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Supplementary Information

Halogen Bonding in Differently Charged Complexes: Basic Profile, Essential Interaction Terms and Intrinsic σ-Hole

Zhengdan Zhu,[#[a,b]] Guimin Wang,[#[a,b]] Zhijian Xu,*[[a,b]] Zhaoqiang Chen,[[a,b]] Jinan Wang,[[a,b]] Jiye Shi,[[a]] and Weiliang Zhu*[[a,b,c]]

[a] CAS Key Laboratory of Receptor Research, Drug Discovery and Design Center, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, China.

[b] University of Chinese Academy of Sciences, Beijing 100049, China.

[c] Open Studio for Druggability Research of Marine Natural Products, Pilot National Laboratory for Marine Science and Technology (Qingdao), 1 Wenhai Road, Aoshanwei, Jimo, Qingdao, 266237, China.

# Z.Z. and G.W. contributed equally to this work.

*Emails: zjxu@simm.ac.cn (Z.X.); wlzhu@simm.ac.cn (W.Z.)

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1. Computational Details

1.1 PDB survey

Complex structures in the Protein Data Bank[1] (PDB, July 2018 release) with halogenated ligands were surveyed to demonstrate the existence of all 9 different charged XB-like interactions. The restriction criterion of interaction distance was set to be less than the sum of atomic van der Waals radii + 0.1 angstrom while that of interaction angle to be larger than 140°. The Epik module in the Schrödinger program suite[2] was applied to predict the protonation status of the complexes. 9 structures with typical halogen bonding patterns and resolutions of 3.0 Å or better were chosen to be presented in Figure S1. However, rather than an exhaustive investigation, we surveyed the PDB only for 9 types of typical structures (which may not be the best) that take halogen "diversity" (4 cases for Cl, 3 for Br, 2 for I in the 9 selected cases) into consideration. The number of cases in each type was not counted.

1.2 Geometry Optimization

Geometry optimization was performed with Gaussian 09 program suite[3] using the M06-2*X* functional[4] either in the gas phase or with implicit solvents, including chloroform (TCM), dichloroethane (DCE), acetone, DMSO and water. The default IEFPCM (Polarizable Continuum Model using the Integral Equation Formalism variant) solvent model[5] was applied to determine solvent effects. Default settings were applied for all parameters in the IEFPCM model including UFF for atomic radii, scaled vdW for cavity type, GePol for cavity algorithm and so on. As suggested by Tomasi et al.,[6] rather than absolute precise values that are comparable with experimental results, what really expected are the trends when

apply theoretical calculations to chemical problems. Calculations showed that there is no significant difference in tendency of intermolecular binding energies with changes in atomic radii applied in the solvent model (Table S27-S29). The triple-ζ basis set 6-311++G(d,p), having considered diffusion functions for the better description of intermolecular weak interactions, especially those involved anionic molecules, was employed for all atoms except iodine, for which the Stuttgart/Dresden effective core pseudopotentials (SDD) and its associated basis set was adopted. Frequency analysis was conducted at the same calculation level with geometry optimizations for the local energy minima confirmation.

However, not all the complex can be optimized to the expected geometry. Disturbed by the potential interactions within the substituent groups of the model molecules, the ideal halogen-bonded geometry is not easy to be obtained owing to its intrinsically weak interaction energy. Yet, optimized structure without imaginary frequencies could be obtained as well by fixing the particular plane angles or dihedral angles (see the annotations following the Cartesian coordinates of the corresponding optimized geometries for details) and conducting constrained optimization using the ModRedundant option. For a portion of extreme cases in vacuum, halogen-boned dimers were not obtained even using constrained optimization, probably owing to the strong intermolecular repulsive or attractive interactions. In these specific cases, single-point energy calculations were performed on the TCM-optimized geometries to estimate the binding energy for reference.

1.3 Binding Energy Calculation

The binding energy was determined by subtracting the electronic energy of the halogen bonding donor

and acceptor from that of the molecular complex (see eq 1 in the manuscript). The basis set superposition error (BSSE) was estimated by counterpoise corrections[7] using the COUNTERPOISE keyword. We performed the corrections in vacuum for all solvent phase cases since conducting counterpoise tasks with implicit solvent models is not allowed in Gaussian 09. The alternative approach to perform counterpoise correlations with implicit solvents via setting ghost atoms marked by Bq (eq S1) is debatable, since the difference in environmental molecular distribution of molecular units and complexes, in other words, the difference in cavities of the solutes in the implicit solvent model, will make the precondition of eq S1 untenable, leading the calculated BSSE to be even negative.

$$\mathrm{BSSE} = E^{\mathrm{S}}_{\mathrm{A\_AB}} - E^{\mathrm{S}}_{\mathrm{A\_Bq}} + E^{\mathrm{S}}_{\mathrm{B\_AB}} - E^{\mathrm{S}}_{\mathrm{B\_Bq}} \qquad \text{S1}$$

Here, $E^{\mathrm{S}}_{\mathrm{A\_AB}}$ and $E^{\mathrm{S}}_{\mathrm{B\_AB}}$ are the electronic energies of the structures extracted from the complex geometry in solvent phase with their respective basis sets, while $E^{\mathrm{S}}_{\mathrm{A\_Bq}}$ and $E^{\mathrm{S}}_{\mathrm{B\_Bq}}$ are those calculated with basis sets superposed.

As a result, all BSSE values were estimated from the equivalent gas phase calculation for all solvent phase optimized geometries.

1.4 Energy Decomposition Analysis

Energy decomposition analysis was performed using the ETS-NOCV method based on ADF program package[8] with optimized geometries obtained from Gaussian 09 results. The PBE functional[9] combined with Grimme's DFT-D3 correction[10] improved by a moderate BJ damping function[11] was applied for the assessment of dispersion terms. Standard double-ζ STO basis set with one set of polarization functions

DZP was used for the hydrogen atom while standard triple-ζ STO basis set with one set of polarization functions TZP was used for other atoms except bromine and iodine, for which relativistic effects were considered with zero-order regular approximation (ZORA) and standard triple-ζ STO basis set with two sets of polarization functions TZ2P was adopted. Solvent effects were evaluated using Conductor like Screening Model (COSMO)[12] of solvation as implemented in ADF program. The empirical scaling factor x (eq S2) is specified as 0.5 for chloroform and the default 0 for other solvents to gain essentially better results, especially in solvents with relative small dielectric constant.[6, 13]

$$f(\varepsilon) = (\varepsilon-1)/(\varepsilon+x) \qquad \text{S2}$$

Here, $f(\varepsilon)$ is the scaling function of energy-related terms, ε is the dielectric constant and x is the empirical scaling factor.

1.5 QTAIM Analysis

The quantum theory of atoms in molecules (QTAIM)[14] has been widely applied to describe the concepts of atoms and bonds in various chemical systems by conducting topologic analysis of molecular electron density. According to the QTAIM theory, electronic properties at the bond critical points (BCPs), including electron density (ρ) and its Laplacian ($\nabla^2\rho$), total energy density (H), potential energy density (V), kinetic energy density (G), and the ratio of the absolute value of the first eigenvalue of the Hessian matrix and the corresponding third eigenvalue ($|\lambda_1|/\lambda_3$), are considered to be highly referential to characterize the interactions. Specially, the Laplacian value represents the curvature of the electron density. Positive or negative Laplacian values stand for locally depleted or concentrated electron density,

respectively. Here in our study, QTAIM analysis was performed using the Multiwfn (version 3.4) program[15] with wave functions obtained from Gaussian 09 results.

