# Electronic Supplementary Information

## Halogen bonding interactions in ion pairs versus conventional charge-assisted and neutral halogen bonds: a theoretical study based on imidazolium species

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**Table S1.** The CSD search results of 2-halo-imidazolium cations[a]

| Code | Donor | Acceptor | Anion | *d*(X···Y) | Reduction (% ) of vdW radii sum | *d*∠(C−X···Y) |
|---|---|---|---|---|---|---|
| | | | **Cl···X⁻** | | | |
| HILMEU | Cl | Cl | $Cl^-$ | 2.798 | 20.1 | 169.5 |
| YILJEK | Cl | Br | $Br^-$ | 3.236 | 10.6 | 169.4 |
| | | | **Cl···Y** | | | |
| AXEFOY | Cl | Cl | $TeCl_6^{2-}$ | 3.196 | 8.7 | 161.9 |
| EHENIO | Cl | Cl | $Cl_2O_2P^-$ | 2.817 | 19.5 | 180.0 |
| KOTDOM | Cl | Cl | $H_2Cl_3CuO^-$ | 3.409 | 2.6 | 169.6 |
| QIVPOB | Cl | Cl | $SeCl_6^{2-}$ | 3.171 | 9.4 | 165.2 |
| GAWHET | Cl | O | $C_6H_6N_3O_5^-$ | 2.881 | 17.7 | 172.7 |
| | | | **Br···X⁻** | | | |
| LAVMEC | Br | Br | $Br^-$ | 3.299 | 11.8 | 161.4 |
| ALOKOC | Br | Br | $Br^-$ | 3.191 | 14.7 | 174.2 |
| ALOKUI | Br | Br | $Br^-$ | 3.217 | 14.0 | 166.8 |
| CIHHAE | Br | Br | $Br^-$ | 3.032 | 18.9 | 177.7 |
| HABNAB | Br | Br | $Br^-$ | 3.297 | 11.8 | 172.6 |
| ICIKEM | Br | Br | $Br^-$ | 3.283 | 12.2 | 174.7 |
| QEGSUS | Br | Br | $Br^-$ | 3.432 | 8.2 | 161.2 |
| QEGTAZ | Br | Br | $Br^-$ | 3.299 | 11.8 | 172.6 |
| VIBPAY | Br | Br | $Br^-$ | 3.106 | 17.0 | 172.6 |
| XEZQOK | Br | Br | $Br^-$ | 3.158 | 15.6 | 168.2 |
| YISQEY | Br | Br | $Br^-$ | 3.222 | 13.9 | 175.9 |
| | | | **Br···Y** | | | |
| ALOLAP | Br | F | $PF_6^-$ | 3.078 | 5.9 | 160.6 |
| CIHHEI | Br | F | $PF_6^-$ | 3.650 | -11.6 | 165.3 |
| CIHHOS | Br | F | $BF_4^-$ | 2.826 | 13.6 | 166.1 |
| CIHHUY | Br | F | $PF_6^-$ | 3.157 | 3.5 | 154.9 |
| CIHJEK | Br | F | $BF_4^-$ | 2.869 | 12.3 | 166.1 |
| VIBNOK | Br | F | $PF_6^-$ | 2.965 | 9.3 | 166.8 |
| YUWZEW | Br | F | $PF_6^-$ | 3.150 | 3.7 | 139.2 |
| YUWZEW01 | Br | F | $PF_6^-$ | 3.286 | -0.5 | 138.2 |
| AXEFIS | Br | Br | $TeBr_6^{2-}$ | 3.419 | 8.6 | 161.7 |
| AYEHOB | Br | Br | $C_6H_6BrO_4^-$ | 2.872 | 23.2 | 153.9 |
| SADYAZ | Br | N | $C_2AgN_2^-$ | 2.959 | 11.1 | 177.7 |
| VIBNUQ | Br | N | $C_2F_6NO_4S_2^-$ | 2.768 | 16.9 | 173.8 |
| FALCIF | Br | O | $NO_3^-$ | 3.005 | 8.7 | 159.1 |
| YILJOU | Br | O | $NO_3^-$ | 2.724 | 17.2 | 175.8 |

| | | | | | | |
|---|---|---|---|---|---|---|
| **I···X⁻** | | | | | | |
| KAQSOM | I | Cl | $Cl^-$ | 3.023 | 20.2 | 174.1 |
| VIBPEC | I | Cl | $Cl^-$ | 3.041 | 19.8 | 176.6 |
| VIBPEC01 | I | Cl | $Cl^-$ | 2.965 | 21.8 | 179.1 |
| XEZRAX | I | Cl | $Cl^-$ | 2.948 | 22.2 | 177.6 |
| KAQSIG | I | Br | $Br^-$ | 3.099 | 20.7 | 178.5 |
| NEDPAP | I | Br | $Br^-$ | 3.121 | 20.2 | 172.0 |
| PETTOZ | I | Br | $Br^-$ | 3.047 | 22.1 | 178.0 |
| PETTUF | I | Br | $Br^-$ | 3.079 | 21.3 | 176.7 |
| PETVAN | I | Br | $Br^-$ | 3.041 | 22.2 | 176.6 |
| WEBFEQ | I | Br | $Br^-$ | 3.095 | 20.8 | 167.5 |
| WEBFIU | I | Br | $Br^-$ | 3.303 | 15.5 | 167.9 |
| YILJIO | I | Br | $Br^-$ | 3.114 | 20.4 | 174.7 |
| ICIKOW | I | I | $I^-$ | 3.357 | 17.7 | 176.3 |
| ICIKUC | I | I | $I^-$ | 3.306 | 19.0 | 179.0 |
| KAQSEC | I | I | $I^-$ | 3.283 | 19.5 | 172.1 |
| KOFPUS | I | I | $I^-$ | 3.263 | 20.0 | 178.1 |
| LOFFUJ | I | I | $I^-$ | 3.373 | 17.3 | 169.4 |
| XEZREB | I | I | $I^-$ | 3.288 | 19.4 | 177.6 |
| **I···Y** | | | | | | |
| WEBFAM | I | F | $PF_6^-$ | 3.045 | 11.5 | 149.4 |
| GAZQIH | I | Br | $Br_2I^-$ | 3.287 | 15.9 | 163.2 |
| FAJCID | I | I | $I_3^-$ | 3.368 | 17.5 | 177.9 |
| KAQSUS | I | O | $H_2O_4P^-$ | 2.602 | 24.8 | 177.8 |
| ITUPAP | I | S | $CF_3SO_3^-$ | 2.838 | 26.1 | 168.7 |

[a] Distances are given in angstroms, and angles in degrees.

**Table S2.** The CSD search results of 4-halo-/5-halo-imidazolium cations[a]

| Code | Donor | Acceptor | Anion | *d*(X···Y) | Reduction (% ) of vdW radii sum | *d*∠(C−X···Y) |
|---|---|---|---|---|---|---|
| **Cl···X⁻** | | | | | | |
| EJEMAI | Cl | Br | $Br^-$ | 3.042 | 16.0 | 177.2 |
| PELLID | Cl | I | $I^-$ | 3.562 | 6.0 | 174.2 |
| WOMYED | Cl | I | $I^-$ | 3.590 | 5.3 | 168.5 |
| **Cl···Y** | | | | | | |
| CUPPEJ | Cl | Cl | $PdCl_4^{2-}$ | 3.283 | 6.2 | 172.7 |
| FUDFUG | Cl | Cl | $SbCl_6^{2-}$ | 3.294 | 5.9 | 161.8 |
| **Br···X⁻** | | | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| CIHHAE | Br | Br | $Br^-$ | 3.201 | 14.4 | 176.6 |
| FEXYIS | Br | Br | $Br^-$ | 3.210 | 14.2 | 177.6 |
| FEXZEP | Br | Br | $Br^-$ | 3.288 | 12.1 | 169.2 |
| FEXZIT | Br | Br | $Br^-$ | 3.283 | 12.2 | 169.5 |
| HABNEF | Br | Br | $Br^-$ | 3.189 | 14.7 | 175.3 |
| QEGTAZ | Br | Br | $Br^-$ | 3.458 | 7.5 | 171.6 |
| QEGTED | Br | Br | $Br^-$ | 3.398 | 9.1 | 165.9 |
| YOXVUD | Br | Br | $Br^-$ | 3.333 | 10.9 | 173.2 |
| YOXWAK | Br | Br | $Br^-$ | 3.209 | 14.2 | 174.7 |
| ZAPSIU | Br | Br | $Br^-$ | 3.321 | 11.2 | 177.8 |
| VUSNIH | Br | I | $I^-$ | 3.559 | 9.0 | 175.6 |
| | | | **Br···Y** | | | |
| CIHHEI | Br | F | $PF_6^-$ | 3.017 | 7.7 | 173.6 |
| CIHHOS | Br | F | $BF_4^-$ | 2.822 | 13.7 | 167.8 |
| CIHHUY | Br | F | $PF_6^-$ | 3.255 | 0.5 | 171.0 |
| CIHJEK | Br | F | $BF_4^-$ | 2.906 | 11.1 | 179.5 |
| CIHJIO | Br | F | $PF_6^-$ | 2.927 | 10.5 | 161.5 |
| HEKJOW | Br | Cl | $PdCl_4^{2-}$ | 3.475 | 4.0 | 156.9 |
| AGOCOQ | Br | N | $C_2F_6NO_4S_2^-$ | 3.003 | 9.8 | 168.1 |
| CIHHIM | Br | N | $C_2F_6NO_4S_2^-$ | 3.612 | -8.5 | 170.1 |
| VURKUP | Br | S | $CF_3SO_3^-$ | 2.994 | 18.4 | 165.7 |
| | | | **I···X$^-$** | | | |
| FEXYOY | I | Br | $Br^-$ | 3.219 | 17.7 | 176.6 |
| YICJUR | I | I | $I^-$ | 3.541 | 13.2 | 177.6 |
| | | | **I···Y** | | | |
| PUZZIU | I | F | $PF_6^-$ | 3.062 | 11.0 | 174.9 |
| AGOCIK | I | N | $C_2F_6NO_4S_2^-$ | 3.127 | 10.7 | 167.4 |
| VURLAW | I | S | $CF_3SO_3^-$ | 2.866 | 25.4 | 174.3 |

