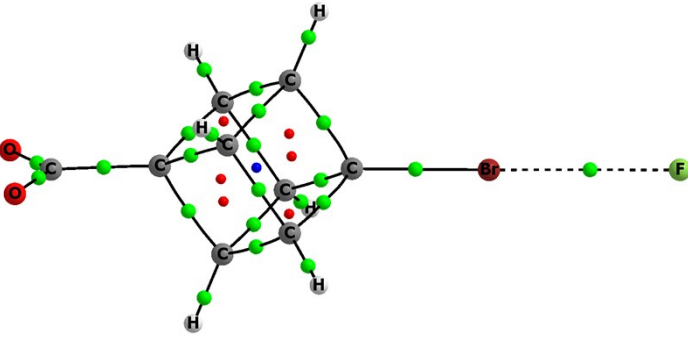
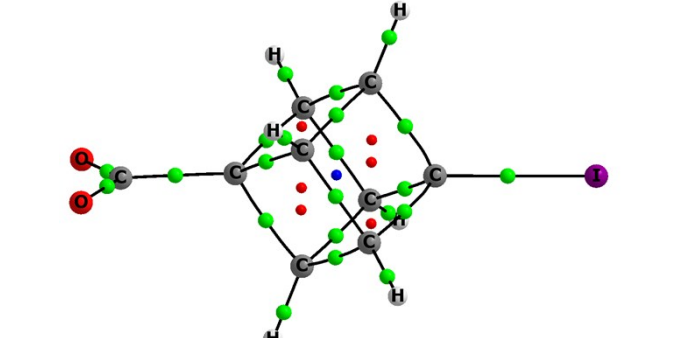
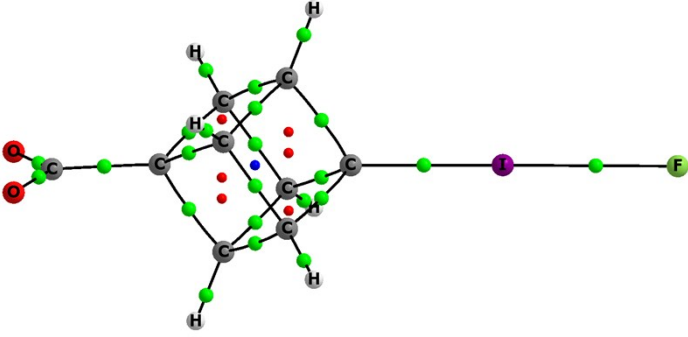


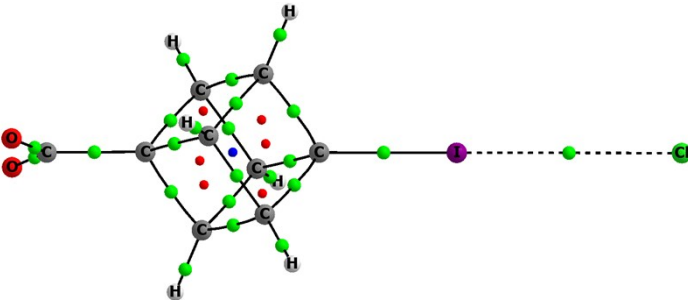
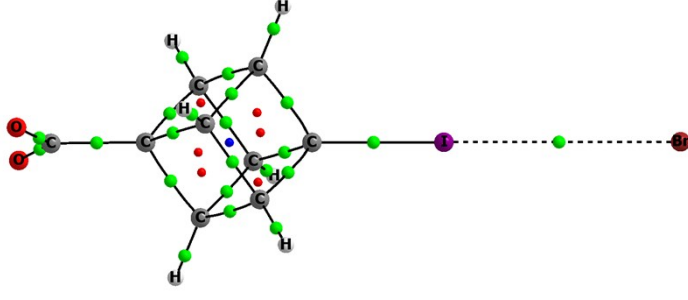
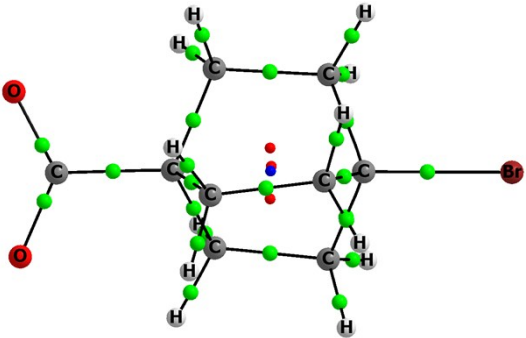
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 C,-0.895863,0.376051,-1.350307
 H,-2.884851,1.077941,-1.883251
 H,-2.688666,-0.669622,-2.039418
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 C,-0.895749,0.981694,0.999652
 H,-0.605815,0.619363,1.984364
 H,-0.393854,1.930827,0.827273
 C,-0.894185,-1.356204,0.348939
 H,-0.391059,-1.680988,1.25666
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 N,-4.450601,-0.00199,0.001175
 H,-4.822731,-0.725575,-0.622288
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 I,1.93144,0.000836,-0.000098
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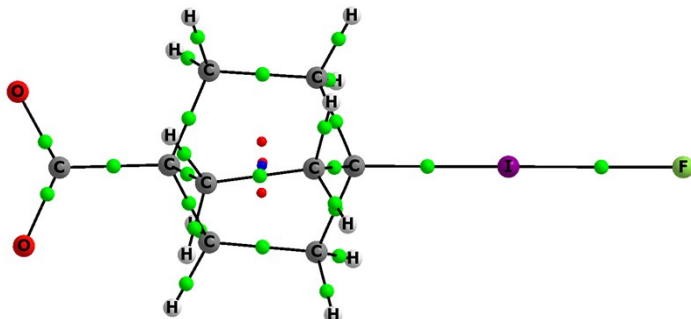
	<p>H,4.579096,-0.351458,0.88688</p> <p>1[CO₂⁻,C-Br]</p> <table border="1"> <tbody> <tr><td>C</td><td>0.00000000</td><td>0.00000000</td><td>-3.37785200</td></tr> <tr><td>O</td><td>0.00000000</td><td>1.12878500</td><td>-3.90236400</td></tr> <tr><td>O</td><td>0.00000000</td><td>-1.12878500</td><td>-3.90236400</td></tr> <tr><td>C</td><td>0.00000000</td><td>0.00000000</td><td>-1.82875900</td></tr> <tr><td>C</td><td>0.00000000</td><td>-1.19549700</td><td>-1.12021500</td></tr> <tr><td>C</td><td>0.00000000</td><td>1.19549700</td><td>-1.12021500</td></tr> <tr><td>C</td><td>0.00000000</td><td>-1.20964900</td><td>0.26906300</td></tr> <tr><td>H</td><td>0.00000000</td><td>-2.11363300</td><td>-1.69299700</td></tr> <tr><td>C</td><td>0.00000000</td><td>1.20964900</td><td>0.26906300</td></tr> <tr><td>H</td><td>0.00000000</td><td>2.11363300</td><td>-1.69299700</td></tr> <tr><td>C</td><td>0.00000000</td><td>0.00000000</td><td>0.94285700</td></tr> <tr><td>H</td><td>0.00000000</td><td>-2.13900300</td><td>0.82179700</td></tr> <tr><td>H</td><td>0.00000000</td><td>2.13900300</td><td>0.82179700</td></tr> <tr><td>Br</td><td>0.00000000</td><td>0.00000000</td><td>2.85647400</td></tr> </tbody> </table>	C	0.00000000	0.00000000	-3.37785200	O	0.00000000	1.12878500	-3.90236400	O	0.00000000	-1.12878500	-3.90236400	C	0.00000000	0.00000000	-1.82875900	C	0.00000000	-1.19549700	-1.12021500	C	0.00000000	1.19549700	-1.12021500	C	0.00000000	-1.20964900	0.26906300	H	0.00000000	-2.11363300	-1.69299700	C	0.00000000	1.20964900	0.26906300	H	0.00000000	2.11363300	-1.69299700	C	0.00000000	0.00000000	0.94285700	H	0.00000000	-2.13900300	0.82179700	H	0.00000000	2.13900300	0.82179700	Br	0.00000000	0.00000000	2.85647400				
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Cl	0.00000000	0.00000000	5.14007000																																																																										
	<table> <tbody> <tr><td colspan="4">1[CO₂⁻,C-I]:Br⁻</td></tr> <tr><td>C</td><td>0.00000000</td><td>0.00000000</td><td>-5.37355600</td></tr> <tr><td>O</td><td>0.00000000</td><td>1.12586500</td><td>-5.91172300</td></tr> <tr><td>O</td><td>0.00000000</td><td>-1.12586500</td><td>-5.91172300</td></tr> <tr><td>C</td><td>0.00000000</td><td>0.00000000</td><td>-3.82792700</td></tr> <tr><td>C</td><td>0.00000000</td><td>-1.19186800</td><td>-3.11201200</td></tr> <tr><td>C</td><td>0.00000000</td><td>1.19186800</td><td>-3.11201200</td></tr> <tr><td>C</td><td>0.00000000</td><td>-1.20023900</td><td>-1.72147900</td></tr> <tr><td>H</td><td>0.00000000</td><td>-2.11451900</td><td>-3.67812400</td></tr> <tr><td>C</td><td>0.00000000</td><td>1.20023900</td><td>-1.72147900</td></tr> <tr><td>H</td><td>0.00000000</td><td>2.11451900</td><td>-3.67812400</td></tr> <tr><td>C</td><td>0.00000000</td><td>0.00000000</td><td>-1.02082400</td></tr> <tr><td>H</td><td>0.00000000</td><td>-2.13705400</td><td>-1.17906500</td></tr> <tr><td>H</td><td>0.00000000</td><td>2.13705400</td><td>-1.17906500</td></tr> <tr><td>I</td><td>0.00000000</td><td>0.00000000</td><td>1.09904200</td></tr> <tr><td>Br</td><td>0.00000000</td><td>0.00000000</td><td>4.72538400</td></tr> </tbody> </table>	1[CO₂⁻,C-I]:Br⁻				C	0.00000000	0.00000000	-5.37355600	O	0.00000000	1.12586500	-5.91172300	O	0.00000000	-1.12586500	-5.91172300	C	0.00000000	0.00000000	-3.82792700	C	0.00000000	-1.19186800	-3.11201200	C	0.00000000	1.19186800	-3.11201200	C	0.00000000	-1.20023900	-1.72147900	H	0.00000000	-2.11451900	-3.67812400	C	0.00000000	1.20023900	-1.72147900	H	0.00000000	2.11451900	-3.67812400	C	0.00000000	0.00000000	-1.02082400	H	0.00000000	-2.13705400	-1.17906500	H	0.00000000	2.13705400	-1.17906500	I	0.00000000	0.00000000	1.09904200	Br	0.00000000	0.00000000	4.72538400												
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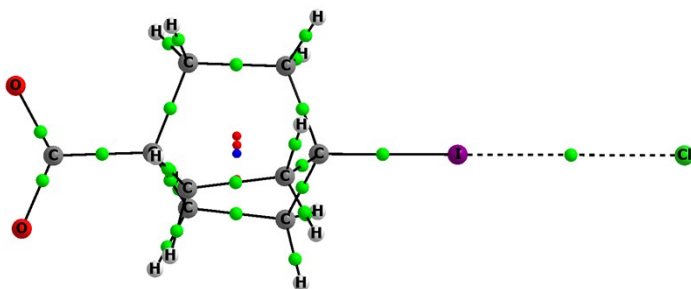
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C	-3.23669600	-0.01012800	0.00145700																																																																																																						
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O	-3.72371900	-1.15911300	0.02245100																																																																																																						
Br	2.90155600	-0.00845300	0.01250500																																																																																																						
	<table> <tbody> <tr><td colspan="4">3[CO₂⁻,C-Br]:F⁻</td></tr> <tr><td>C</td><td>0.53774800</td><td>0.00718300</td><td>-0.00732300</td></tr> <tr><td>C</td><td>-2.08471300</td><td>0.02852000</td><td>-0.02563300</td></tr> <tr><td>C</td><td>0.01149700</td><td>1.38701800</td><td>-0.40539500</td></tr> <tr><td>C</td><td>0.00415200</td><td>-1.02310800</td><td>-1.00277200</td></tr> <tr><td>C</td><td>-0.00545900</td><td>-0.33762000</td><td>1.37969200</td></tr> <tr><td>C</td><td>-1.52365800</td><td>1.44140400</td><td>-0.19825500</td></tr> <tr><td>C</td><td>-1.52722600</td><td>-0.84572700</td><td>-1.15720300</td></tr> <tr><td>C</td><td>-1.54080900</td><td>-0.53272500</td><td>1.29861900</td></tr> <tr><td>H</td><td>0.27735000</td><td>1.56743400</td><td>-1.45028700</td></tr> <tr><td>H</td><td>0.52093000</td><td>2.14975700</td><td>0.18545500</td></tr> <tr><td>H</td><td>0.25258100</td><td>-2.02148400</td><td>-0.63391000</td></tr> <tr><td>H</td><td>0.51746800</td><td>-0.90095400</td><td>-1.95775400</td></tr> <tr><td>H</td><td>0.25622500</td><td>0.47277000</td><td>2.06447400</td></tr> <tr><td>H</td><td>0.49041000</td><td>-1.23742100</td><td>1.74730400</td></tr> <tr><td>H</td><td>-1.78071900</td><td>2.02879600</td><td>0.68515200</td></tr> <tr><td>H</td><td>-2.02291500</td><td>1.92574700</td><td>-1.03764600</td></tr> <tr><td>H</td><td>-1.75899300</td><td>-0.36628600</td><td>-2.11340700</td></tr> <tr><td>H</td><td>-2.04833100</td><td>-1.80224500</td><td>-1.13974000</td></tr> <tr><td>H</td><td>-1.81217800</td><td>-1.58816600</td><td>1.35522300</td></tr> <tr><td>H</td><td>-2.03823600</td><td>-0.03015600</td><td>2.13183300</td></tr> <tr><td>C</td><td>-3.64591200</td><td>-0.01441200</td><td>0.00559200</td></tr> <tr><td>O</td><td>-4.23919900</td><td>1.08567300</td><td>0.03189700</td></tr> <tr><td>O</td><td>-4.14692600</td><td>-1.16137000</td><td>0.02683600</td></tr> <tr><td>Br</td><td>2.50862800</td><td>-0.00216900</td><td>0.00509200</td></tr> <tr><td>F</td><td>5.23107900</td><td>-0.01994300</td><td>0.02125400</td></tr> </tbody> </table>	3[CO₂⁻,C-Br]:F⁻				C	0.53774800	0.00718300	-0.00732300	C	-2.08471300	0.02852000	-0.02563300	C	0.01149700	1.38701800	-0.40539500	C	0.00415200	-1.02310800	-1.00277200	C	-0.00545900	-0.33762000	1.37969200	C	-1.52365800	1.44140400	-0.19825500	C	-1.52722600	-0.84572700	-1.15720300	C	-1.54080900	-0.53272500	1.29861900	H	0.27735000	1.56743400	-1.45028700	H	0.52093000	2.14975700	0.18545500	H	0.25258100	-2.02148400	-0.63391000	H	0.51746800	-0.90095400	-1.95775400	H	0.25622500	0.47277000	2.06447400	H	0.49041000	-1.23742100	1.74730400	H	-1.78071900	2.02879600	0.68515200	H	-2.02291500	1.92574700	-1.03764600	H	-1.75899300	-0.36628600	-2.11340700	H	-2.04833100	-1.80224500	-1.13974000	H	-1.81217800	-1.58816600	1.35522300	H	-2.03823600	-0.03015600	2.13183300	C	-3.64591200	-0.01441200	0.00559200	O	-4.23919900	1.08567300	0.03189700	O	-4.14692600	-1.16137000	0.02683600	Br	2.50862800	-0.00216900	0.00509200	F	5.23107900	-0.01994300	0.02125400
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I	2.64106900	-0.00651500	0.00819700																																																																																																						