1.6 NCI Analysis

The non-covalent interactions (NCI) method could be applied[16] to distinguish non-covalent interactions from various terms by a combination of reduced density gradient (RDG) and electron density (ρ) multiplied by the sign of the second eigenvalue of the Hessian matrix (sign(λ_2)).[17] We carried out the NCI analysis using the Multiwfn (version 3.4) program[15] with wave functions obtained from Gaussian 09 results. In order to plot the relevant results with high quality and to economize on computation and storage space, we specially focused the probe points in the halogen-bonded region, rather than the whole molecular system. Hence, a million probe points, consisted of 100 points in each dimension, were applied in a grid space centered on the midpoint of the halogen and the corresponding acceptor oxygen atom, with the extension distance of 4.5 Bohr in the respective *X*, *Y*, *Z* direction. Plots of the RDG versus the electron density (ρ) multiplied by the sign of the second eigenvalue of the Hessian matrix (sign(λ_2)), which distinguishes attractive or repulsive interactions with its negative or positive value, respectively, were presented in our study to probe into the non-covalent profiles (Figure S3-S5).

1.7 Hirshfled Population Analysis

The Hirshfled population analysis (HPA)[18] was conducted for further confirming the results observed in natural population analysis (NPA). This process was performed by Multiwfn[15] with wave functions obtained from Gaussian 09 results using the build-in atomic densities in free-states in the Multiwfn

programe.

1.8 Electron Density Difference Calculation

The electron density difference (EDD) was calculated by subtracting electron density of the individual molecular subunits from the whole system. This process was conducted by Multiwfn[15] with wave functions obtained from Gaussian 09 results.

1.9 Surface Electrostatic Potential Calculation

The electrostatic potentials (ESPs) were calculated using the Multiwfn (version 3.4) program[15] with wave functions obtained from Gaussian 09 results. In our study, all the ESPs were generated on the 0.001 electrons/Bohr^3 isosurface of electronic density.

1.10 Calculation of $E_{\mathbf{bind\_X}}$

The net binding energy ($E_{\mathrm{bind\_X}}$) between the halogen atom and the corresponding XB acceptor is calculated by excluding the contribution of intermolecular Coulombic interactions and other potential non-covalent terms (the background interactions) from the total binding energy (see eq 3 in the manuscript). Albeit Coulombic interactions are well-defined by the reported[19] point-charge model in charged molecules, the precise characterization of the point-charge position is challenging and without any rigorous and universal standard, owing to the charge delocalization in the whole molecule. On the other hand, electrostatic effects involving the neutral molecules could not be easily described by the point-charge model. Correlations leaving out these systems will certainly reduce the systematic comparability and consequently preclude the application of the point-charge strategy in neutral halogen

bonding complexes. The "free radical" strategy enables us to estimate the contribution of the background interaction (E_{bg}) at the same calculation level with total binding energies. In detail, E_{bg} is calculated by subtracting the orbital interaction (E_{orb_SCF}) from the binding energy of free radicalized complex (E_{bind_FR}) (see eq 2 in the manuscript) for the applied molecules (Figure S8). E_{orb_SCF}, originates from the mix of occupied and virtual molecular orbitals, is determined by eq S3, according to that is defined in Multiwfn.[15]

$$E_{orb\_SCF} = E_{SCF\_Last} - E_{SCF\_First} \qquad \text{S3}$$

Here, E_{orb_SCF} is the orbital interaction term evaluated at the same calculation level with total binding energy. E_{SCF_Last} and E_{SCF_First} are the corresponding electronic energy of wave functions obtained after and before the SCF iteration process, in other words, after and before the mix of molecular orbitals, respectively. In detail, E_{SCF_Last} equals to the electronic energy of the free radicalized complex, while combined fragment wave functions are applied as the complex wave function before the SCF iteration process.

1.11 Evaluating the Shape of Halogen Atoms

The axial (r_{ax}) and radial (r_{rad}) distances from the halogen atom to the molecular surface, and their ratios, are employed to evaluate the shape of the halogen atoms. In detail, r_{ax} and r_{rad} stand for the closest distances from nuclei position of the halogen atom to its molecular surface along axial and radial directions of the C-X covalent bond, respectively, as illustrated in Figure S7. Notably, r_{rad} is determined by calculating the distance from the nuclei position to all probe points on the halogen atomic surface

along the radial direction, and then figuring out the shortest, rather than simply (which is not simple in technique) measuring those coplanar with the donor ring. Same with that has been mentioned in ESP calculations, the molecular surface was defined as the 0.001 electrons/Bohr^3 isosurface of electronic density, and was calculated using the Multiwfn (version 3.4) program with wave functions obtained from Gaussian 09 results. The r_{ax} and r_{rad} values are provided respectively in Table S7 and Table S8.

1.12 Distribution of Electrostatic Potential on the Surface of Halogen Atoms

The distribution of electrostatic potential on the surface of halogen atoms are presented to probe into the solvent effects in halogen bonding interaction. The electrostatic potential surface was obtained using the Multiwfn (version 3.4) program[15] as mentioned above. Cartesian coordinates for the probe points (*A*) as well as the corresponding ESP values composing the electrostatic potential surface are all available in the Multiwfn analysis results. The *AXC* angle (Figure S14), is then measured for all probe points on the halogen atomic surface based on the corresponding Cartesian coordinates, rather than simply consider those coplanar with the donor ring. We thus plot the scatter diagrams (Figure S15) simply by extracting probe points with *AXC* angle values ranging from 90° to 180°, and presenting their ESP values, to explore the ESP distribution of the halogen atom.

1.13 Calculation of outer-sphere electron transfer activation barriers from the Marcus theory

The outer-sphere electron transfer activation barriers from the Marcus theory[20] were calculated with Gaussian 09 following the similar scheme with that utilized by Rosokha et al.[21] The G4MP2 theory was applied[22] to calculate the gas-phase thermodynamic energy terms, while conductor-like polarizable

continuum model (CPCM) at HF/6-31+G(d) level with UAHF radii was used for solvation energies[23] and B3LYP/6-311G(d) level for intramolecular reorganization energy and effective molecular radii.

In detail, the outer-sphere electron transfer activation barrier ΔG^* can be evaluated by eq. S4:

$$\Delta G^* = \lambda/4 \{1 + (\Delta G^o + w_p)/\lambda\}^2 \qquad \text{S4}$$

Here, ΔG^o is the free energy that drives the electron transfer reaction in solvents, which was calculated with eq. S5. The G4MP2 theory was applied to evaluate the gas-phase free energy difference (ΔG_{gas}) between the reactants and products while CPCM for solvation energy difference (ΔG_{solv}). $\Delta G_{1atm\text{-}1M}$ in eq. S5 refers to the free energy change from the standard state of gas phase to that of solvent phase while the multiple factor n refers to the equivalent difference between the products and reactants:

$$\Delta G^o = \Delta G_{gas} + \Delta G_{solv} + n \times \Delta G_{1atm\text{-}1M} \qquad \text{S5}$$

w_p in eq S4 describes the work of bring the ionic reactants and products together, which was evaluated through the Coulomb formula as the electric potential difference between the reactants and products based on the effective molecular radii and van der Walls radius of the corresponding molecules and halogen atom respectively. The effective molecular radii were calculated at B3LYP/6-311G(d) level based on the structures optimized in the G4MP2 scheme with 2000 points per Bohr^3 for Monte-Carlo calculation of molar volume (IOp(6/45)=2000). Notably, the work term w_p equals to zero if no ion-ion interaction was presented among either reactants or products.