[a] Distances are given in angstroms, and angles in degrees.

**Table S3.** Geometric and energetic data calculated with B3LYP for all the studied systems[a]

| | $\Delta E$ | $d$(X···X) | Reduction (% ) of vdw radii sum | ∠(C-X···X) |
|---|---|---|---|---|
| | | Ion-pair complexes | | |
| **1**-$Cl^-$ | -76.7 | 2.618 | 25.2 | 179.1 |
| **2**-$Br^-$ | -82.6 | 2.713 | 27.5 | 180. 0 |
| **3**-$I^-$ | -89.9 | 2.966 | 27.3 | 179.9 |
| **4**-$Cl^-$ | -69.2 | 2.652 | 24.2 | 175. 0 |
| **5**-$Br^-$ | -74.6 | 2.741 | 26.7 | 177.8 |

| | | | | |
|---|---|---|---|---|
| **6**-$I^-$ | -80.5 | 3.008 | 26.3 | 179. 0 |
| Charge-assisted complexes | | | | |
| **1**-HCl | -0.4 | 3.455 | 1.3 | 171.7 |
| **2**-HBr | -2.2 | 3.519 | 5.9 | 175.9 |
| **3**-HI | -3.8 | 3.633 | 11.0 | 177.8 |
| **4**-HCl | -1.5 | 3.513 | -0.4 | 170. 0 |
| **5**-HBr | -1.7 | 3.576 | 4.4 | 172.5 |
| **6**-HI | -2.8 | 3.704 | 9.2 | 179. 0 |
| **7**-$Cl^-$ | --- | --- | --- | --- |
| **8**-$Br^-$ | -6.6 | 3.227 | 13.7 | 173.1 |
| **9**-$I^-$ | -10.5 | 3.409 | 16.4 | 177.2 |
| **10**-$Cl^-$ | --- | --- | --- | --- |
| **11**-$Br^-$ | -10.3 | 3.143 | 16.0 | 173.5 |
| **12**-$I^-$ | -14.6 | 3.33 | 18.4 | 176.9 |
| Neutral complexes | | | | |
| **7**-HCl | --- | --- | --- | --- |
| **8**-HBr | --- | --- | --- | --- |
| **9**-HI | -0.3 | 4.188 | -2.6 | 179.6 |
| **10**-HCl | --- | --- | --- | --- |
| **11**-HBr | --- | --- | --- | --- |
| **12**-HI | --- | --- | --- | --- |

[a] Energies are given in kcal/mol, distances in angstroms, and angles in degrees. The complexes **7**-$Cl^-$ and **10**-$Cl^-$, together with almost all the neutral complexes, cannot be obtained at the level of B3LYP/aug-cc-pVDZ(-PP).

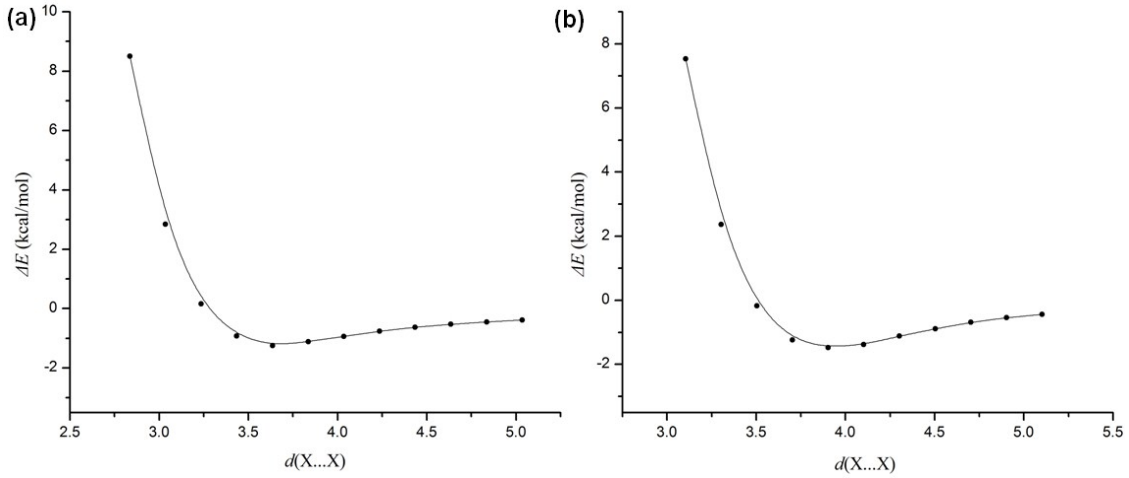


**Fig. S1** Plot of the interaction energy versus the intermolecular X···X distance (a) for **8**-HBr and (b) for **9**-HI.