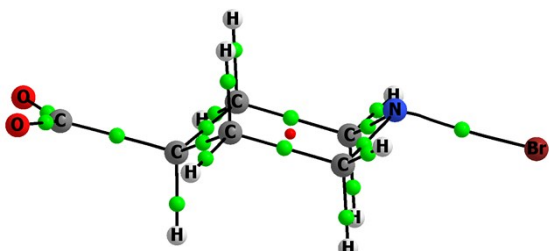
3[CO₂⁻,C-I]:F⁻

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C	-2.48769900	0.02881400	-0.02583300
C	-0.38930900	1.38600300	-0.40593200
C	-0.39632400	-1.02107900	-1.00104700
C	-0.40584200	-0.33515100	1.37794400
C	-1.92590600	1.44127800	-0.19851600
C	-1.92903300	-0.84484400	-1.15712800
C	-1.94253700	-0.53179800	1.29802800
H	-0.12966000	1.56884700	-1.45279000
H	0.11296300	2.15957800	0.17896400
H	-0.15336300	-2.02238000	-0.63420300
H	0.11048300	-0.90756800	-1.96154900
H	-0.15041400	0.47526600	2.06638500
H	0.08310600	-1.23528000	1.75640200
H	-2.18272800	2.02835700	0.68565100
H	-2.42633600	1.92635100	-1.03740400
H	-2.16043600	-0.36423000	-2.11332500
H	-2.45067400	-1.80152300	-1.14139500
H	-2.21306800	-1.58782100	1.35438700
H	-2.44140700	-0.03010700	2.13157900
C	-4.04863400	-0.01467500	0.00538900
O	-4.64437600	1.08478900	0.03169600
O	-4.55144700	-1.16148400	0.02653200
I	2.34563000	-0.00317800	0.00468900
F	4.83449400	-0.01419500	0.01551900



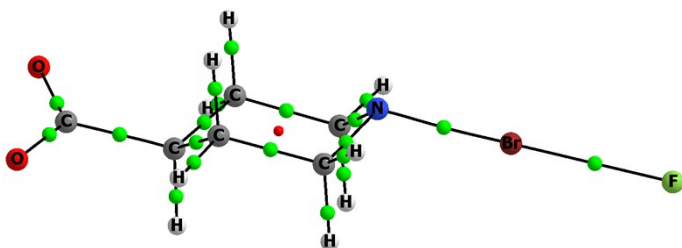
3[CO₂⁻,C-I]:Cl⁻

C	-0.23083100	0.00913000	-0.00830900
C	-2.84489900	0.02783500	-0.02416200
C	-0.75099400	1.39242400	-0.40326900
C	-0.75655700	-1.02117400	-1.00797900
C	-0.76447200	-0.34072900	1.38111300
C	-2.28733500	1.44158700	-0.19394200
C	-2.28943200	-0.84331700	-1.15782700
C	-2.30102700	-0.53574200	1.29801500
H	-0.48946300	1.57607500	-1.44835400
H	-0.24805700	2.15903800	0.18779700
H	-0.50883100	-2.02093000	-0.64327300
H	-0.25058100	-0.89760300	-1.96621100
H	-0.50562900	0.46722500	2.06948200
H	-0.27375000	-1.24284200	1.74878100
H	-2.54337800	2.02711700	0.69061900
H	-2.78612700	1.92701200	-1.03261000
H	-2.52208000	-0.36346200	-2.11316700
H	-2.80776900	-1.80113800	-1.14013200
H	-2.57076300	-1.59139500	1.35319700
H	-2.79598200	-0.03448000	2.13302500
C	-4.40650300	-0.01714400	0.00780300
O	-4.99840200	1.08269400	0.03446200
O	-4.90276800	-1.16531800	0.02874500
I	1.95183100	-0.00017900	0.00144700
Cl	5.52100300	-0.01243200	0.01351900