λ in eq S4 is the total reorganization energy, which was evaluated with eq S6 following the suggestions of Saveant et al.[21, 24] to take into consideration the bond dissociation energy (D_{RBr}) of the carbon-halogen

bond in XB donors. The C-X bond dissociation energies were calculated as the difference in enthalpies in the bond dissociation process applying the G4MP2 theory in gas phase. Intramolecular reorganization energies (λ_i) of electron donors (XB acceptors) were calculated at B3LYP/6-311G(d) level based on the structures optimized in the G4MP2 scheme. λ_s refers to the solvent reorganization energy, which was evaluated with eq S7. [20a, 25]

$$\lambda = \lambda_i + \lambda_s + D_{RBr} \qquad \text{S6}$$

$$\lambda_s = (1/\varepsilon_\infty - 1/\varepsilon_0)\,(Q_{CT} + u)\,(Q_{CT} - v)\,(1/2r_D + 1/2r_A - 1/r_{DA}) \qquad \text{S7}$$

Here, ε_∞ and ε_0 are the optical and static dielectric constants of solvents. Q_{CT} is the transferred charge in the NPA results (Table S18) while u and v refer to the original charge bears on the electron donor and acceptor, respectively. r_D and r_A are the effective molecular radii of the electron donor (XB acceptor) and electron acceptor (XB donor) respectively while r_{DA} refers to their separation.

The final results of outer-sphere electron transfer activation barriers from the Marcus theory are summarized in Table S26.

2. Figures

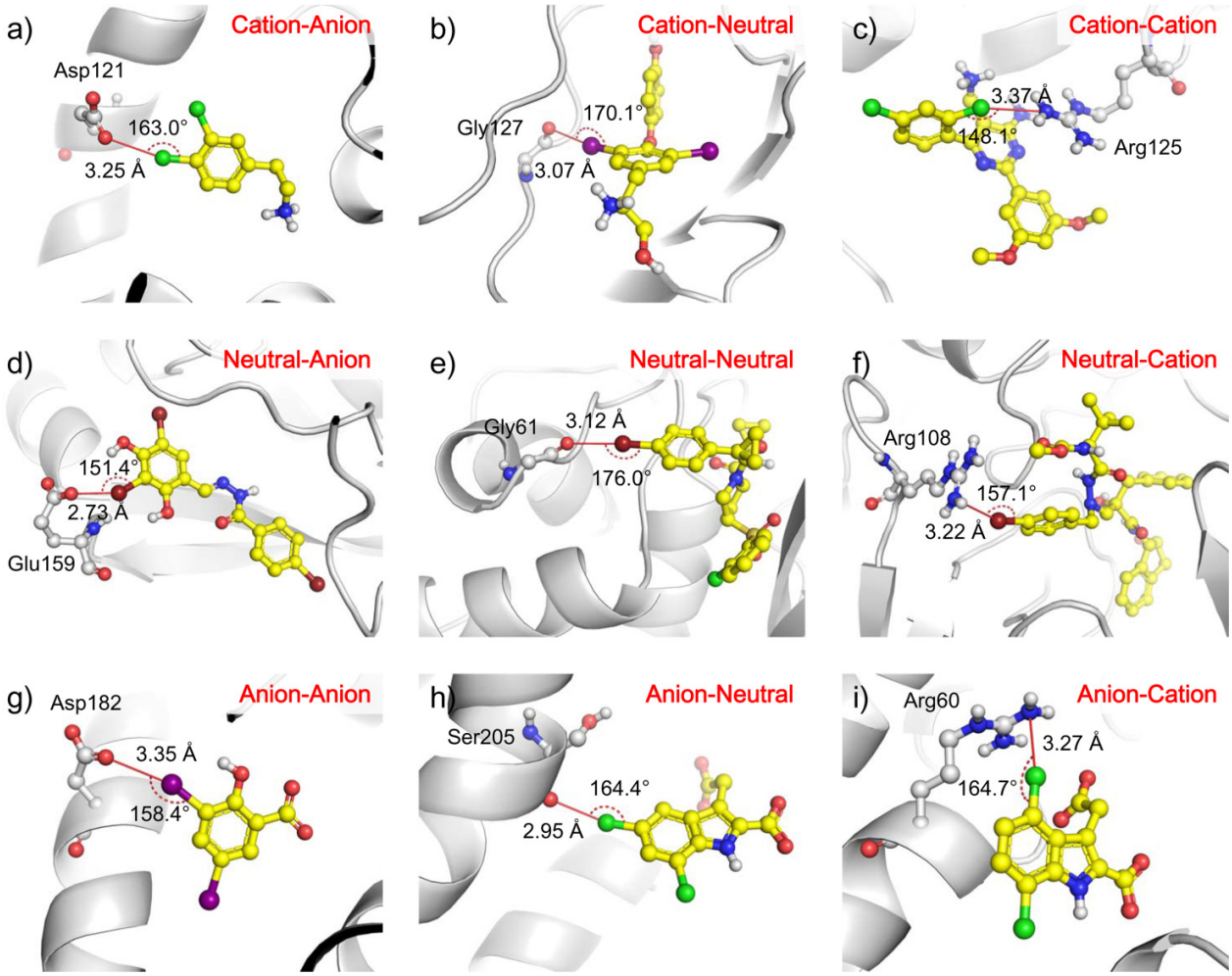

Figure S1. Selected cases for 9 types of differently charged XB-like interactions in PDB, including (a) 4XPA: cation-anion (hereinafter refer to that between cationic donor and anionic acceptor and so forth for others); (b) 3WGW: cation-neutral; (c) 1RWQ: cation-cation; (d) 3DP2: neutral-anion; (e)2YJ2: neutral-neutral; (f) 2CEJ: neutral-cation; (g) 4J2V: anion-anion; (h) 3N5J: anion-neutral; (i) 3N5H: anion-cation. Ligands and the contacting residues are presented as balls and sticks whereas the protein backbones are shown in cartoon. Carbon atoms in ligands and residues are colored in yellow and white, respectively, while oxygen in red, nitrogen in blue, chloride in green, bromine in brown, iodine in purple and polar hydrogen in white. The protonation status of the ligands and residues are predicted with the Epik module in the Schrödinger program suite at pH 7.0 ± 2.0.[2]