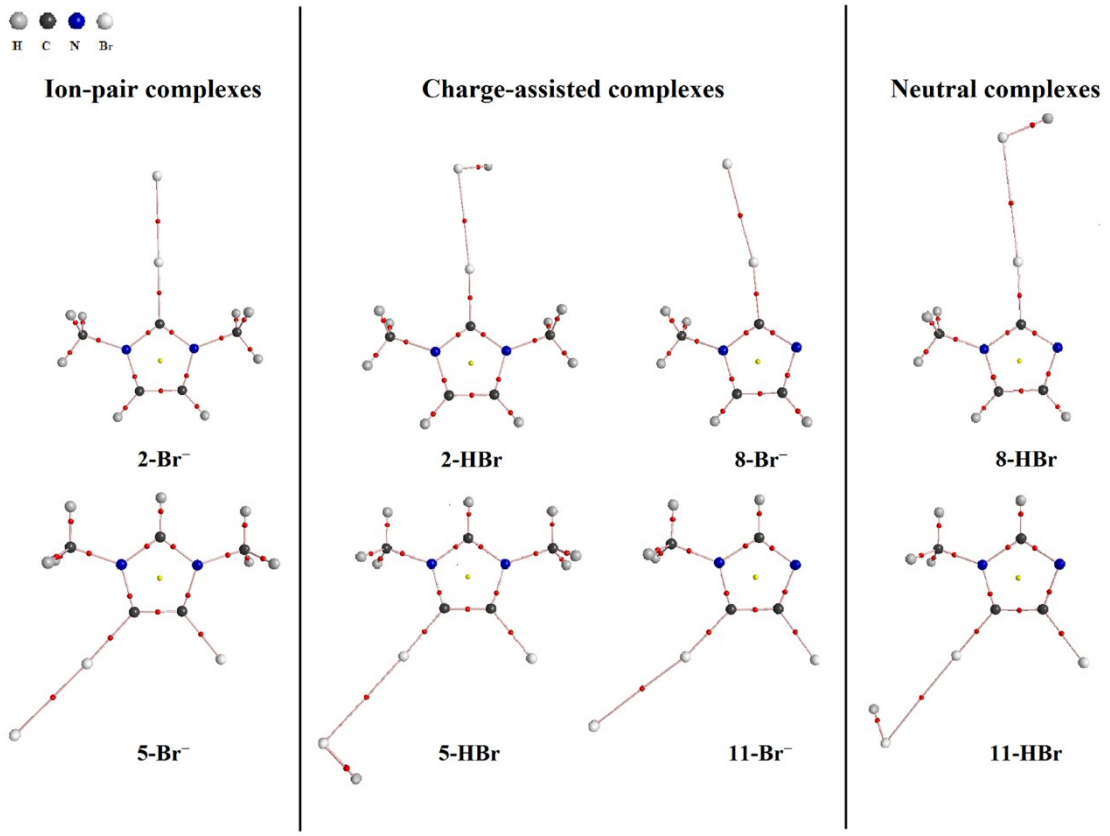


**Fig. S2** Molecular graphs of eight brominated complexes.

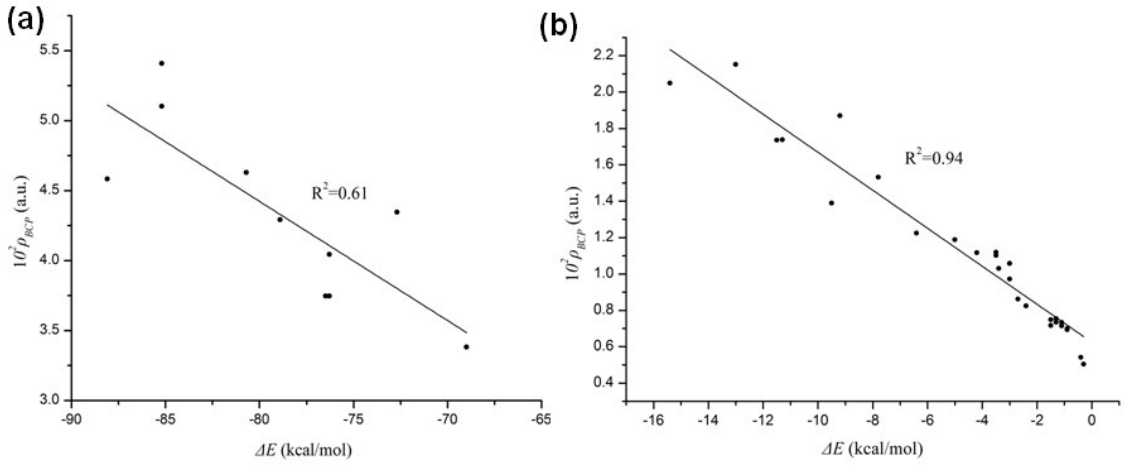


**Fig. S3** Correlation between the interaction energies and the values of $\rho_{BCP}$ (a) for ion-pair complexes and (b) for charge-assisted and neutral systems.

Cartesian coordinates of the optimized structures for all the studied complexes with the M06-2X/aug-cc-pvDZ(-PP) method:

**Ion-pair complexes**

**1**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.394260 | 0.684019 | -0.101070 |
| 2 | 6 | 2.392534 | -0.676244 | -0.106629 |
| 3 | 6 | 0.287889 | 0.006012 | 0.028686 |
| 4 | 7 | 1.076201 | 1.089242 | -0.016071 |
| 5 | 1 | 3.211062 | 1.391467 | -0.149628 |
| 6 | 1 | 3.207481 | -1.385400 | -0.161105 |
| 7 | 7 | 1.073383 | -1.078819 | -0.024906 |
| 8 | 6 | 0.573617 | 2.460796 | 0.022378 |
| 9 | 1 | -0.057545 | 2.642901 | -0.852618 |
| 10 | 1 | -0.019602 | 2.602889 | 0.930496 |
| 11 | 1 | 1.431909 | 3.135495 | 0.018994 |
| 12 | 6 | 0.567412 | -2.449359 | 0.001434 |
| 13 | 1 | 1.424066 | -3.126124 | -0.005395 |
| 14 | 1 | -0.028126 | -2.597356 | 0.907081 |
| 15 | 1 | -0.062133 | -2.622930 | -0.876481 |
| 16 | 17 | -1.425918 | 0.009298 | 0.167750 |
| 17 | 17 | -4.061475 | 0.023598 | 0.469992 |

**2**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.385590 | 0.683067 | -0.112150 |
| 2 | 6 | 2.389774 | -0.677014 | -0.118063 |
| 3 | 6 | 0.272080 | -0.004233 | 0.047908 |
| 4 | 7 | 1.065821 | 1.077504 | -0.008560 |
| 5 | 1 | 3.198299 | 1.394487 | -0.172717 |

| | | | | |
|---|---|---|---|---|
| 6 | 1 | 3.206752 | -1.382966 | -0.184619 |
| 7 | 7 | 1.072490 | -1.080444 | -0.018082 |
| 8 | 6 | 0.571247 | 2.450188 | 0.035783 |
| 9 | 1 | -0.091289 | 2.627599 | -0.816571 |
| 10 | 1 | 0.012443 | 2.605151 | 0.963373 |
| 11 | 1 | 1.430088 | 3.123599 | -0.005531 |
| 12 | 6 | 0.586407 | -2.456541 | 0.013266 |
| 13 | 1 | 1.449653 | -3.124195 | -0.029804 |
| 14 | 1 | 0.024836 | -2.622467 | 0.937285 |
| 15 | 1 | -0.071537 | -2.631404 | -0.843195 |
| 16 | 35 | -1.671080 | -0.011216 | 0.211151 |
| 17 | 17 | -4.224407 | -0.021885 | 0.441447 |

**2**-$Br^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.392765 | 0.684982 | -0.128733 |
| 2 | 6 | 2.401569 | -0.675230 | -0.134789 |
| 3 | 6 | 0.286302 | -0.009716 | 0.063042 |
| 4 | 7 | 1.073487 | 1.075250 | -0.005312 |
| 5 | 1 | 3.201849 | 1.399407 | -0.201578 |
| 6 | 1 | 3.219746 | -1.378554 | -0.213483 |
| 7 | 7 | 1.087508 | -1.083621 | -0.014971 |
| 8 | 6 | 0.574318 | 2.446426 | 0.045734 |
| 9 | 1 | -0.100893 | 2.621061 | -0.797181 |
| 10 | 1 | 0.028906 | 2.599583 | 0.981530 |
| 11 | 1 | 1.430156 | 3.122706 | -0.008153 |
| 12 | 6 | 0.606263 | -2.461649 | 0.022713 |
| 13 | 1 | 1.471319 | -3.126128 | -0.031055 |
| 14 | 1 | 0.057519 | -2.629224 | 0.954092 |
| 15 | 1 | -0.061584 | -2.638923 | -0.825539 |
| 16 | 35 | -1.653965 | -0.022141 | 0.247527 |
| 17 | 35 | -4.372190 | -0.036356 | 0.513336 |

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**2**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 3.452916 | 0.856547 | -0.117159 |
| 2 | 6 | 3.455564 | -0.503820 | -0.122624 |
| 3 | 6 | 1.342819 | 0.171496 | 0.055362 |
| 4 | 7 | 2.134242 | 1.252824 | -0.005815 |
| 5 | 1 | 4.266041 | 1.567176 | -0.182703 |
| 6 | 1 | 4.271411 | -1.210761 | -0.193793 |
| 7 | 7 | 2.138452 | -0.906148 | -0.014657 |
| 8 | 6 | 1.640953 | 2.626698 | 0.040955 |
| 9 | 1 | 0.975643 | 2.805072 | -0.808994 |
| 10 | 1 | 1.087054 | 2.782021 | 0.971384 |
| 11 | 1 | 2.500575 | 3.298775 | -0.003798 |
| 12 | 6 | 1.650666 | -2.282334 | 0.019706 |
| 13 | 1 | 2.513316 | -2.950516 | -0.025085 |
| 14 | 1 | 1.092479 | -2.446569 | 0.946038 |
| 15 | 1 | 0.990684 | -2.457605 | -0.835077 |
| 16 | 35 | -0.611863 | 0.167910 | 0.233098 |
| 17 | 53 | -3.529538 | 0.163771 | 0.519346 |