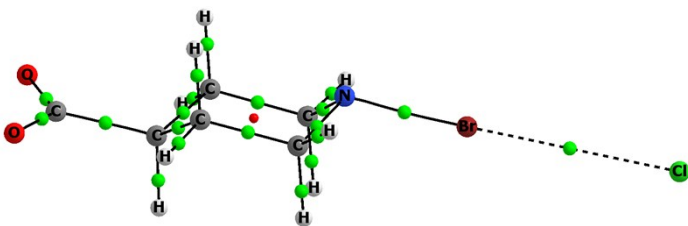
4[CO₂⁻,N-Br]

N	-0.45239700	0.95418600	0.00000000
C	0.15447200	0.38667000	1.21272200
C	-0.10315700	-1.11580000	1.24024500
C	0.45307400	-1.79754900	0.00000000
C	-0.10315700	-1.11580000	-1.24024500
C	0.15447200	0.38667000	-1.21272200
H	0.34151000	-1.55023200	2.13437000
H	1.23689300	0.58193400	1.22835700
H	-0.29509700	0.88266800	2.07258700
H	1.54412300	-1.66474100	0.00000000
H	0.34151000	-1.55023200	-2.13437000
H	-1.17900600	-1.29755800	-1.30044000
H	1.23689300	0.58193400	-1.22835700
H	-0.29509700	0.88266800	-2.07258700
H	-1.17900600	-1.29755800	1.30044000
C	0.21974100	-3.34381500	0.00000000
O	0.15447200	-3.87256500	-1.12721200
O	0.15447200	-3.87256500	1.12721200
Br	-0.16314800	2.83744600	0.00000000



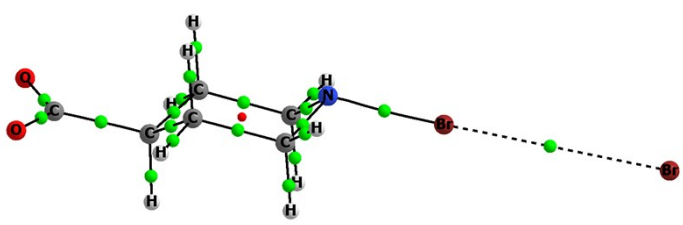
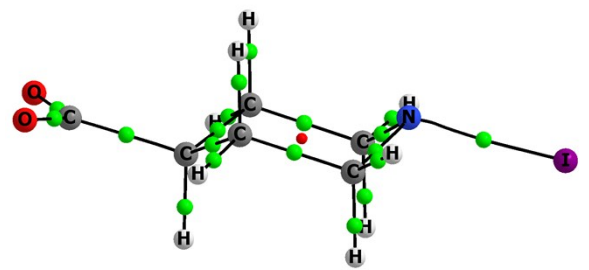
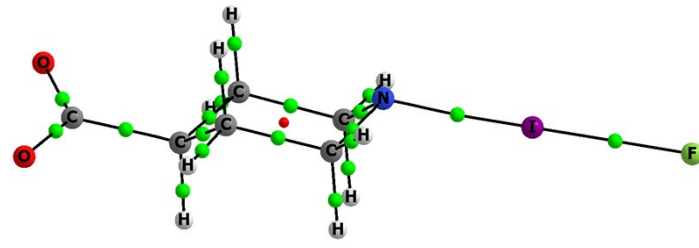
4[CO₂⁻,N-Br]:F⁻

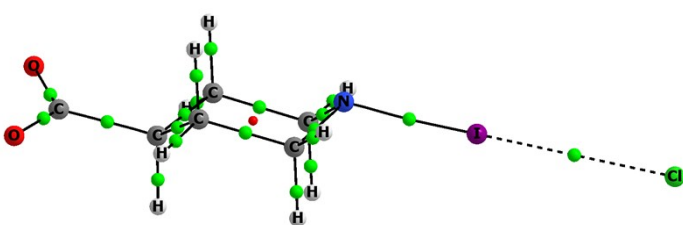
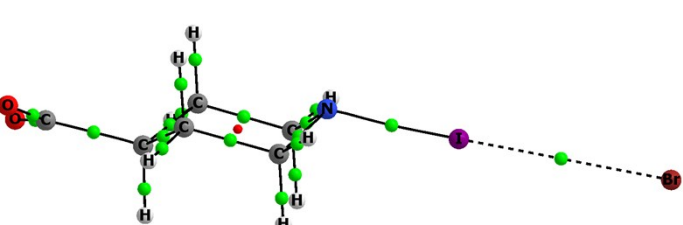
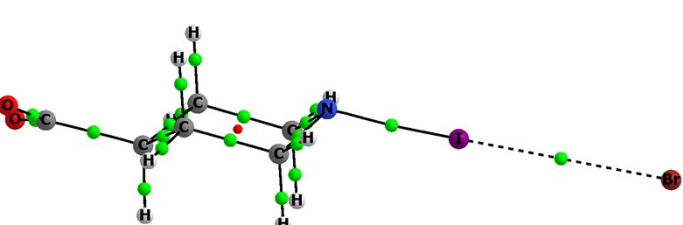
N	-0.56359100	0.05691500	-0.43117300
C	0.05468900	-1.19057300	-0.00376200
C	1.55101800	-1.19220100	-0.30953700
C	2.25688500	-0.01444600	0.35825300
C	1.53903300	1.27113600	-0.02776500
C	0.04227400	1.18201700	0.26858700
H	2.01013000	-2.12386700	0.02312500
H	-0.09218000	-1.34834100	1.08127200
H	-0.44959600	-2.01078100	-0.51822000
H	2.15531000	-0.15343100	1.44357400
H	1.97905500	2.11886100	0.50037600
H	1.69010500	1.45363800	-1.09432400
H	-0.10830800	1.08731900	1.36064600
H	-0.47176800	2.09166600	-0.04775800
H	1.69167500	-1.12220700	-1.39309600
C	3.79077900	-0.01275100	0.07837300
O	4.29480300	1.06244800	-0.31322400
O	4.37198000	-1.10054300	0.29801500
Br	-2.46522300	0.00524100	-0.08418100
F	-4.76875900	-0.05878200	0.28285900



4[CO₂⁻,N-Br]:Cl⁻

N	-0.10874300	0.03622200	-0.46802700
C	0.48695600	-1.20125800	0.03635300
C	1.98594300	-1.21575000	-0.24775400
C	2.68365100	-0.01190100	0.37496100
C	1.98183300	1.25819400	-0.08320700
C	0.48223300	1.19878300	0.19574600
H	2.43310500	-2.13409900	0.13191600
H	0.31603700	-1.29934200	1.12152400
H	-0.01456400	-2.03689100	-0.45254900
H	2.56440800	-0.09301800	1.46480500
H	2.41997600	2.12585200	0.41012400
H	2.14698600	1.38954600	-1.15547200
H	0.30830400	1.15126900	1.28389600
H	-0.02253500	2.08966500	-0.17910700
H	2.14452600	-1.19996100	-1.33018300
C	4.22478700	-0.01336800	0.12695900
O	4.75017800	1.09510700	-0.11049100