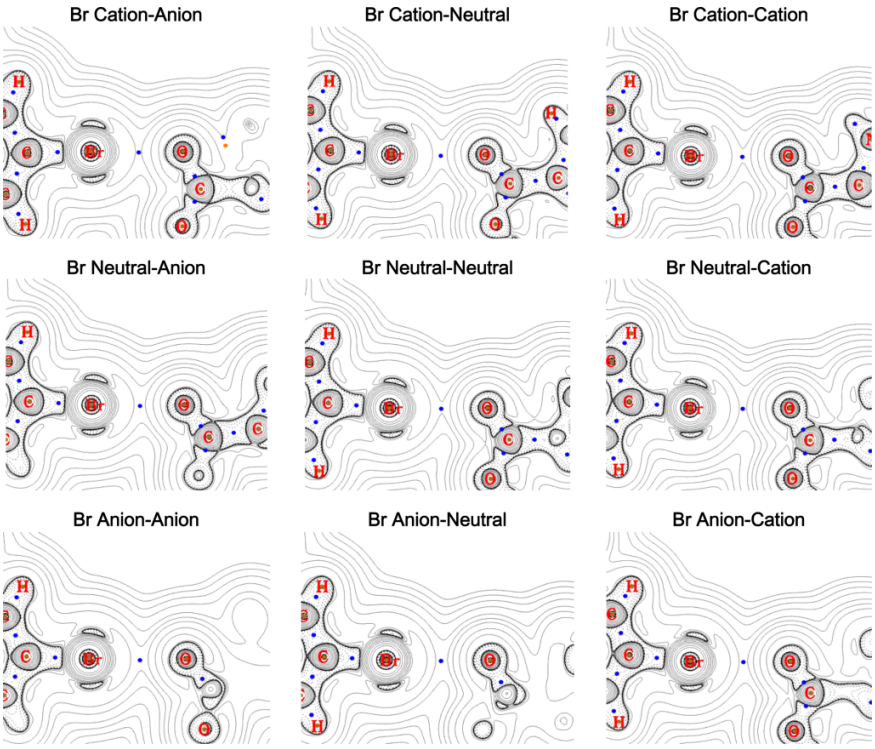

Figure S2. Contour maps of Laplacian distribution for the plane of intermolecular interaction in complexes represented by that between differently charged 3-amino-5-bromobenzoic acid and glycine. Solid and dashed lines stand for positive and negative regions of Laplacian, respectively. Blue points lying on the covalent and halogen bonds represent the bond critical points. Wave functions of optimized geometries in TCM are applied on behalf of all the systems, considering the single-point cases in vacuum. As shown in the figure, the bond critical point, where the electron density gradient modulus is zero, lies between the halogen atom and its corresponding oxygen, in the same way as that of covalent bonds. This means, whatever the molecular charge state is, the second saddle point of the electron density function always exists between the halogen and oxygen atom, where the curvature of the function is positive in one dimension and negative in the other two. Electrons are obviously more concentrated in the radial direction of the bromine atom than that along the C-Br covalent bond, revealing the anisotropic distribution of electrons. All these observations provide further evidence for the formation of intermolecular XBs as well as the intrinsic electrophilicity of a halogen's σ-hole region in all differently charged systems.

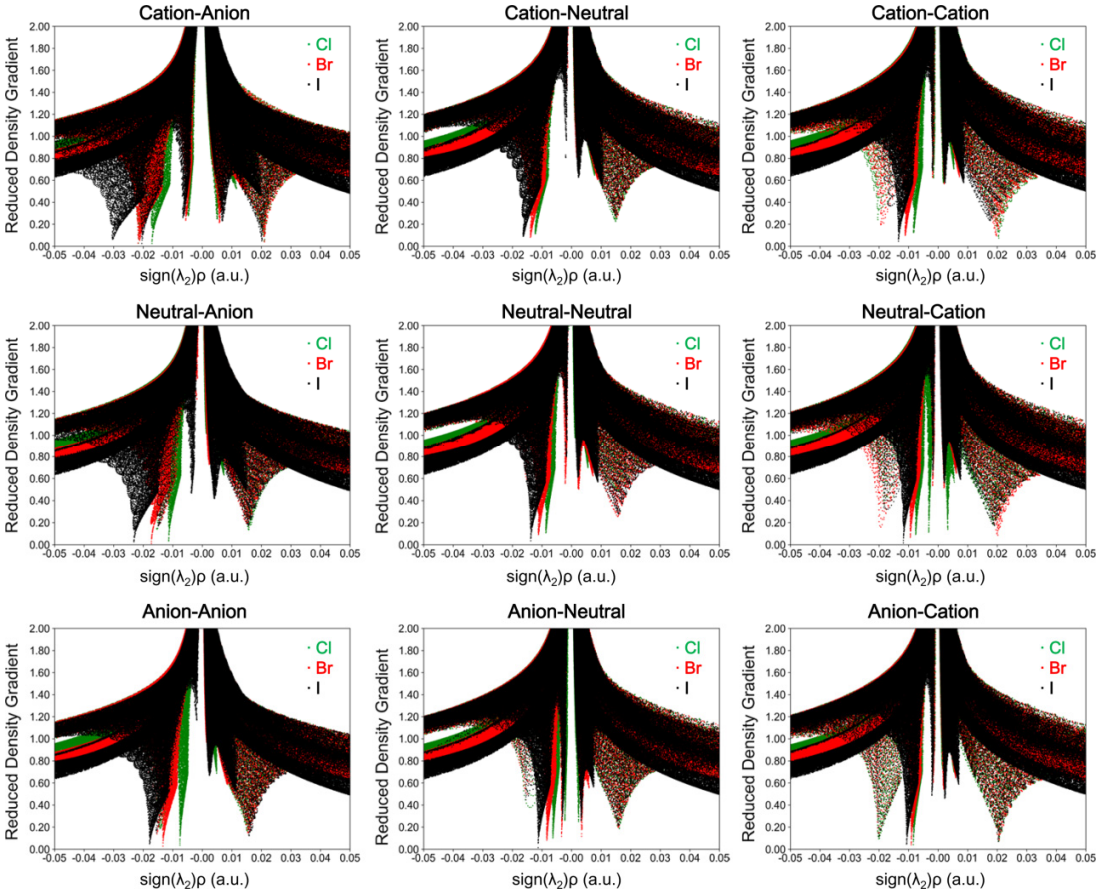

Figure S3. Plots of reduced density gradient (RDG) versus the electron density multiplied by the sign of the second eigenvalue of the Hessian matrix (sign(λ_2)ρ) for complexes between differently charged 3-amino-5-halobenzoic acid (green for Cl, red for Br, black for I) and glycine in TCM. The peaks with negative sign(λ_2)ρ and medium RDG value in the figure indicates the existence of attractive non-covalent interactions. For all the systems, the corresponding |sign(λ_2)ρ| value for the halogen bonding peak (see Figure S4-S5 for discussions on peak attribution) follows the trend of I > Br > Cl, demonstrating that complexes involving iodine may form the strongest halogen bonding interaction. In general, cation-anion complexes have the largest |sign(λ_2)ρ| values while anion-cation cases have the smallest, which are in good agreement with the observation from net binding energy ($E_{\text{bind\_X}}$) (Table 3, Table S9-S10) and amount of electron transferred (Table S17-S19, Table S20-S22). The narrow peak with negative

sign(λ_2)ρ value might be the peak of the secondary halogen bond that forms between the halogen atom and the other carboxyl oxygen atom in the acceptor (Figure S4).