**3**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.793740 | -2.457814 | 0.045975 |
| 2 | 6 | 0.565726 | -2.425152 | 0.058147 |
| 3 | 6 | -0.164856 | -0.308615 | -0.007792 |
| 4 | 7 | -1.219168 | -1.144878 | 0.005421 |
| 5 | 1 | -1.482683 | -3.291753 | 0.064617 |
| 6 | 1 | 1.293602 | -3.225114 | 0.089629 |
| 7 | 7 | 0.928506 | -1.092992 | 0.025906 |
| 8 | 6 | 2.295301 | -0.582492 | 0.009104 |
| 9 | 1 | 2.979014 | -1.423099 | 0.149005 |
| 10 | 1 | 2.494207 | -0.092206 | -0.948939 |
| 11 | 1 | 2.422103 | 0.143227 | 0.817390 |
| 12 | 6 | -2.608613 | -0.700132 | -0.021133 |
| 13 | 1 | -2.805515 | -0.061347 | 0.844968 |
| 14 | 1 | -2.794164 | -0.131770 | -0.937490 |
| 15 | 1 | -3.252815 | -1.581942 | 0.009008 |
| 16 | 53 | -0.219196 | 1.953537 | -0.067497 |
| 17 | 53 | -0.284251 | 4.906524 | -0.138428 |

**4**-$Cl^-$

| Center | Atomic | Coordinates (Angstroms) |
|---|---|---|

| Number | Number | X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.910868 | -0.932126 | 0.160624 |
| 2 | 6 | 0.460442 | -0.907771 | 0.173107 |
| 3 | 6 | -0.227602 | 1.180434 | 0.099568 |
| 4 | 7 | -1.303809 | 0.392978 | 0.114623 |
| 5 | 7 | 0.864392 | 0.412860 | 0.134338 |
| 6 | 6 | 2.247730 | 0.875273 | 0.134733 |
| 7 | 1 | 2.737745 | 0.546925 | 1.056214 |
| 8 | 1 | 2.767461 | 0.452646 | -0.730174 |
| 9 | 1 | 2.245878 | 1.965969 | 0.077007 |
| 10 | 6 | -2.703046 | 0.820961 | 0.091344 |
| 11 | 1 | -3.201970 | 0.442418 | 0.988166 |
| 12 | 1 | -2.728531 | 1.912644 | 0.061041 |
| 13 | 1 | -3.188459 | 0.393548 | -0.790767 |
| 14 | 1 | -0.231940 | 2.262044 | 0.064699 |
| 15 | 17 | -2.067941 | -2.204615 | 0.189787 |
| 16 | 17 | 1.568641 | -2.192996 | 0.234401 |
| 17 | 17 | -4.084052 | -3.996238 | 0.216997 |

**5**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.987141 | -0.904931 | 0.093945 |
| 2 | 6 | 0.383314 | -0.851522 | 0.065286 |
| 3 | 6 | -0.332977 | 1.221919 | -0.053252 |
| 4 | 7 | -1.393650 | 0.415982 | 0.018238 |
| 5 | 7 | 0.771908 | 0.473061 | -0.026802 |
| 6 | 6 | 2.142114 | 0.965847 | -0.091168 |
| 7 | 1 | 2.680199 | 0.658865 | 0.810508 |

| | | | | |
|---|---|---|---|---|
| 8 | 1 | 2.635280 | 0.545998 | -0.973130 |
| 9 | 1 | 2.113646 | 2.055865 | -0.159358 |
| 10 | 6 | -2.792179 | 0.840425 | 0.023282 |
| 11 | 1 | -3.263869 | 0.488105 | 0.945025 |
| 12 | 1 | -2.824471 | 1.931100 | -0.037609 |
| 13 | 1 | -3.302847 | 0.387649 | -0.831289 |
| 14 | 1 | -0.355372 | 2.301908 | -0.121658 |
| 15 | 35 | -2.262722 | -2.372388 | 0.202303 |
| 16 | 35 | 1.607210 | -2.238756 | 0.146228 |
| 17 | 17 | -4.049294 | -4.245809 | 0.327365 |

**5**-$Br^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.002663 | -0.904595 | 0.046064 |
| 2 | 6 | 0.367892 | -0.861709 | 0.030499 |
| 3 | 6 | -0.334738 | 1.218892 | -0.043405 |
| 4 | 7 | -1.401724 | 0.419211 | -0.001064 |
| 5 | 7 | 0.765029 | 0.462121 | -0.025575 |
| 6 | 6 | 2.139497 | 0.946910 | -0.061430 |
| 7 | 1 | 2.661841 | 0.620637 | 0.842841 |
| 8 | 1 | 2.642422 | 0.538813 | -0.943310 |
| 9 | 1 | 2.119010 | 2.038068 | -0.111126 |
| 10 | 6 | -2.798049 | 0.852258 | 0.001212 |
| 11 | 1 | -3.279209 | 0.486369 | 0.912758 |
| 12 | 1 | -2.822827 | 1.943978 | -0.040044 |
| 13 | 1 | -3.304231 | 0.418785 | -0.866015 |
| 14 | 1 | -0.349420 | 2.300385 | -0.085436 |
| 15 | 35 | -2.284755 | -2.364435 | 0.121021 |
| 16 | 35 | 1.579589 | -2.260194 | 0.082197 |

| | | | | |
|---|---|---|---|---|
| 17 | 35 | -4.207301 | -4.345083 | 0.232614 |

**5**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.981210 | -0.901440 | 0.065741 |
| 2 | 6 | 0.388147 | -0.850227 | 0.042529 |
| 3 | 6 | -0.330825 | 1.224266 | -0.049572 |
| 4 | 7 | -1.391707 | 0.417384 | 0.006859 |
| 5 | 7 | 0.774869 | 0.476039 | -0.029612 |
| 6 | 6 | 2.145642 | 0.971093 | -0.077868 |
| 7 | 1 | 2.676808 | 0.652436 | 0.823900 |
| 8 | 1 | 2.645056 | 0.563169 | -0.961816 |
| 9 | 1 | 2.116506 | 2.061846 | -0.131655 |
| 10 | 6 | -2.791652 | 0.840096 | 0.013725 |
| 11 | 1 | -3.264878 | 0.476459 | 0.930307 |
| 12 | 1 | -2.824649 | 1.931285 | -0.033909 |
| 13 | 1 | -3.299237 | 0.398032 | -0.848313 |
| 14 | 1 | -0.353896 | 2.305239 | -0.102748 |
| 15 | 35 | -2.257035 | -2.373868 | 0.178091 |
| 16 | 35 | 1.610456 | -2.239029 | 0.107497 |
| 17 | 53 | -4.318879 | -4.503287 | 0.371660 |

**6**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.998197 | -0.892764 | 0.029929 |
| 2 | 6 | 0.374568 | -0.844704 | 0.019410 |
| 3 | 6 | -0.322282 | 1.238548 | -0.040824 |
| 4 | 7 | -1.388191 | 0.436609 | -0.008800 |
| 5 | 7 | 0.776364 | 0.481049 | -0.024584 |
| 6 | 6 | 2.146426 | 0.976014 | -0.052715 |
| 7 | 1 | 2.671896 | 0.639777 | 0.846159 |
| 8 | 1 | 2.653766 | 0.584910 | -0.939829 |
| 9 | 1 | 2.120351 | 2.067889 | -0.085909 |
| 10 | 6 | -2.778227 | 0.884057 | -0.008848 |
| 11 | 1 | -3.264578 | 0.530403 | 0.904795 |
| 12 | 1 | -2.796369 | 1.976046 | -0.056725 |
| 13 | 1 | -3.288775 | 0.451585 | -0.873914 |
| 14 | 1 | -0.335540 | 2.320530 | -0.074495 |
| 15 | 53 | -2.447141 | -2.598898 | 0.100038 |
| 16 | 53 | 1.713766 | -2.416303 | 0.072425 |
| 17 | 53 | -4.415498 | -4.846948 | 0.192035 |

**Charge-assisted complexes**

**1**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 3.823566 | 1.433644 | 0.035092 |
| 2 | 6 | 3.966890 | 0.079542 | 0.016082 |
| 3 | 6 | 1.818208 | 0.535629 | 0.121142 |
| 4 | 7 | 2.471890 | 1.700566 | 0.100326 |
| 5 | 1 | 4.561520 | 2.225019 | 0.007061 |
| 6 | 1 | 4.854052 | -0.538729 | -0.029569 |
| 7 | 7 | 2.700948 | -0.466051 | 0.070720 |
| 8 | 6 | 1.841790 | 3.022842 | 0.153798 |
| 9 | 1 | 1.116167 | 3.110988 | -0.659660 |
| 10 | 1 | 1.344829 | 3.150411 | 1.120076 |
| 11 | 1 | 2.627071 | 3.771193 | 0.035218 |
| 12 | 6 | 2.361109 | -1.891443 | 0.069757 |
| 13 | 1 | 3.294370 | -2.456187 | 0.038409 |
| 14 | 1 | 1.808466 | -2.133412 | 0.982056 |
| 15 | 1 | 1.755772 | -2.120707 | -0.812014 |
| 16 | 17 | 0.141335 | 0.360756 | 0.194832 |
| 17 | 17 | -3.136912 | 0.759842 | 0.461853 |
| 18 | 1 | -3.938495 | -0.225004 | 0.224456 |