	<p>O 4.77996800 -1.12978300 0.22441700</p> <p>Br -1.98937600 0.01192400 -0.16044600</p> <p>Cl -5.24826400 -0.02792400 0.25100500</p>
	<p>4[CO₂⁻,N-Br]:Br⁻</p> <p>N 0.68148700 0.03666500 -0.50082800</p> <p>C 1.26387600 -1.20186800 0.02052600</p> <p>C 2.76710500 -1.21810500 -0.23841400</p> <p>C 3.45499900 -0.01344400 0.39262800</p> <p>C 2.76467600 1.25628400 -0.08293300</p> <p>C 1.26067500 1.20264100 0.17040700</p> <p>H 3.20582200 -2.13608600 0.15144000</p> <p>H 1.07334700 -1.29332000 1.10231200</p> <p>H 0.76888200 -2.03743900 -0.47458200</p> <p>H 3.31665900 -0.08980400 1.48052400</p> <p>H 3.19545400 2.12491700 0.41472800</p> <p>H 2.94866700 1.38343400 -1.15257100</p> <p>H 1.06649900 1.15863700 1.25455400</p> <p>H 0.76426100 2.09186000 -0.21859800</p> <p>H 2.94438000 -1.20650400 -1.31784500</p> <p>C 5.00044900 -0.01678100 0.17109200</p> <p>O 5.53116600 1.09369800 -0.04186800</p> <p>O 5.54984500 -1.13604800 0.26294500</p> <p>Br -1.20093600 0.01696900 -0.22273000</p> <p>Br -4.84972500 -0.01599500 0.16265500</p>
	<p>4[CO₂⁻,N-I]</p> <p>N -0.40848200 0.45195600 0.00000000</p> <p>C 0.20125100 -0.11738200 1.21242700</p> <p>C -0.05474900 -1.62093400 1.23996900</p> <p>C 0.50126900 -2.30264000 0.00000000</p> <p>C -0.05474900 -1.62093400 -1.23996900</p> <p>C 0.20125100 -0.11738200 -1.21242700</p> <p>H 0.39042600 -2.05476500 2.13452700</p> <p>H 1.28483400 0.07424000 1.23199500</p> <p>H -0.24554700 0.37274200 2.07767500</p> <p>H 1.59251900 -2.17062200 0.00000000</p> <p>H 0.39042600 -2.05476500 -2.13452700</p> <p>H -1.13068500 -1.80241900 -1.30007100</p> <p>H 1.28483400 0.07424000 -1.23199500</p> <p>H -0.24554700 0.37274200 -2.07767500</p> <p>H -1.13068500 -1.80241900 1.30007100</p> <p>C 0.26663000 -3.84875200 0.00000000</p> <p>O 0.20125100 -4.37758700 -1.12720500</p> <p>O 0.20125100 -4.37758700 1.12720500</p> <p>I -0.16823800 2.52145000 0.00000000</p>
	<p>4[CO₂⁻,N-F]</p> <p>N -0.13278900 0.05209100 -0.37865000</p> <p>C 0.50488200 -1.19236100 0.01815100</p> <p>C 1.99895300 -1.18860000 -0.30800600</p> <p>C 2.71092300 -0.01392400 0.36031700</p> <p>C 1.98063500 1.27221200 -0.00021400</p> <p>C 0.48727200 1.16884300 0.31632600</p> <p>H 2.46797500 -2.12132800 0.00951400</p> <p>H 0.38427700 -1.37445400 1.10583800</p> <p>H 0.00395300 -2.01644600 -0.49637200</p> <p>H 2.62755300 -0.16593200 1.44545800</p> <p>H 2.42552300 2.11658900 0.53082700</p> <p>H 2.11329500 1.46617800 -1.06719800</p> <p>H 0.36381000 1.07119500 1.41483300</p> <p>H -0.02937500 2.08627100 0.02305700</p>

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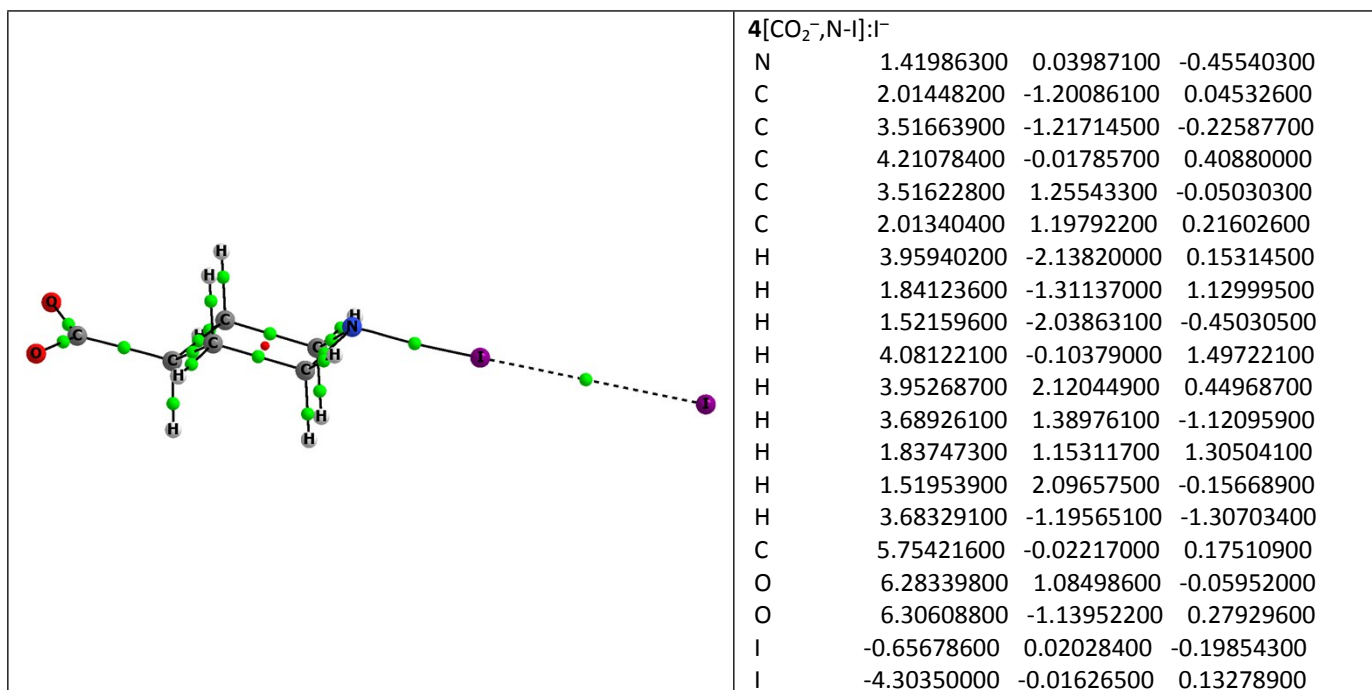


Table S2. Difference between the binding energy of hydrogen-bonded (HB) and halogen-bonded cation-cation complexes (E_{rel} in $\text{kJ}\cdot\text{mol}^{-1}$). Negative values indicate that HB is more stable than halogen-bonded systems.

	E_{rel}
1[NH ₃ (+), N]:ClNH ₃ (+) HB	5.5
1[NH ₃ (+), N]:BrNH ₃ (+) HB	34.5
1[NH ₃ (+), N]:INH ₃ (+) HB	55.4
2[NH ₃ (+), N]:ClNH ₃ (+) HB	-1.1
2[NH ₃ (+), N]:BrNH ₃ (+) HB	49.2
2[NH ₃ (+), N]:INH ₃ (+) HB	74.2
3[NH ₃ (+), N]:ClNH ₃ (+) HB	-1.8
3[NH ₃ (+), N]:BrNH ₃ (+) HB	36.2
3[NH ₃ (+), N]:INH ₃ (+) HB	71.8

Table S3. Basis set superposition error (BSSE in $\text{kJ}\cdot\text{mol}^{-1}$) for selected ion-ion complexes and their corresponding transition states (TS).

	Minimum	TS
1[NH ₃ ⁺ ,N]:ClNH ₃ ⁺	0.9	0.2
1[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	1.4	0.2
1[NH ₃ ⁺ ,N]:INH ₃ ⁺	0.7	0.2
1[CO ₂ ⁻ ,Cl]:F ⁻	0.9	0.1
1[CO ₂ ⁻ ,Cl]:Cl ⁻	0.3	0.1
1[CO ₂ ⁻ ,Cl]:Br ⁻	0.4	0.2

Table S4. Relative binding energies (E_{rel} in $\text{kJ}\cdot\text{mol}^{-1}$) of complexes **1** $[\text{NH}_3^+, \text{N}]:\text{XNH}_3^+$ and **4** $[\text{CO}_2^-, \text{NI}]:\text{Y}^-$ with three explicit water molecules. Complex A shows halogen bond and complex B shows a water molecule linking the two charged systems.

	$E_{rel}(\text{kJ}\cdot\text{mol}^{-1})$
1 $[\text{NH}_3^+, \text{N}]:\text{ClNH}_3^+_{_A}$	0.0
1 $[\text{NH}_3^+, \text{N}]:\text{ClNH}_3^+_{_B}$	16.9
1 $[\text{NH}_3^+, \text{N}]:\text{BrNH}_3^+_{_A}$	0.0
1 $[\text{NH}_3^+, \text{N}]:\text{BrNH}_3^+_{_B}$	12.8
1 $[\text{NH}_3^+, \text{N}]:\text{INH}_3^+_{_A}$	0.0
1 $[\text{NH}_3^+, \text{N}]:\text{INH}_3^+_{_B}$	5.4
4 $[\text{CO}_2^-, \text{NI}]:\text{F}^-_{_A}$	0.0
4 $[\text{CO}_2^-, \text{NI}]:\text{F}^-_{_B}$	6.8
4 $[\text{CO}_2^-, \text{NI}]:\text{Cl}^-_{_A}$	0.0
4 $[\text{CO}_2^-, \text{NI}]:\text{Cl}^-_{_B}$	0.6
4 $[\text{CO}_2^-, \text{NI}]:\text{Br}^-_{_A}$	0.0
4 $[\text{CO}_2^-, \text{NI}]:\text{Br}^-_{_B}$	-0.8
4 $[\text{CO}_2^-, \text{NI}]:\text{I}^-_{_A}$	0.0
4 $[\text{CO}_2^-, \text{NI}]:\text{I}^-_{_B}$	-3.0
1 $[\text{NH}_3^+, \text{N}]:\text{ClNH}_3^+_{_A}$ (PCM)	0.0
1 $[\text{NH}_3^+, \text{N}]:\text{ClNH}_3^+_{_B}$ (PCM)	13.2
4 $[\text{CO}_2^-, \text{NI}]:\text{F}^-_{_A}$ (PCM)	0.0
4 $[\text{CO}_2^-, \text{NI}]:\text{F}^-_{_B}$ (PCM)	8.7

Table S5. Electron density (ρ_{BCP}), Laplacian ($\nabla^2\rho_{\text{BCP}}$) and total electron density energy (H_{BCP}), in a.u., for the intermolecular bond critical point in all complexes in gas phase.