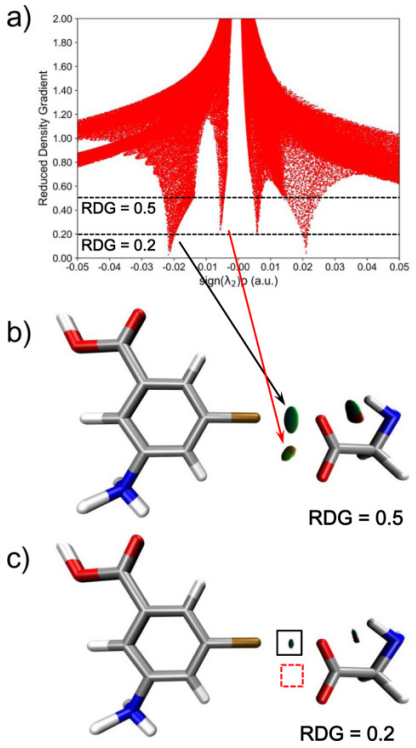

Figure S4. (a) Plots of RDG versus sign(λ_2)ρ for the example system, scatter peaks of the typical and secondary halogen bonds were pointed out by black and red arrows, respectively, associated with (b) the corresponding interaction isosurface for RDG = 0.5 and -0.05 < sign(λ_2)ρ < 0.05 prepared with VMD.[26] Colors vary from blue, green and red stand respectively for attractive, weak dispersion or van der Waals, and repulsive interactions. (c) Similar with b, RDG = 0.2. Interaction isosurface of the typical halogen bond remains (black solid wireframe) while that of secondary halogen bond disappears (red dashed wireframe), which thus attributes the broad peak to halogen bond and the narrow peak to the interaction within the halogen atom and the other carboxyl oxygen atom in the acceptor, or in other words, the secondary halogen bond. Wave function and optimized geometry of the complex between cationic 3-amino-5-bromobenzoic acid donor, and anionic glycine acceptor in TCM was applied for instance, considering the obvious difference of RDG between the corresponding scatter peaks.

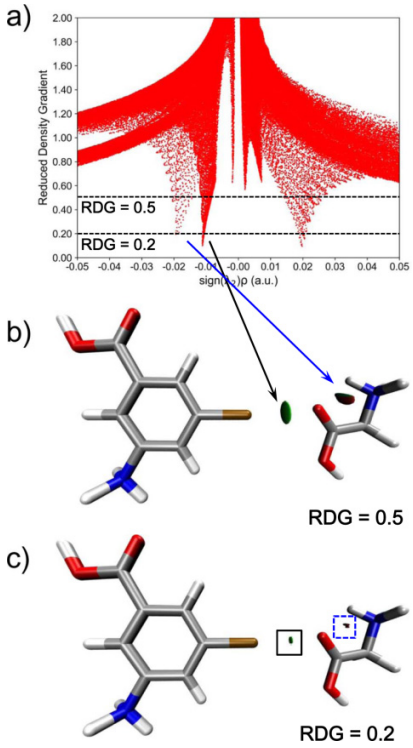

Figure S5. (a) Plots of RDG versus sign(λ_2)ρ for the example system, scatter peaks of intermolecular halogen bond and intramolecular hydrogen bond were pointed out by black and blue arrows, respectively, associated with (b) the corresponding interaction isosurface for RDG = 0.5 and -0.05 < sign(λ_2)ρ < 0.05 prepared with VMD.[26] Colors vary from blue, green and red stand respectively for attractive, weak dispersion or van der Waals, and repulsive interactions. (c) Similar with b, RDG = 0.2. Interaction isosurface of the intermolecular halogen bond remains (black solid wireframe) while that of intramolecular hydrogen bond disappears (blue dashed wireframe, the remaining isosurface colored in red is possibly for the ring critical point), which thus attributes the dark scatter peak with negative λ_2 to intermolecular halogen bond and the lightish one intramolecular hydrogen bond. Scatter peaks with positive λ_2 probably represent various (3,+1) critical points according to the QTAIM theory,[14] namely, the ring critical points or cage critical points. Wave function and optimized geometry of the complex between cationic 3-amino-5-bromobenzoic acid donor, and cationic glycine acceptor in TCM was applied for instance, considering the obvious difference of RDG between the corresponding scatter peaks. However, not all the NCI scatter diagrams are plotted with the hydrogen bonding peaks, since we

have concentrated the limited probe points to the halogen-bonded region as mentioned above in the computational details.

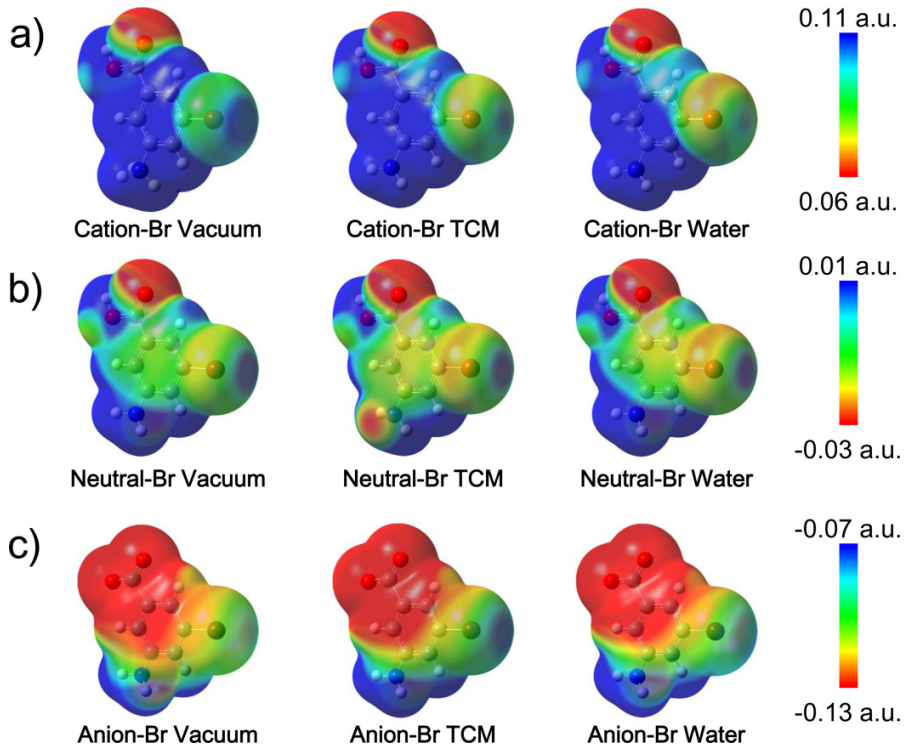

Figure S6. Electrostatic potentials (ESPs) mapped on the 0.001 electrons/Bohr^3 isosurface of electronic density for differently charged XB donors represented by the 3-amino-5-bromobenzoic acid in different environments, including (a) cationic XB donor in vacuum (left), TCM (middle) and water (right); (b) neutral XB donor in vacuum (left), TCM (middle) and water (right); (c) anionic XB donor in in vacuum (left), TCM (middle) and water (right). The scales between the maxima and minima of plotted ESP values have been adjusted to visualize the anisotropy of halogen's electron density more clearly. As a result, a locally less negatively charged region is presented on the halogen atomic surface of all differently charged organobromine donors in different environments. Local electrostatic potential maxima of the halogen atom in XB donors are listed in Table S5. All these evidences suggest the "σ-hole" region (or at least, the local less negatively charged region) exists on halogen atoms in XB donors in all studied systems.