**2**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.314380 | 1.490572 | -4.267603 |
| 2 | 6 | 0.491796 | 0.145868 | -4.389256 |
| 3 | 6 | -1.083323 | 0.491524 | -2.888011 |
| 4 | 7 | -0.672696 | 1.687431 | -3.325631 |
| 5 | 1 | 0.802737 | 2.317625 | -4.766447 |
| 6 | 1 | 1.163284 | -0.427482 | -5.015207 |
| 7 | 7 | -0.389611 | -0.461706 | -3.520521 |
| 8 | 6 | -1.196065 | 2.979510 | -2.875237 |
| 9 | 1 | -2.265139 | 3.037145 | -3.099922 |
| 10 | 1 | -1.030283 | 3.083727 | -1.799034 |
| 11 | 1 | -0.659343 | 3.763122 | -3.412651 |
| 12 | 6 | -0.549121 | -1.903840 | -3.316925 |
| 13 | 1 | 0.149749 | -2.413458 | -3.982605 |
| 14 | 1 | -0.322451 | -2.151359 | -2.275845 |
| 15 | 1 | -1.575623 | -2.193358 | -3.559761 |
| 16 | 35 | -2.394759 | 0.204916 | -1.623404 |
| 17 | 17 | -4.873363 | -0.422083 | 0.426454 |
| 18 | 1 | -4.433342 | -0.429951 | 1.641359 |

**2**-HBr

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 3.622279 | 1.867649 | 0.222252 |
| 2 | 6 | 3.714347 | 0.509144 | 0.200397 |
| 3 | 6 | 1.577742 | 1.046452 | 0.232997 |
| 4 | 7 | 2.280760 | 2.184822 | 0.242458 |
| 5 | 1 | 4.390565 | 2.630292 | 0.225244 |
| 6 | 1 | 4.578593 | -0.141998 | 0.181392 |
| 7 | 7 | 2.427962 | 0.013743 | 0.207314 |
| 8 | 6 | 1.709277 | 3.533494 | 0.270180 |

| | | | | |
|---|---|---|---|---|
| 9 | 1 | 1.086726 | 3.682680 | -0.616995 |
| 10 | 1 | 1.110105 | 3.655368 | 1.177386 |
| 11 | 1 | 2.535954 | 4.246020 | 0.269966 |
| 12 | 6 | 2.044040 | -1.399755 | 0.190474 |
| 13 | 1 | 2.958928 | -1.993988 | 0.160709 |
| 14 | 1 | 1.476482 | -1.633734 | 1.095858 |
| 15 | 1 | 1.438331 | -1.601647 | -0.697828 |
| 16 | 35 | -0.263154 | 0.925278 | 0.246563 |
| 17 | 1 | -4.164298 | -0.086835 | 0.826523 |
| 18 | 35 | -3.663157 | 1.026542 | 0.085060 |

**2**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 3.846403 | 0.942407 | -0.365878 |
| 2 | 6 | 3.888205 | -0.418574 | -0.369589 |
| 3 | 6 | 1.781710 | 0.197152 | -0.169287 |
| 4 | 7 | 2.523104 | 1.308787 | -0.240100 |
| 5 | 1 | 4.638021 | 1.676512 | -0.443000 |
| 6 | 1 | 4.723495 | -1.102286 | -0.448679 |
| 7 | 7 | 2.590124 | -0.866240 | -0.245793 |
| 8 | 6 | 2.004449 | 2.677789 | -0.190051 |
| 9 | 1 | 1.324624 | 2.840877 | -1.031521 |
| 10 | 1 | 1.478233 | 2.831545 | 0.756533 |
| 11 | 1 | 2.854064 | 3.359368 | -0.258802 |
| 12 | 6 | 2.156858 | -2.264918 | -0.206027 |
| 13 | 1 | 3.048025 | -2.892222 | -0.265204 |
| 14 | 1 | 1.629174 | -2.454762 | 0.733211 |
| 15 | 1 | 1.499605 | -2.467050 | -1.056938 |
| 16 | 35 | -0.055676 | 0.143392 | 0.008691 |
| 17 | 53 | -3.640801 | 0.156679 | 0.348065 |

| | | | | |
|---|---|---|---|---|
| 18 | 1 | -3.857965 | -1.415534 | 0.035985 |

**3**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.046306 | -1.126076 | -0.176051 |
| 2 | 6 | 0.313308 | -1.062333 | -0.146500 |
| 3 | 6 | -0.463860 | 1.007700 | -0.213820 |
| 4 | 7 | -1.511044 | 0.170043 | -0.218147 |
| 5 | 1 | -1.715802 | -1.976353 | -0.170666 |
| 6 | 1 | 1.058985 | -1.846064 | -0.108730 |
| 7 | 7 | 0.656621 | 0.271930 | -0.170567 |
| 8 | 6 | 2.021706 | 0.801062 | -0.154871 |
| 9 | 1 | 2.708740 | -0.045580 | -0.103632 |
| 10 | 1 | 2.203133 | 1.372073 | -1.070376 |
| 11 | 1 | 2.154599 | 1.442151 | 0.721628 |
| 12 | 6 | -2.918947 | 0.569446 | -0.260652 |
| 13 | 1 | -3.155504 | 1.171678 | 0.621477 |
| 14 | 1 | -3.107777 | 1.144788 | -1.171886 |
| 15 | 1 | -3.525384 | -0.338046 | -0.263137 |
| 16 | 53 | -0.557214 | 3.078476 | -0.269221 |
| 17 | 53 | -0.556705 | 6.702756 | -0.442819 |
| 18 | 1 | -1.966431 | 6.940964 | 0.314787 |

**4**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.389534 | -1.443433 | -0.061966 |
| 2 | 6 | 0.601823 | -2.368421 | -0.256529 |
| 3 | 6 | -1.286061 | -3.450520 | 0.074504 |
| 4 | 7 | -1.558389 | -2.146747 | 0.142678 |
| 5 | 7 | 0.015717 | -3.614061 | -0.165929 |
| 6 | 6 | 0.715576 | -4.893019 | -0.313282 |
| 7 | 1 | 1.160254 | -4.943619 | -1.311334 |
| 8 | 1 | 1.495121 | -4.962836 | 0.450619 |
| 9 | 1 | -0.013459 | -5.695612 | -0.183540 |
| 10 | 6 | -2.872525 | -1.546061 | 0.386885 |
| 11 | 1 | -3.144847 | -0.926281 | -0.471978 |
| 12 | 1 | -3.597539 | -2.352213 | 0.516527 |
| 13 | 1 | -2.821120 | -0.933039 | 1.291027 |
| 14 | 1 | -2.007720 | -4.249211 | 0.195498 |
| 15 | 17 | -0.324858 | 0.246692 | -0.050008 |
| 16 | 17 | 2.251572 | -2.147600 | -0.557700 |
| 17 | 17 | -0.933321 | 3.529145 | 0.010684 |
| 18 | 1 | 0.054285 | 4.326335 | 0.249916 |

**5**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.241353 | -1.109248 | 0.094640 |
| 2 | 6 | 0.127466 | -1.182612 | 0.119430 |
| 3 | 6 | -0.438983 | 0.942999 | 0.033852 |
| 4 | 7 | -1.567091 | 0.231418 | 0.040508 |
| 5 | 7 | 0.603294 | 0.112272 | 0.081143 |
| 6 | 6 | 2.014926 | 0.503635 | 0.094757 |
| 7 | 1 | 2.472758 | 0.153080 | 1.024349 |
| 8 | 1 | 2.517163 | 0.051472 | -0.765227 |
| 9 | 1 | 2.067851 | 1.592770 | 0.034058 |
| 10 | 6 | -2.926188 | 0.776030 | -0.010095 |
| 11 | 1 | -3.467866 | 0.470118 | 0.889422 |
| 12 | 1 | -2.855691 | 1.864844 | -0.057887 |
| 13 | 1 | -3.430284 | 0.389827 | -0.900735 |
| 14 | 1 | -0.378262 | 2.023975 | -0.004367 |
| 15 | 35 | -2.500185 | -2.459216 | 0.120445 |
| 16 | 35 | 1.226365 | -2.662546 | 0.176015 |
| 17 | 17 | -4.894974 | -4.732045 | -0.043639 |
| 18 | 1 | -4.712683 | -5.632769 | 0.864243 |