Complex	ρ_{BCP}	$\nabla^2\rho_{\text{BCP}}$	H_{BCP}
1[NH ₃ ⁺ ,N]:CINH ₃ ⁺	0.0627	0.1256	-0.0119
1[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	0.0761	0.1026	-0.0235
1[NH ₃ ⁺ ,N]:INH ₃ ⁺	0.0638	0.1130	-0.0181
2[NH ₃ ⁺ ,N]:CINH ₃ ⁺	0.1171	0.1011	-0.0467
2[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	0.0986	0.0853	-0.0410
2[NH ₃ ⁺ ,N]:INH ₃ ⁺	0.0764	0.1185	-0.0269
3[NH ₃ ⁺ ,N]:CINH ₃ ⁺	0.1148	0.0879	-0.0445
3[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	0.0950	0.0730	-0.0376
3[NH ₃ ⁺ ,N]:INH ₃ ⁺	0.0737	0.0986	-0.0251
1[CO ₂ ⁻ ,C-Br]:F ⁻	0.0262	0.1059	0.0024
1[CO ₂ ⁻ ,C-I]:F ⁻	0.0452	0.1554	-0.0027
1[CO ₂ ⁻ ,C-I]:Cl ⁻	0.0135	0.0388	0.0011
1[CO ₂ ⁻ ,C-I]:Br ⁻	0.0103	0.0271	0.0009
2[CO ₂ ⁻ ,C-Br]:F ⁻	0.0221	0.0882	0.0023
2[CO ₂ ⁻ ,C-I]:F ⁻	0.0400	0.1412	-0.0009
2[CO ₂ ⁻ ,C-I]:Cl ⁻	0.0106	0.0305	0.0011
2[CO ₂ ⁻ ,C-I]:Br ⁻	0.0071	0.0184	0.0008
3[CO ₂ ⁻ ,C-Br]:F ⁻	0.0204	0.0804	0.0022
3[CO ₂ ⁻ ,C-I]:F ⁻	0.0393	0.1382	-0.0008
3[CO ₂ ⁻ ,C-I]:Cl ⁻	0.0095	0.0268	0.0011
4[CO ₂ ⁻ ,N-Br]:F ⁻	0.0468	0.1622	-0.0016
4[CO ₂ ⁻ ,N-Br]:Cl ⁻	0.0125	0.0384	0.0013
4[CO ₂ ⁻ ,N-Br]:Br ⁻	0.0076	0.0216	0.0009
4[CO ₂ ⁻ ,N-I]:F ⁻	0.0609	0.1869	-0.0104
4[CO ₂ ⁻ ,N-I]:Cl ⁻	0.0214	0.0551	0.0001
4[CO ₂ ⁻ ,N-I]:Br ⁻	0.0165	0.0397	0.0004
4[CO ₂ ⁻ ,N-I]:I ⁻	0.0123	0.0275	0.0005

Table S6. DF-DFT-symmetry-adapted perturbation theory (SAPT) electrostatic, exchange, induction, and Hartree-Fock higher-order energy contributions (E_{el} , E_{exch} , E_i , and δHF , respectively) of ion-ion complexes. Energies in $\text{kJ}\cdot\text{mol}^{-1}$.

Comp.	E_{el}	E_{exch}	E_i	δHF
1[NH ₃ ⁺ ,N]:CINH ₃ ⁺	60.7	197.5	-49.8	-46.3
1[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	1.2	290.7	-105.8	-45.1
1[NH ₃ ⁺ ,N]:INH ₃ ⁺	1.5	224.6	-228.2	115.3
1[NH ₃ ⁺ ,N]:CINH ₃ ⁺ (TS)	141.9	1.7	-5.4	-0.3
1[NH ₃ ⁺ ,N]:BrNH ₃ ⁺ (TS)	138.4	0.5	-5.5	-0.4
1[NH ₃ ⁺ ,N]:INH ₃ ⁺ (TS)	140.1	1.1	-5.4	0.0
2[NH ₃ ⁺ ,N]:CINH ₃ ⁺	-106.3	505.7	-179.6	-117.5
2[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	-101.0	441.0	-200.1	-45.3
2[NH ₃ ⁺ ,N]:INH ₃ ⁺	-74.5	296.8	-361.9	225.1
2[NH ₃ ⁺ ,N]:CINH ₃ ⁺ (TS)	135.2	0.5	-3.9	-0.2
2[NH ₃ ⁺ ,N]:BrNH ₃ ⁺ (TS)	133.1	0.3	-3.8	-0.1
2[NH ₃ ⁺ ,N]:INH ₃ ⁺ (TS)	132.7	0.3	-4.4	-0.1
3[NH ₃ ⁺ ,N]:CINH ₃ ⁺	-93.3	504.3	-174.4	-125.9
3[NH ₃ ⁺ ,N]:BrNH ₃ ⁺	-79.3	428.2	-185.2	-54.5
3[NH ₃ ⁺ ,N]:INH ₃ ⁺	-52.5	293.8	-348.5	209.8
3[NH ₃ ⁺ ,N]:CINH ₃ ⁺ (TS)	147.8	0.8	-5.3	-0.2
3[NH ₃ ⁺ ,N]:BrNH ₃ ⁺ (TS)	146.3	0.6	-5.5	-0.3
3[NH ₃ ⁺ ,N]:INH ₃ ⁺ (TS)	145.3	0.4	-6.0	-0.1
1[CO ₂ ⁻ ,C-Br]:F ⁻	127.4	104.9	-56.6	62.3
1[CO ₂ ⁻ ,C-I]:F ⁻	9.8	217.6	-283.2	115.9
1[CO ₂ ⁻ ,C-I]:Cl ⁻	129.7	42.5	-72.5	36.7
1[CO ₂ ⁻ ,C-I]:Br ⁻	135.0	29.8	-56.0	30.7
1[CO ₂ ⁻ ,C-Br]:F ⁻ (TS)	163.2	5.7	-18.7	0.6
1[CO ₂ ⁻ ,C-I]:F ⁻ (TS)	149.6	1.7	-18.4	1.4
1[CO ₂ ⁻ ,C-I]:Cl ⁻ (TS)	146.7	3.4	-18.8	3.7
1[CO ₂ ⁻ ,C-I]:Br ⁻ (TS)	144.8	4.2	-19.1	5.1
2[CO ₂ ⁻ ,C-Br]:F ⁻	152.7	85.0	-52.8	-6.5
2[CO ₂ ⁻ ,C-I]:F ⁻	51.5	192.6	-248.8	94.0
2[CO ₂ ⁻ ,C-I]:Cl ⁻	149.5	31.9	-59.7	26.6
2[CO ₂ ⁻ ,C-I]:Br ⁻	152.4	18.8	-41.9	7.3
2[CO ₂ ⁻ ,C-Br]:F ⁻ (TS)	175.2	8.7	-23.2	1.0
2[CO ₂ ⁻ ,C-I]:F ⁻ (TS)	162.6	2.7	-24.6	2.5
2[CO ₂ ⁻ ,C-I]:Cl ⁻ (TS)	157.6	5.4	-24.2	5.6
2[CO ₂ ⁻ ,C-I]:Br ⁻ (TS)	155.1	8.0	-26.8	3.4
3[CO ₂ ⁻ ,C-Br]:F ⁻	163.5	75.9	-49.3	-5.8
3[CO ₂ ⁻ ,C-I]:F ⁻	59.6	187.2	-240.5	89.9
3[CO ₂ ⁻ ,C-I]:Cl ⁻	156.5	25.5	-51.3	21.5
3[CO ₂ ⁻ ,C-Br]:F ⁻ (TS)	181.0	9.9	-23.7	0.9
3[CO ₂ ⁻ ,C-I]:F ⁻ (TS)	166.7	3.2	-25.3	2.7
3[CO ₂ ⁻ ,C-I]:Cl ⁻ (TS)	161.4	6.9	-26.3	6.8
4[CO ₂ ⁻ ,N-Br]:F ⁻	64.2	221.9	-94.8	-24.9
4[CO ₂ ⁻ ,N-Br]:Cl ⁻	149.3	43.2	-25.6	-5.1
4[CO ₂ ⁻ ,N-Br]:Br ⁻	153.2	22.8	-17.8	-2.4

4[CO ₂ ⁻ ,N-Br]:F ⁻ (TS)	162.5	4.6	-17.8	0.8
4[CO ₂ ⁻ ,N-Br]:Cl ⁻ (TS)	157.6	9.7	-15.9	-0.4
4[CO ₂ ⁻ ,N-Br]:Br ⁻ (TS)	154.8	13.1	-15.1	-1.0
4[CO ₂ ⁻ ,N-I]:F ⁻	-71.6	323.6	-415.8	184.7
4[CO ₂ ⁻ ,N-I]:Cl ⁻	98.4	83.7	-124.0	70.9
4[CO ₂ ⁻ ,N-I]:Br ⁻	111.7	59.8	-96.6	59.9
4[CO ₂ ⁻ ,N-I]:I ⁻	119.4	41.3	-81.0	58.9
4[CO ₂ ⁻ ,N-I]:F ⁻ (TS)	146.5	1.2	-16.8	1.3
4[CO ₂ ⁻ ,N-I]:Cl ⁻ (TS)	143.3	1.9	-15.5	2.4
4[CO ₂ ⁻ ,N-I]:Br ⁻ (TS)	141.8	2.5	-15.6	3.3
4[CO ₂ ⁻ ,N-I]:I ⁻ (TS)	139.3	3.1	-16.0	5.0

Table S7. CSD reference codes, contact distances (in Å) and type of intermolecular contact.