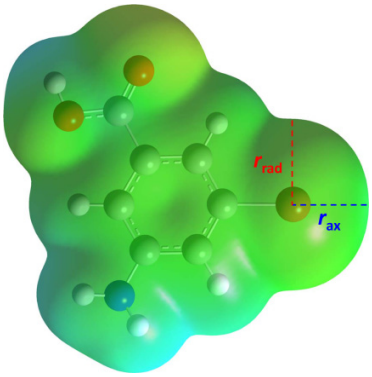

Figure S7. The schematic diagram for the axial (r_{ax}, blue dashed line) and radial distance (r_{rad}, red dashed line) from the nuclei position of the halogen atom to the molecular surface along axial and radial directions, respectively. The values of r_{ax} and r_{rad} and their ratio (r_{ax}/r_{rad}) are applied to evaluate the atomic electron density distribution for differently charged XB donors (Table S6-S8). Notably, r_{rad} is determined by figuring out the probe points with the shortest distance from the nuclei position among all those along the radial direction, rather than simply measuring the points coplanar with the donor ring.

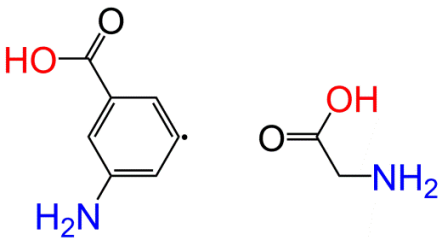

Figure S8. Schematic models of the corresponding free radicalized complexes for applied molecules. The halogen atom is replaced with a free radical to maintain the substituent charge of the XB donor. Both of the subunits could be protonated or deprotonated to mimic differently charged systems.

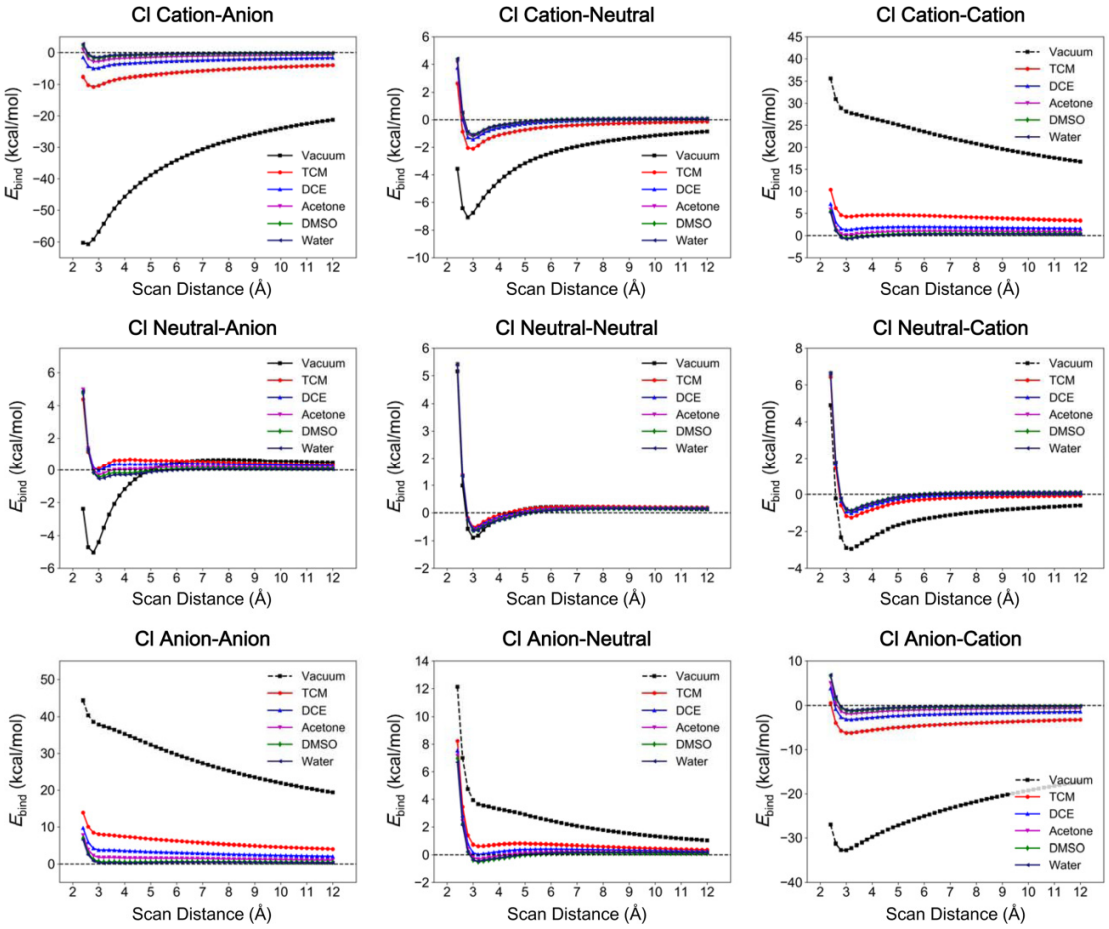

Figure S9. Overall binding energy (E_{bind}) versus intermolecular Cl···O distance of complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine in different environments including vacuum (black, those based on optimized structures in TCM are shown in dashed line), TCM (red), DCE (blue), acetone (magenta), DMSO (green), water (midnightblue).