**5**-HBr

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 1 | 6 | 0.433901 | -7.061791 | 0.208009 |
| 2 | 6 | 1.382656 | -6.113903 | -0.076099 |
| 3 | 6 | 2.391993 | -8.063930 | 0.120282 |
| 4 | 7 | 1.090618 | -8.270276 | 0.325473 |
| 5 | 7 | 2.596974 | -6.769130 | -0.124725 |
| 6 | 6 | 3.892170 | -6.141903 | -0.399289 |
| 7 | 1 | 3.868273 | -5.696599 | -1.398151 |
| 8 | 1 | 4.077923 | -5.369412 | 0.352115 |
| 9 | 1 | 4.663092 | -6.913766 | -0.346287 |
| 10 | 6 | 0.461751 | -9.558587 | 0.626957 |
| 11 | 1 | -0.274338 | -9.785309 | -0.149607 |
| 12 | 1 | 1.241570 | -10.323262 | 0.643605 |
| 13 | 1 | -0.028431 | -9.496017 | 1.602862 |
| 14 | 1 | 3.160552 | -8.827103 | 0.150266 |
| 15 | 35 | -1.388705 | -6.879513 | 0.421592 |
| 16 | 35 | 1.198751 | -4.297263 | -0.358230 |
| 17 | 1 | -0.424052 | -0.768463 | -0.917749 |
| 18 | 35 | 0.991327 | -0.899093 | -0.790289 |

**5**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.144809 | -0.409636 | 0.138997 |
| 2 | 6 | 1.224998 | -0.422336 | 0.085148 |
| 3 | 6 | 0.556253 | 1.669059 | -0.078557 |
| 4 | 7 | -0.534837 | 0.910817 | 0.034719 |
| 5 | 7 | 1.637145 | 0.888052 | -0.051015 |
| 6 | 6 | 3.026668 | 1.341007 | -0.148930 |
| 7 | 1 | 3.564667 | 1.039363 | 0.754251 |
| 8 | 1 | 3.488612 | 0.886970 | -1.030435 |
| 9 | 1 | 3.024804 | 2.429202 | -0.241509 |

| | | | | |
|---|---|---|---|---|
| 10 | 6 | -1.918287 | 1.392492 | 0.047765 |
| 11 | 1 | -2.385734 | 1.106681 | 0.994495 |
| 12 | 1 | -1.902343 | 2.479738 | -0.053785 |
| 13 | 1 | -2.459798 | 0.941079 | -0.788450 |
| 14 | 1 | 0.564325 | 2.747817 | -0.177121 |
| 15 | 35 | -1.337747 | -1.809756 | 0.323560 |
| 16 | 35 | 2.393341 | -1.846078 | 0.170283 |
| 17 | 53 | -3.511911 | -4.660251 | 0.886076 |
| 18 | 1 | -4.387793 | -4.646775 | -0.475326 |

**6**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.546781 | 2.724801 | -0.122011 |
| 2 | 6 | 2.919902 | 2.740068 | -0.076165 |
| 3 | 6 | 2.214509 | 4.827855 | -0.005280 |
| 4 | 7 | 1.137555 | 4.045338 | -0.076680 |
| 5 | 7 | 3.308121 | 4.065397 | -0.002560 |
| 6 | 6 | 4.683736 | 4.559597 | 0.076541 |
| 7 | 1 | 5.156017 | 4.156416 | 0.977171 |
| 8 | 1 | 5.233576 | 4.235795 | -0.811752 |
| 9 | 1 | 4.653618 | 5.650498 | 0.123621 |
| 10 | 6 | -0.248348 | 4.516159 | -0.106481 |
| 11 | 1 | -0.786945 | 4.094573 | 0.747147 |
| 12 | 1 | -0.241993 | 5.606852 | -0.047448 |
| 13 | 1 | -0.715708 | 4.191144 | -1.040531 |
| 14 | 1 | 2.203647 | 5.910016 | 0.043170 |
| 15 | 53 | 0.237170 | 1.121327 | -0.226524 |
| 16 | 53 | 4.250017 | 1.166502 | -0.113436 |
| 17 | 53 | -2.124331 | -1.673160 | -0.347557 |
| 18 | 1 | -1.054137 | -2.730098 | 0.256706 |

---

**7**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.829115 | 0.988114 | 0.559483 |
| 2 | 6 | 2.639432 | -0.121031 | 0.510343 |
| 3 | 6 | 0.743690 | -0.757844 | -0.166455 |
| 4 | 7 | 0.598576 | 0.559085 | 0.116362 |
| 5 | 1 | 1.964678 | 2.030754 | 0.850727 |
| 6 | 1 | 3.686395 | -0.194843 | 0.779815 |
| 7 | 7 | 1.944383 | -1.222597 | 0.049976 |
| 8 | 6 | -0.598384 | 1.378333 | -0.012090 |
| 9 | 1 | -0.931811 | 1.379970 | -1.056097 |
| 10 | 1 | -1.393201 | 0.970009 | 0.622461 |
| 11 | 1 | -0.335163 | 2.396336 | 0.309013 |
| 12 | 17 | -0.593119 | -1.687411 | -0.760303 |
| 13 | 17 | 0.930775 | 4.307101 | 1.115926 |

**8**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.456839 | 0.739125 | -0.117190 |
| 2 | 6 | 2.491677 | -0.632747 | -0.124582 |
| 3 | 6 | 0.428532 | -0.101504 | 0.034779 |
| 4 | 7 | 1.124319 | 1.071754 | -0.015931 |
| 5 | 1 | 3.231730 | 1.493413 | -0.176393 |
| 6 | 1 | 3.361116 | -1.277660 | -0.192345 |
| 7 | 7 | 1.221695 | -1.149867 | -0.029456 |
| 8 | 6 | 0.558350 | 2.405414 | 0.047502 |
| 9 | 1 | -0.183278 | 2.537703 | -0.746907 |
| 10 | 1 | 0.060701 | 2.561192 | 1.011006 |
| 11 | 1 | 1.369938 | 3.128512 | -0.074318 |
| 12 | 35 | -1.447165 | -0.069843 | 0.179976 |
| 13 | 17 | -4.461054 | 0.386783 | 0.409766 |

**8**-$Br^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.383699 | 0.729558 | -0.100783 |
| 2 | 6 | 2.422953 | -0.642216 | -0.113214 |
| 3 | 6 | 0.358780 | -0.117241 | 0.023444 |
| 4 | 7 | 1.049458 | 1.058688 | -0.014182 |
| 5 | 1 | 3.157078 | 1.486227 | -0.147370 |
| 6 | 1 | 3.294841 | -1.284375 | -0.173268 |
| 7 | 7 | 1.153372 | -1.163467 | -0.035420 |
| 8 | 6 | 0.478445 | 2.390696 | 0.050022 |
| 9 | 1 | -0.261571 | 2.521402 | -0.746012 |
| 10 | 1 | -0.021429 | 2.543639 | 1.012793 |
| 11 | 1 | 1.287918 | 3.116377 | -0.069230 |
| 12 | 35 | -1.516093 | -0.091847 | 0.145266 |
| 13 | 35 | -4.724603 | 0.498888 | 0.343849 |

**8**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.457317 | 0.752183 | -0.117746 |

| | | | | |
|---|---|---|---|---|
| 2 | 6 | 2.531346 | -0.618366 | -0.126789 |
| 3 | 6 | 0.459013 | -0.144509 | 0.033924 |
| 4 | 7 | 1.116907 | 1.048694 | -0.015306 |
| 5 | 1 | 3.210718 | 1.527857 | -0.176155 |
| 6 | 1 | 3.418135 | -1.238722 | -0.195477 |
| 7 | 7 | 1.276202 | -1.171262 | -0.031541 |
| 8 | 6 | 0.512426 | 2.366480 | 0.051513 |
| 9 | 1 | -0.233767 | 2.479529 | -0.741467 |
| 10 | 1 | 0.013633 | 2.506640 | 1.016648 |
| 11 | 1 | 1.303326 | 3.111565 | -0.071015 |
| 12 | 35 | -1.412662 | -0.163169 | 0.175442 |
| 13 | 53 | -4.855061 | 0.602315 | 0.402020 |