NUPVUF	3.35	F...F
ANCLA	3.27	F...F
AYUYUP	3.166	F..F
COLKEV	3.340	F...F
FENCOS	2.950	F...F
HOBAC	3.012	F...F
HOBEG	3.305	F...F
HOBBIK	3.299	F..F
ISOXOE	3.242	F...F
LOYWH	3.410	F...F
PIPLIJ	3.066	F...F
RAVKAB	2.861	F...F
RUPSEB	3.481	F...F
RUPSOL	3.215	F...F
RUQCAI	3.325	F...F
VENTUF	3.077	F...F
VUYJEF	3.247	F...F
VUYJEF01	3.125	F...F
XIXYIM	3.381	F...F
YEPBEB	3.217	F...F
ZOGPIU	2.746	F...F
ZUFKES	3.056	F...F
LESRIM	3.190	F...Cl
VAJXIP	3.138	F...Br
CEBIMA	3.482	Cl...Cl
XAZDOT	3.476	Cl...Cl
SAQLAX	3.454	Cl...Cl
UHIVUE	3.398	Cl...Cl
UJIKAZ	3.427	Cl...Cl
QUBROV	3.376	Cl...Cl
JACROV	3.379	Cl...Cl
LIJGAN	3.465	Cl...Cl
LIJGAN01	3.472	Cl...Cl
XEMREM	3.483	Cl...Br
XEMRIQ	3.477	Cl...Br
YOGDEF	3.469	Br...Br
QAVRUC	3.496	Br...Br
QUWTUY	3.413	Br...Br
ROBZOX	3.323	Cl...N
BIBVEN	3.459	Br...N
EFUXIN	3.477	I...N

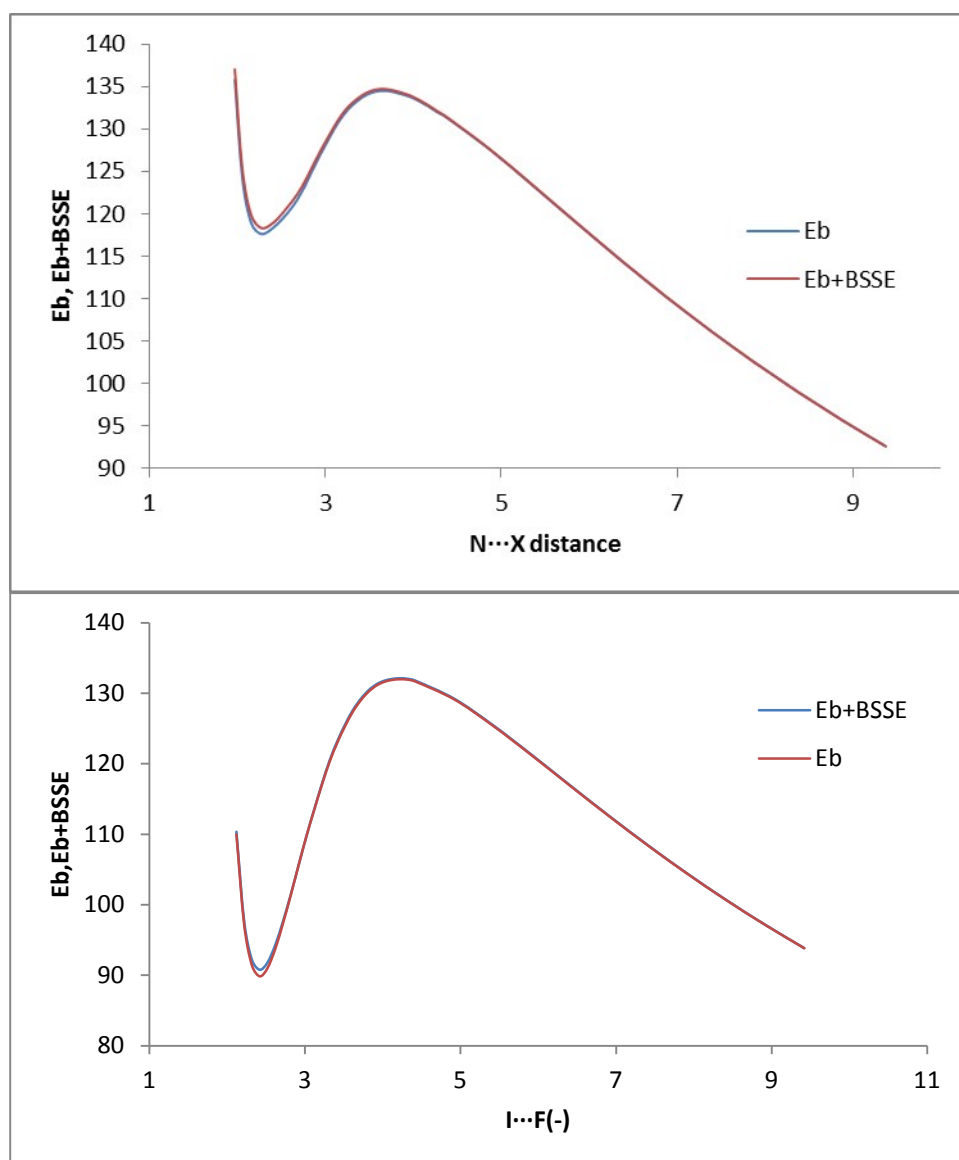


Figure S1. Energy (kJ/mol) dissociation profile with BSSE and without BSSE correction of **1**[NH₃(+), N]:ClNH₃(+) vs. the N...Cl distance (Å) (top) and Energy (kJ/mol) dissociation profile of **1**[CO₂(-), Cl]:F(-) vs. the I...F(-) distance (Å) (bottom).

Figure S2. Binding energy along the dissociation path. E_b in $\text{kJ}\cdot\text{mol}^{-1}$ and distances in \AA .

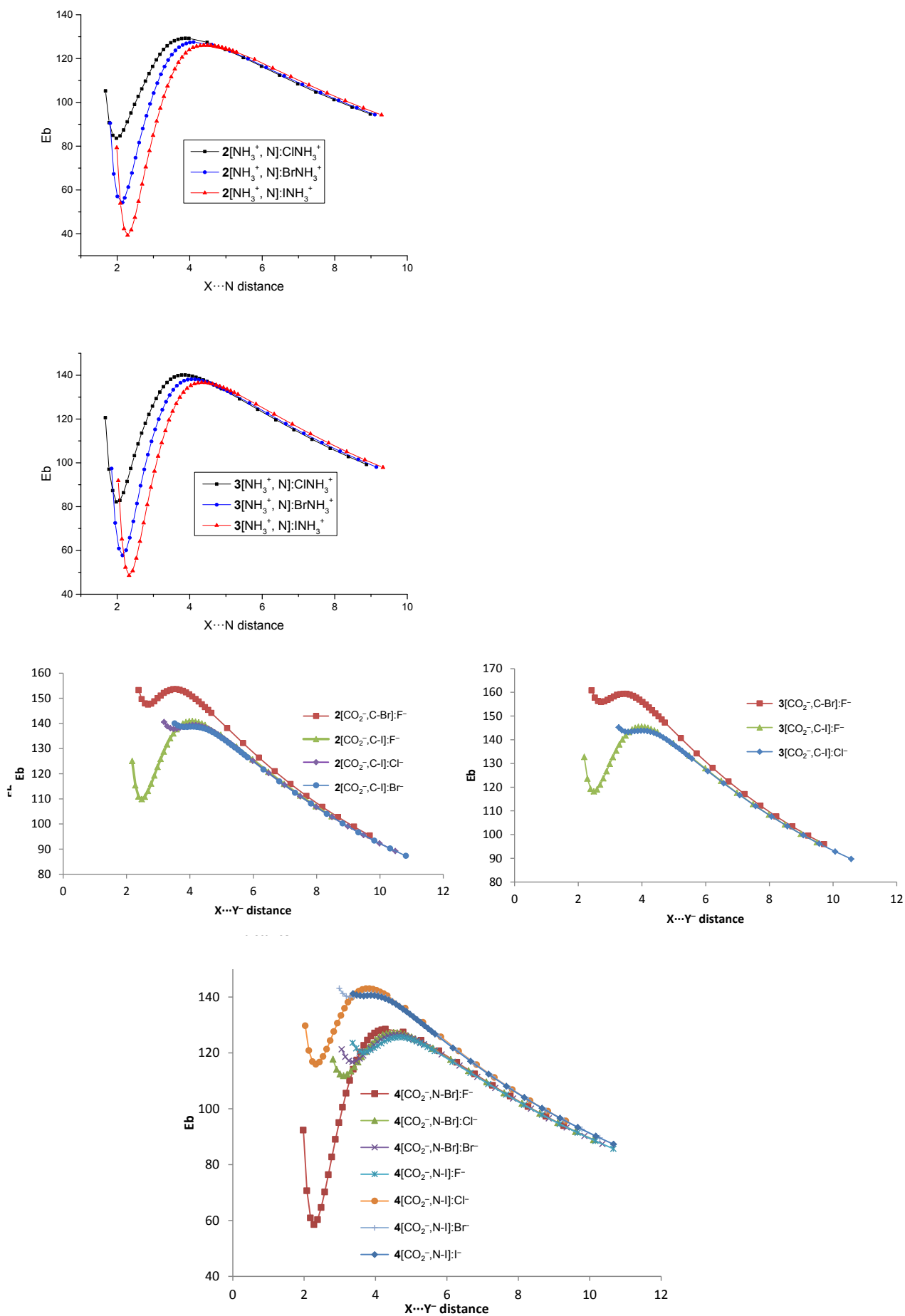
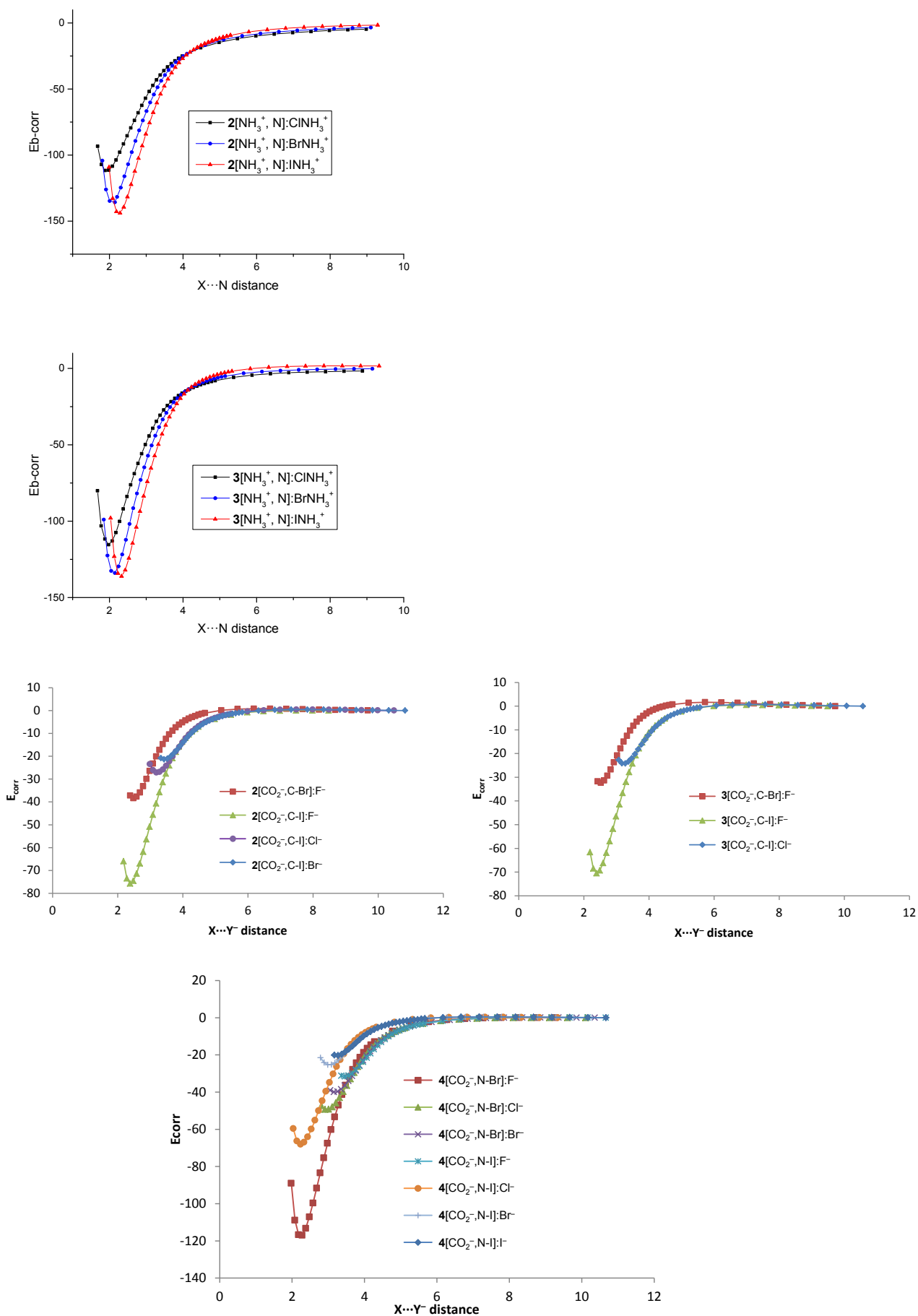