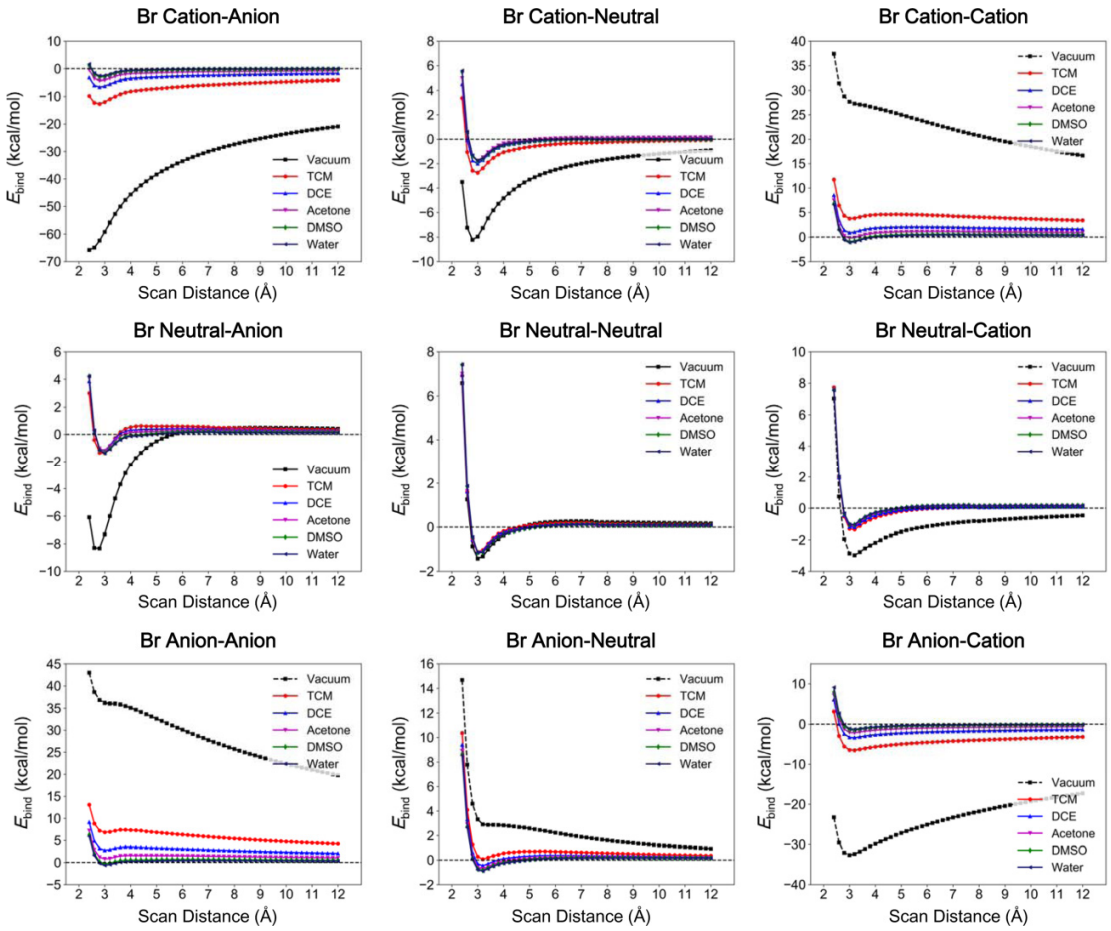

Figure S10. Overall binding energy (E_{bind}) versus intermolecular Br···O distance of complexes between differently charged 3-amino-5-bromobenzoic acid and glycine in different environments including vacuum (black, those based on optimized structures in TCM are shown in dashed line), TCM (red), DCE (blue), acetone (magenta), DMSO (green), water (midnightblue).

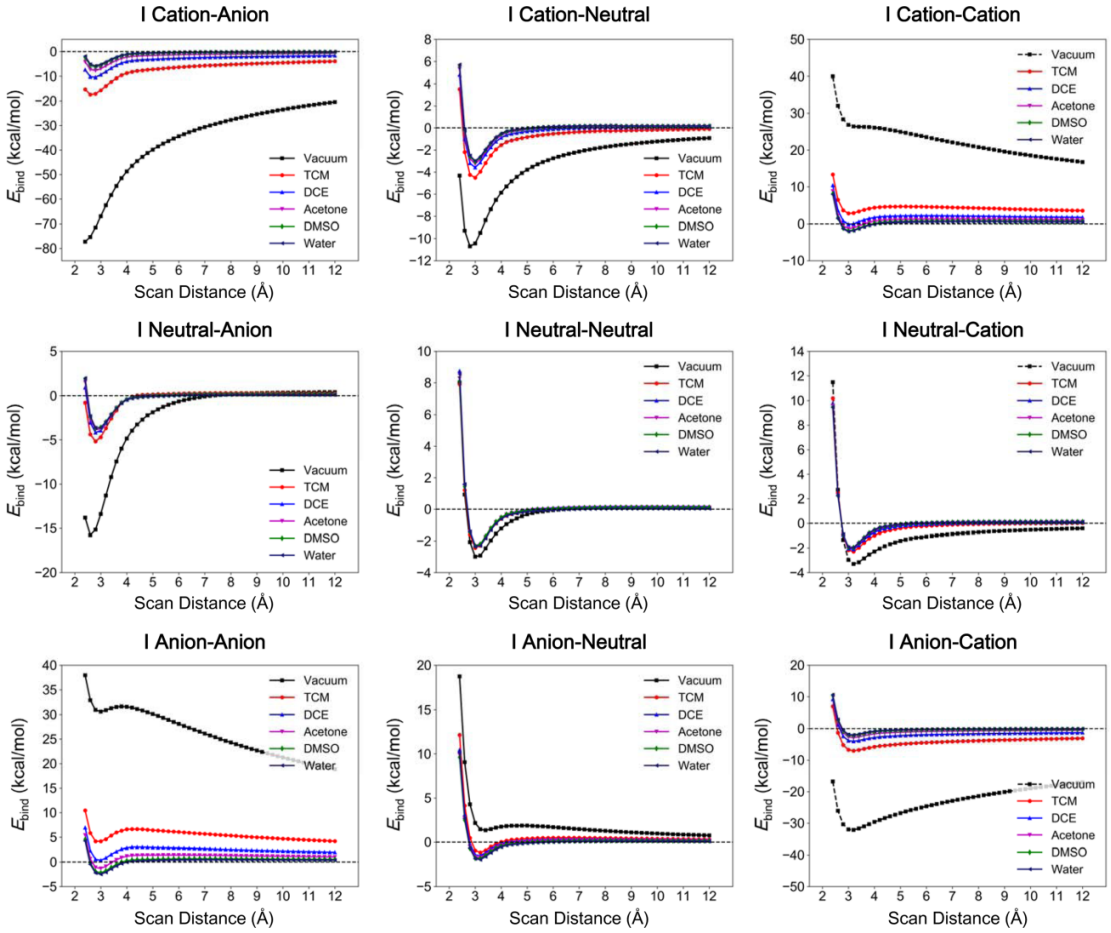

Figure S11. Overall binding energy (E_{bind}) versus intermolecular I···O distance of complexes between differently charged 3-amino-5-iodobenzoic acid and glycine in different environments including vacuum (black, those based on optimized structures in TCM are shown in dashed line), TCM (red), DCE (blue), acetone (magenta), DMSO (green), water (midnightblue).