**9**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.446908 | 0.744469 | -0.110152 |
| 2 | 6 | 2.485985 | -0.627294 | -0.117701 |
| 3 | 6 | 0.413832 | -0.100548 | 0.029491 |
| 4 | 7 | 1.113273 | 1.073644 | -0.017244 |
| 5 | 1 | 3.220429 | 1.500731 | -0.164561 |
| 6 | 1 | 3.357651 | -1.269976 | -0.180503 |
| 7 | 7 | 1.216365 | -1.144993 | -0.030754 |
| 8 | 6 | 0.560655 | 2.412788 | 0.045025 |
| 9 | 1 | -0.182985 | 2.552327 | -0.746541 |
| 10 | 1 | 0.072556 | 2.580707 | 1.011829 |

| | | | | |
|---|---|---|---|---|
| 11 | 1 | 1.378006 | 3.128209 | -0.085080 |
| 12 | 53 | -1.697657 | -0.108454 | 0.179789 |
| 13 | 53 | -5.128966 | 0.130007 | 0.434289 |

**10**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.519530 | 0.034192 | -0.159054 |
| 2 | 6 | 1.595115 | -0.953968 | -0.383437 |
| 3 | 7 | 1.807862 | 1.204580 | -0.105991 |
| 4 | 7 | 0.346890 | -0.435369 | -0.470076 |
| 5 | 6 | 2.338362 | 2.543061 | 0.111867 |
| 6 | 1 | 1.487420 | 3.240764 | 0.087683 |
| 7 | 1 | 2.842051 | 2.581289 | 1.084682 |
| 8 | 1 | 3.057081 | 2.782276 | -0.680303 |
| 9 | 6 | 0.504130 | 0.870859 | -0.298778 |
| 10 | 1 | -0.266120 | 1.644516 | -0.300346 |
| 11 | 17 | 4.224411 | -0.027476 | 0.032961 |
| 12 | 17 | 1.924337 | -2.645004 | -0.540150 |
| 13 | 17 | -0.707182 | 4.116979 | -0.090459 |

**11**-$Cl^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.292191 | 0.576913 | 0.007638 |
| 2 | 6 | 2.164785 | -0.789273 | -0.122232 |
| 3 | 7 | 0.996170 | 1.039764 | -0.026969 |
| 4 | 7 | 0.861886 | -1.170600 | -0.232121 |
| 5 | 6 | 0.596694 | 2.430187 | 0.071053 |
| 6 | 1 | -0.495049 | 2.475973 | 0.014294 |
| 7 | 1 | 0.944176 | 2.853140 | 1.019553 |
| 8 | 1 | 1.041525 | 3.006143 | -0.747455 |
| 9 | 35 | 3.739909 | 1.757442 | 0.199252 |
| 10 | 35 | 3.574657 | -2.025355 | -0.156517 |
| 11 | 6 | 0.184376 | -0.041782 | -0.170565 |
| 12 | 1 | -0.894805 | 0.051451 | -0.224930 |
| 13 | 17 | 5.792756 | 3.903471 | 0.513929 |

**11**-$Br^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.433604 | -3.570420 | 0.080661 |
| 2 | 6 | 2.420471 | -2.615580 | 0.196029 |
| 3 | 7 | 0.266212 | -2.845320 | 0.007298 |
| 4 | 7 | 1.906350 | -1.354810 | 0.196146 |
| 5 | 6 | -1.065905 | -3.401723 | -0.131745 |
| 6 | 1 | -1.778138 | -2.572089 | -0.170321 |
| 7 | 1 | -1.129050 | -3.996057 | -1.049335 |
| 8 | 1 | -1.291843 | -4.052661 | 0.719308 |
| 9 | 35 | 1.417930 | -5.442854 | 0.012703 |
| 10 | 35 | 4.261632 | -2.941583 | 0.328628 |
| 11 | 6 | 0.605498 | -1.530448 | 0.080770 |
| 12 | 1 | -0.137734 | -0.741509 | 0.042878 |
| 13 | 35 | 0.887683 | -8.595118 | -0.157279 |

**11**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.266133 | 0.524323 | 0.008590 |
| 2 | 6 | 2.113066 | -0.839544 | -0.108275 |
| 3 | 7 | 0.983450 | 1.019683 | -0.034103 |
| 4 | 7 | 0.802233 | -1.189719 | -0.218637 |
| 5 | 6 | 0.615206 | 2.420632 | 0.051372 |
| 6 | 1 | -0.474722 | 2.489573 | -0.011582 |
| 7 | 1 | 0.966258 | 2.842693 | 0.998879 |
| 8 | 1 | 1.076456 | 2.979849 | -0.769415 |
| 9 | 35 | 3.734444 | 1.668909 | 0.191596 |
| 10 | 35 | 3.494452 | -2.105733 | -0.125545 |
| 11 | 6 | 0.149832 | -0.045429 | -0.169910 |
| 12 | 1 | -0.926784 | 0.070774 | -0.228519 |
| 13 | 53 | 5.964482 | 4.290435 | 0.564516 |

**12**-$I^-$

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.339371 | 0.580991 | -0.086443 |
| 2 | 6 | 2.257233 | -0.788131 | -0.246024 |

| | | | | |
|---|---|---|---|---|
| 3 | 7 | 1.027266 | 0.997870 | -0.165265 |
| 4 | 7 | 0.971233 | -1.211295 | -0.415598 |
| 5 | 6 | 0.558735 | 2.365924 | -0.062173 |
| 6 | 1 | -0.532056 | 2.361484 | -0.151719 |
| 7 | 1 | 0.853158 | 2.791977 | 0.902969 |
| 8 | 1 | 0.996441 | 2.975772 | -0.859997 |
| 9 | 53 | 3.935871 | 1.943841 | 0.213126 |
| 10 | 53 | 3.859624 | -2.120380 | -0.239446 |
| 11 | 6 | 0.256638 | -0.105742 | -0.361532 |
| 12 | 1 | -0.822419 | -0.045305 | -0.456895 |
| 13 | 53 | 6.316435 | 4.270377 | 0.685273 |

**Neutral complexes**

**7**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 5.560195 | 1.718064 | -0.349854 |
| 2 | 6 | 5.192704 | 0.404085 | -0.207177 |
| 3 | 6 | 3.394474 | 1.521376 | -0.200229 |
| 4 | 7 | 4.385543 | 2.439002 | -0.344852 |
| 5 | 1 | 6.523195 | 2.201824 | -0.453994 |
| 6 | 1 | 5.831910 | -0.469774 | -0.168568 |
| 7 | 7 | 3.824335 | 0.292687 | -0.113817 |
| 8 | 6 | 4.233073 | 3.877505 | -0.460248 |
| 9 | 1 | 3.611379 | 4.123274 | -1.327363 |

| | | | | |
|---|---|---|---|---|
| 10 | 1 | 3.768090 | 4.283762 | 0.444412 |
| 11 | 1 | 5.225770 | 4.315477 | -0.587696 |
| 12 | 17 | 1.746111 | 2.015097 | -0.151966 |
| 13 | 17 | -1.423112 | 0.386186 | -0.198244 |
| 14 | 1 | -2.695805 | 0.177627 | -0.199283 |

**8**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 3.346182 | 6.504918 | 0.520716 |
| 2 | 6 | 4.163661 | 5.404588 | 0.579102 |
| 3 | 6 | 2.178414 | 4.662257 | 0.539985 |
| 4 | 7 | 2.058686 | 6.016098 | 0.496056 |
| 5 | 1 | 3.549967 | 7.567885 | 0.495945 |
| 6 | 1 | 5.246101 | 5.374988 | 0.613701 |
| 7 | 7 | 3.416449 | 4.249760 | 0.590659 |
| 8 | 6 | 0.831059 | 6.787774 | 0.433503 |
| 9 | 1 | 0.278304 | 6.548842 | -0.481360 |
| 10 | 1 | 0.202169 | 6.566717 | 1.302269 |
| 11 | 1 | 1.095592 | 7.847879 | 0.434109 |
| 12 | 35 | 0.662880 | 3.562569 | 0.527669 |
| 13 | 17 | -2.563398 | 2.143911 | 0.398835 |
| 14 | 1 | -2.748310 | 0.866953 | 0.400177 |