Figure S3. Corrected binding energy along the dissociation path. E_{corr} in $\text{kJ}\cdot\text{mol}^{-1}$ and distances in \AA .



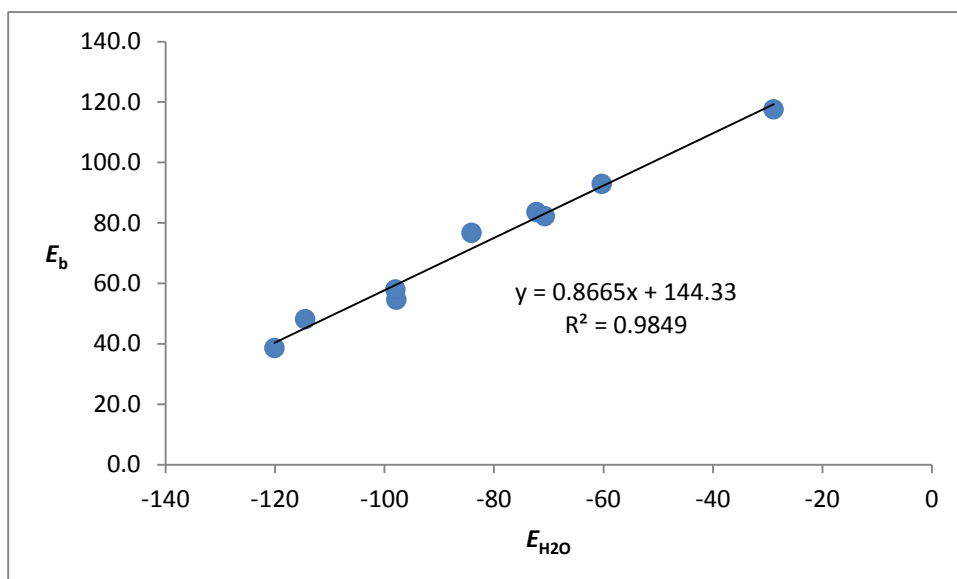


Figure S4. Representation of the binding energy in water (E_{H_2O} , kJ·mol⁻¹) versus the binding energy in gas phase (E_b , kJ·mol⁻¹) for the cation-cation complexes.

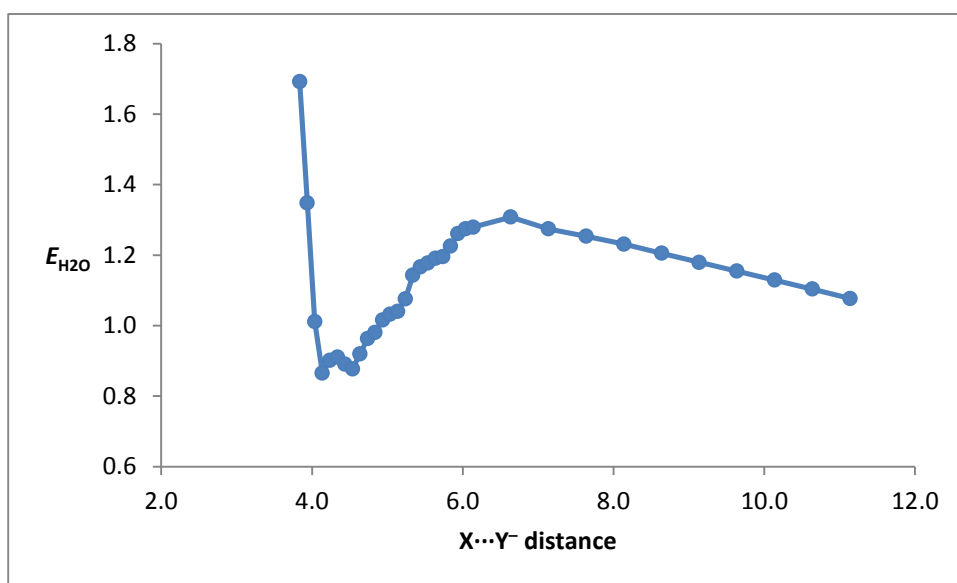


Figure S5. Binding energy along the dissociation path of $3[CO_2^-, C-Br]:F^-$ in water. E_{H_2O} in kJ·mol⁻¹ and distances in Å.

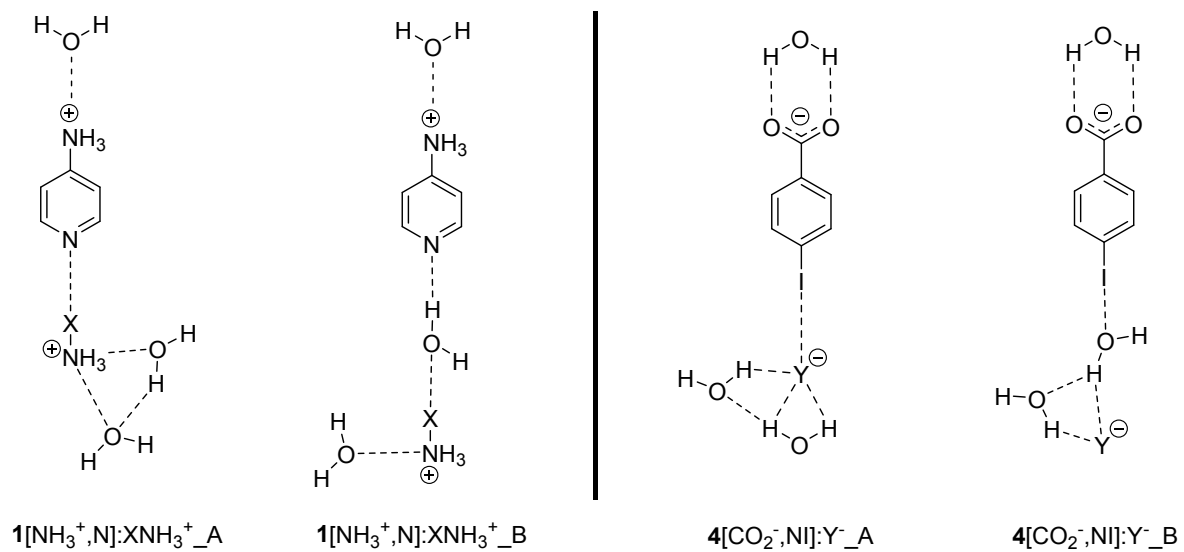


Figure S6. Schematic representation of the explicit solvent complexes under study.