**8**-HBr

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -3.995820 | 0.349507 | -0.038250 |
| 2 | 6 | -3.956140 | -1.021882 | -0.039917 |
| 3 | 6 | -1.937847 | -0.374286 | 0.002333 |
| 4 | 7 | -2.682187 | 0.763422 | -0.010659 |
| 5 | 1 | -4.813968 | 1.058419 | -0.054806 |
| 6 | 1 | -4.787229 | -1.716841 | -0.057603 |
| 7 | 7 | -2.654485 | -1.466052 | -0.014808 |
| 8 | 6 | -2.195214 | 2.130465 | 0.004441 |
| 9 | 1 | -1.613057 | 2.314284 | 0.913643 |
| 10 | 1 | -1.564162 | 2.316858 | -0.870861 |
| 11 | 1 | -3.058347 | 2.799911 | -0.018324 |
| 12 | 35 | -0.067452 | -0.299627 | 0.040874 |
| 13 | 1 | 3.972203 | -1.260886 | -0.075511 |
| 14 | 35 | 3.545492 | 0.096879 | -0.018871 |

**8**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.572409 | 0.852461 | -0.158585 |
| 2 | 6 | 2.646418 | -0.517630 | -0.154614 |
| 3 | 6 | 0.591166 | -0.038142 | 0.044850 |
| 4 | 7 | 1.235271 | 1.156935 | -0.029818 |
| 5 | 1 | 3.325591 | 1.625849 | -0.241479 |
| 6 | 1 | 3.528754 | -1.141333 | -0.235306 |
| 7 | 7 | 1.392020 | -1.067295 | -0.026155 |
| 8 | 6 | 0.639970 | 2.478970 | 0.030894 |
| 9 | 1 | -0.100171 | 2.596322 | -0.767342 |
| 10 | 1 | 0.151853 | 2.630450 | 0.999641 |
| 11 | 1 | 1.435113 | 3.217191 | -0.096991 |
| 12 | 35 | -1.272095 | -0.116969 | 0.227924 |
| 13 | 53 | -5.059884 | -0.098573 | 0.493873 |
| 14 | 1 | -5.303718 | -1.696097 | 0.491117 |

**9**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 5.682061 | 3.187928 | -0.200127 |
| 2 | 6 | 5.775766 | 1.819057 | -0.175703 |
| 3 | 6 | 3.707981 | 2.273649 | 0.012104 |
| 4 | 7 | 4.341348 | 3.476204 | -0.079531 |
| 5 | 1 | 6.425221 | 3.969938 | -0.292733 |
| 6 | 1 | 6.666897 | 1.206377 | -0.245087 |
| 7 | 7 | 4.528940 | 1.256076 | -0.042042 |
| 8 | 6 | 3.740987 | 4.796691 | -0.035038 |
| 9 | 1 | 2.984384 | 4.894526 | -0.820350 |
| 10 | 1 | 3.272407 | 4.970328 | 0.940042 |
| 11 | 1 | 4.529822 | 5.535462 | -0.196315 |
| 12 | 53 | 1.640803 | 2.128185 | 0.218595 |
| 13 | 53 | -2.191924 | 2.629547 | 0.757040 |
| 14 | 1 | -3.066668 | 1.268513 | 0.753756 |

**10**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 2.437158 | -3.963406 | -0.008725 |
| 2 | 6 | 3.312113 | -2.936128 | -0.265617 |
| 3 | 7 | 3.181100 | -5.114784 | -0.084959 |

| | | | | |
|---|---|---|---|---|
| 4 | 7 | 4.561108 | -3.416690 | -0.496027 |
| 5 | 6 | 2.693770 | -6.467351 | 0.106894 |
| 6 | 1 | 3.541058 | -7.150067 | 0.002547 |
| 7 | 1 | 2.259016 | -6.571852 | 1.106359 |
| 8 | 1 | 1.934760 | -6.705196 | -0.646031 |
| 9 | 6 | 4.449796 | -4.723978 | -0.381275 |
| 10 | 1 | 5.254504 | -5.440207 | -0.502803 |
| 11 | 17 | 0.765422 | -3.972614 | 0.346395 |
| 12 | 17 | 2.931914 | -1.261248 | -0.296443 |
| 13 | 17 | -2.394467 | -2.541644 | 0.903098 |
| 14 | 1 | -3.644075 | -2.790225 | 1.104440 |

**11**-HCl

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 1.017166 | -1.301949 | -0.398906 |
| 2 | 6 | 1.085470 | -2.669785 | -0.521013 |
| 3 | 7 | -0.318914 | -0.989873 | -0.475585 |
| 4 | 7 | -0.155701 | -3.201964 | -0.668479 |
| 5 | 6 | -0.905449 | 0.334645 | -0.399720 |
| 6 | 1 | -1.988618 | 0.230890 | -0.506124 |
| 7 | 1 | -0.673397 | 0.795485 | 0.566376 |
| 8 | 1 | -0.516044 | 0.965861 | -1.205580 |
| 9 | 35 | 2.339719 | -0.015870 | -0.170718 |
| 10 | 35 | 2.637497 | -3.709891 | -0.500396 |
| 11 | 6 | -0.974028 | -2.170485 | -0.637129 |
| 12 | 1 | -2.053640 | -2.218516 | -0.726482 |

| | | | | |
|---|---|---|---|---|
| 13 | 17 | 5.358271 | 1.701636 | 0.301145 |
| 14 | 1 | 5.556786 | 2.976343 | 0.293180 |

**11**-HBr

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -0.788369 | 0.834452 | -0.056250 |
| 2 | 6 | -0.834251 | -0.539700 | -0.038316 |
| 3 | 7 | -2.096587 | 1.246804 | -0.138701 |
| 4 | 7 | -2.117839 | -0.979522 | -0.105058 |
| 5 | 6 | -2.571312 | 2.616239 | -0.197711 |
| 6 | 1 | -3.661772 | 2.592754 | -0.271477 |
| 7 | 1 | -2.275467 | 3.158368 | 0.706600 |
| 8 | 1 | -2.153871 | 3.121010 | -1.075541 |
| 9 | 35 | 0.641570 | 2.020418 | 0.004993 |
| 10 | 35 | 0.631439 | -1.694475 | 0.051167 |
| 11 | 6 | -2.849213 | 0.114281 | -0.164404 |
| 12 | 1 | -3.931226 | 0.147387 | -0.227467 |
| 13 | 1 | 3.139793 | 5.204807 | 0.890722 |
| 14 | 35 | 3.499324 | 4.232797 | -0.089826 |

**11**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | 0.872766 | -0.426514 | -0.916844 |
| 2 | 6 | 1.665437 | -1.539421 | -1.069261 |
| 3 | 7 | -0.421479 | -0.878039 | -1.008663 |
| 4 | 7 | 0.904654 | -2.650333 | -1.249812 |
| 5 | 6 | -1.627877 | -0.077150 | -0.918940 |
| 6 | 1 | -2.485604 | -0.746502 | -1.026048 |
| 7 | 1 | -1.674352 | 0.427146 | 0.052055 |
| 8 | 1 | -1.643588 | 0.671679 | -1.718111 |
| 9 | 35 | 1.297282 | 1.361800 | -0.636900 |
| 10 | 35 | 3.532461 | -1.581272 | -1.043071 |
| 11 | 6 | -0.339725 | -2.220584 | -1.208815 |
| 12 | 1 | -1.224661 | -2.838222 | -1.316254 |
| 13 | 53 | 3.409573 | 4.443400 | -0.236405 |
| 14 | 1 | 2.837723 | 5.949547 | -0.099576 |

**12**-HI

| Center Number | Atomic Number | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | 6 | -1.816752 | 1.686712 | -0.095420 |
| 2 | 6 | -0.933052 | 2.742879 | -0.033619 |
| 3 | 7 | -3.061684 | 2.260022 | -0.221564 |
| 4 | 7 | -1.593564 | 3.929751 | -0.116575 |
| 5 | 6 | -4.333878 | 1.570983 | -0.329755 |
| 6 | 1 | -5.121702 | 2.324933 | -0.409918 |
| 7 | 1 | -4.344001 | 0.934335 | -1.220874 |
| 8 | 1 | -4.505135 | 0.953659 | 0.558647 |
| 9 | 53 | -1.509001 | -0.358958 | -0.027446 |
| 10 | 53 | 1.131989 | 2.631048 | 0.157508 |
| 11 | 6 | -2.864954 | 3.605045 | -0.228507 |
| 12 | 1 | -3.689081 | 4.304459 | -0.317490 |
| 13 | 53 | 0.067435 | -3.887858 | 0.258473 |
| 14 | 1 | -0.883180 | -5.121666 | -0.175465 |