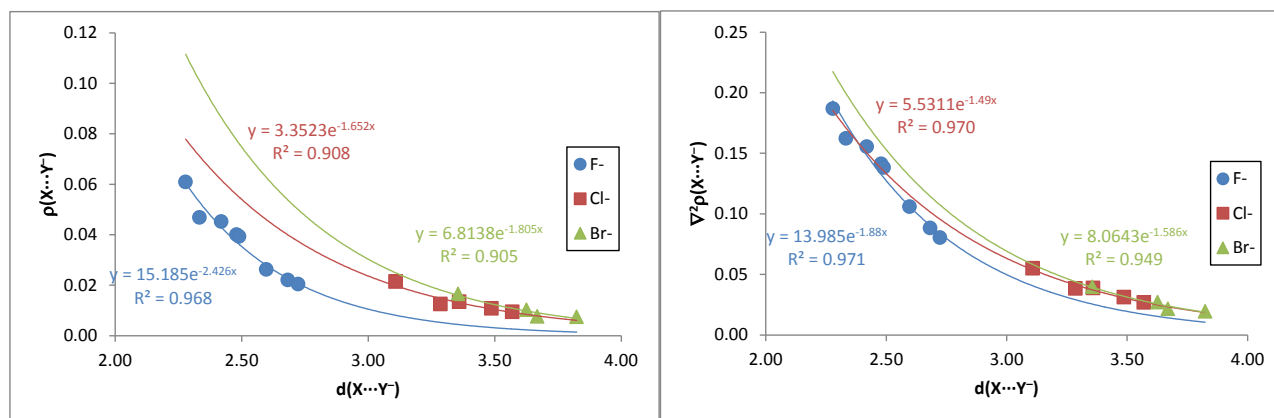


Figure S7. Exponential relationship between $X...Y^-$ intermolecular distance and the electron density and laplacian at the BCP (ρ and $\nabla^2\rho$, respectively, in a.u.) for the anion-anion complexes in gas phase.

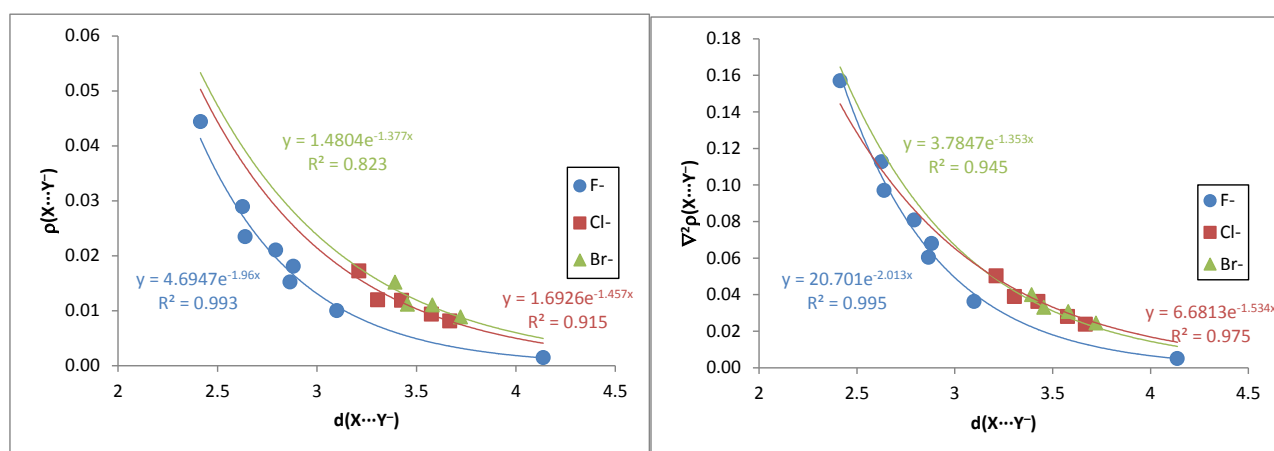


Figure S8. Exponential relationship between $X...Y^-$ intermolecular distance and the electron density and laplacian at the BCP (ρ and $\nabla^2\rho$, respectively, in a.u.) for the anion-anion complexes in water.

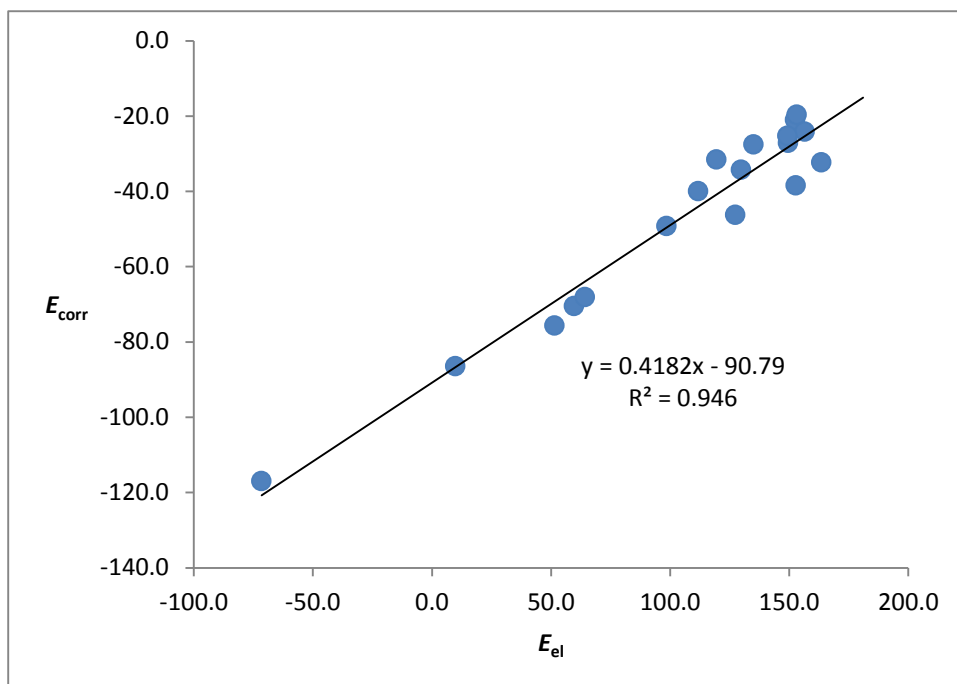


Figure S9. Corrected binding energy (E_{corr} , $\text{kJ}\cdot\text{mol}^{-1}$) vs the electrostatic contribution (E_{el} , $\text{kJ}\cdot\text{mol}^{-1}$) for anion-anion complexes in gas phase.

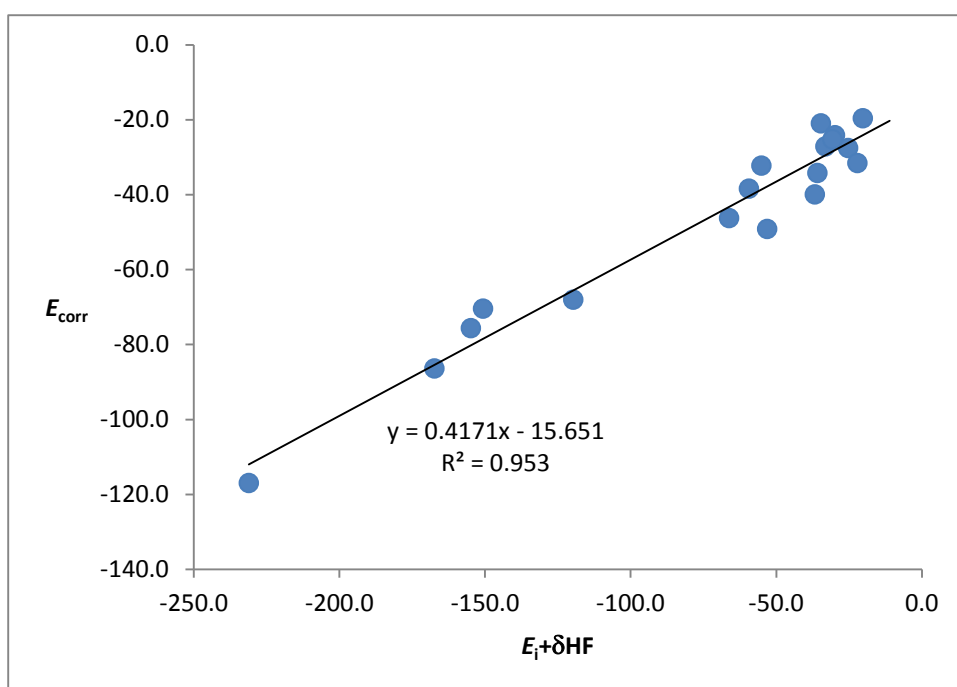


Figure S10. Corrected binding energy (E_{corr} , $\text{kJ}\cdot\text{mol}^{-1}$) vs the induction contribution ($E_i + \delta\text{HF}$, $\text{kJ}\cdot\text{mol}^{-1}$) for anion-anion complexes in gas phase.