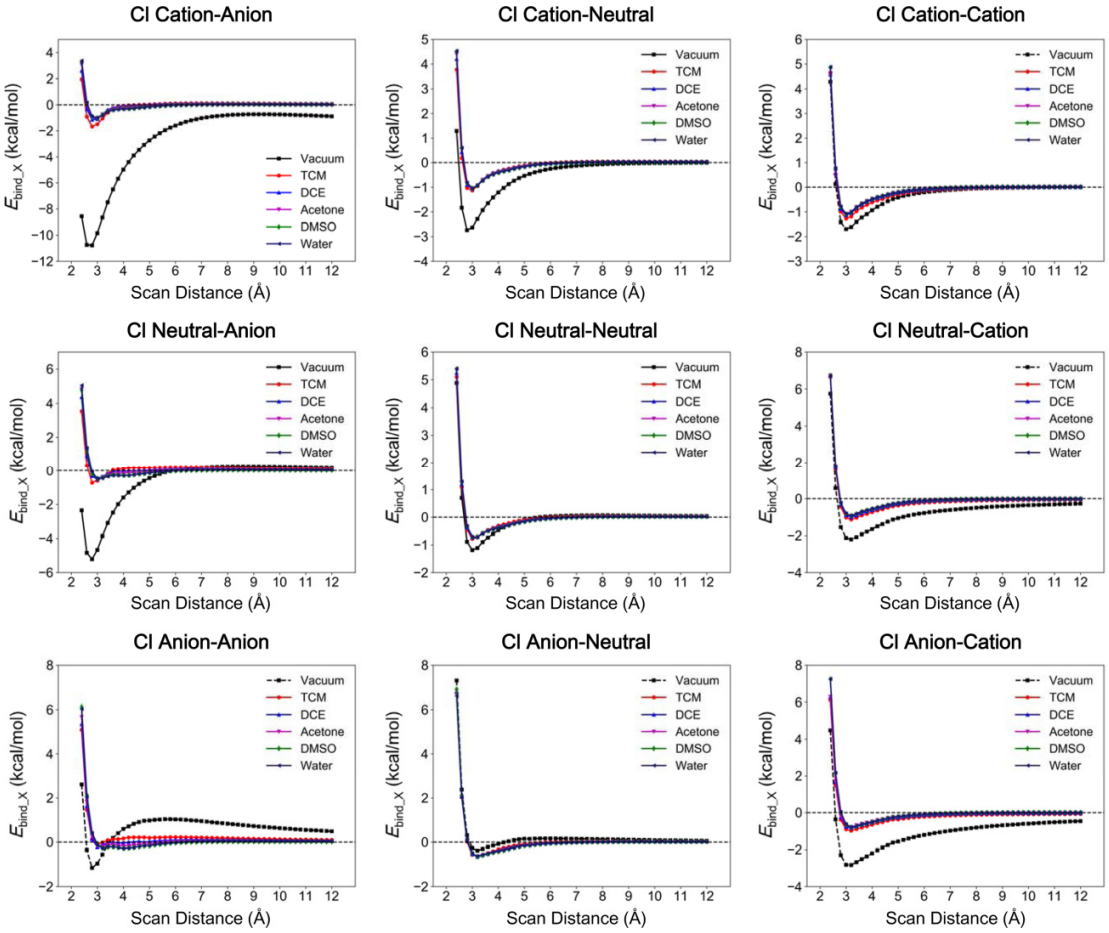

Figure S12. Net binding energy (E_{bind_X}) between the Cl atom and acceptor versus intermolecular Cl···O distance of complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine in different environments including vacuum (black, those based on optimized structures in TCM are shown in dashed line), TCM (red), DCE (blue), acetone (magenta), DMSO (green), water (midnightblue).

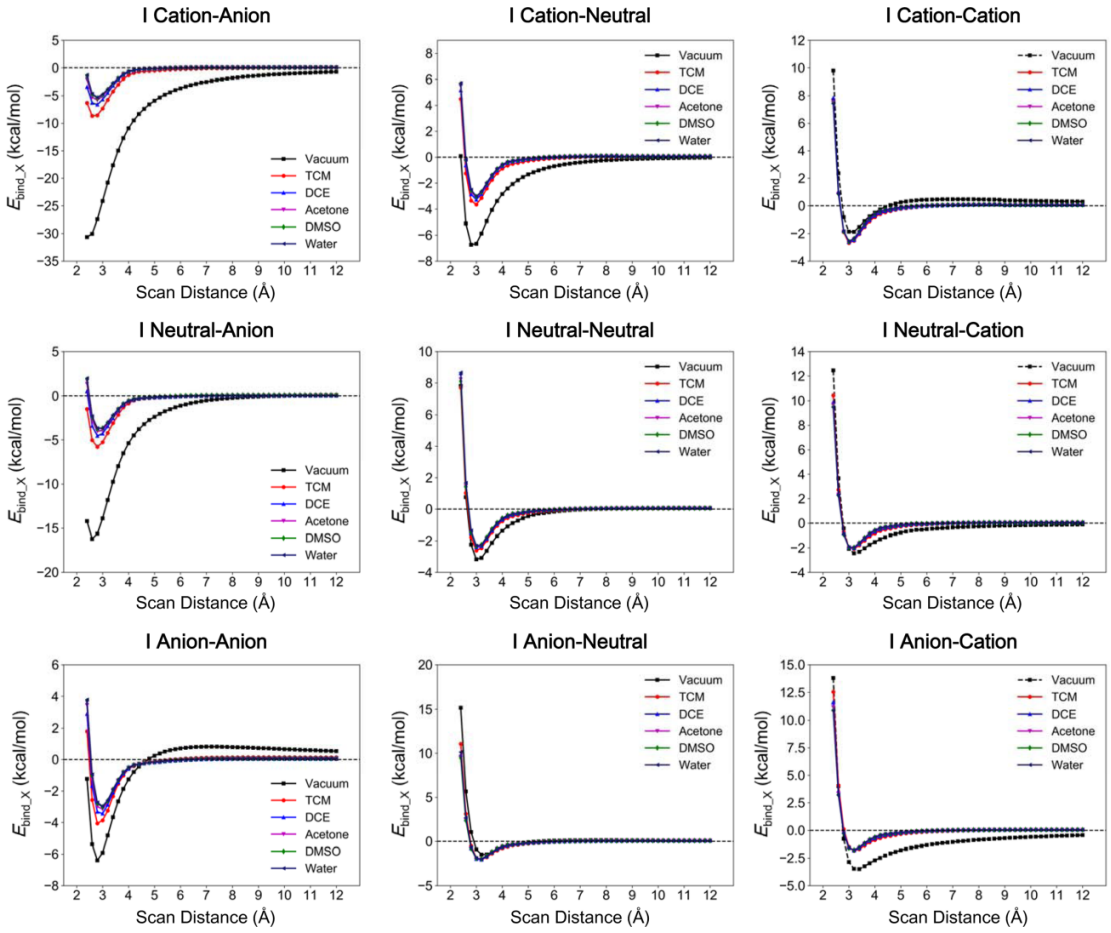

Figure S13. Net binding energy between the I atom and acceptor ($E_{\text{bind, X}}$) versus intermolecular I···O distance of complexes between differently charged 3-amino-5-iodobenzoic acid and glycine in different environments including vacuum (black, those based on optimized structures in TCM are shown in dashed line), TCM (red), DCE (blue), acetone (magenta), DMSO (green), water (midnightblue).

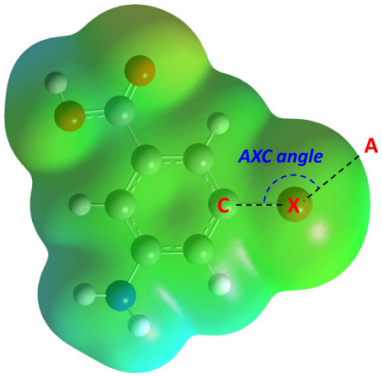

Figure S14. The schematic diagram for the *AXC* angle which stands for the angle among the probe point on the molecular surface (*A*), the halogen atom (*X*), and its covalent bonded carbon atom (*C*). The *AXC* angle is designed to describe the relative position of probe points on the halogen atomic surface for the purpose of evaluating the atomic electrostatic potential distribution (Figure S15). Notably, the *AXC* angle is measured for all probe points on the halogen atomic surface rather than simply consider those coplanar with the donor ring.

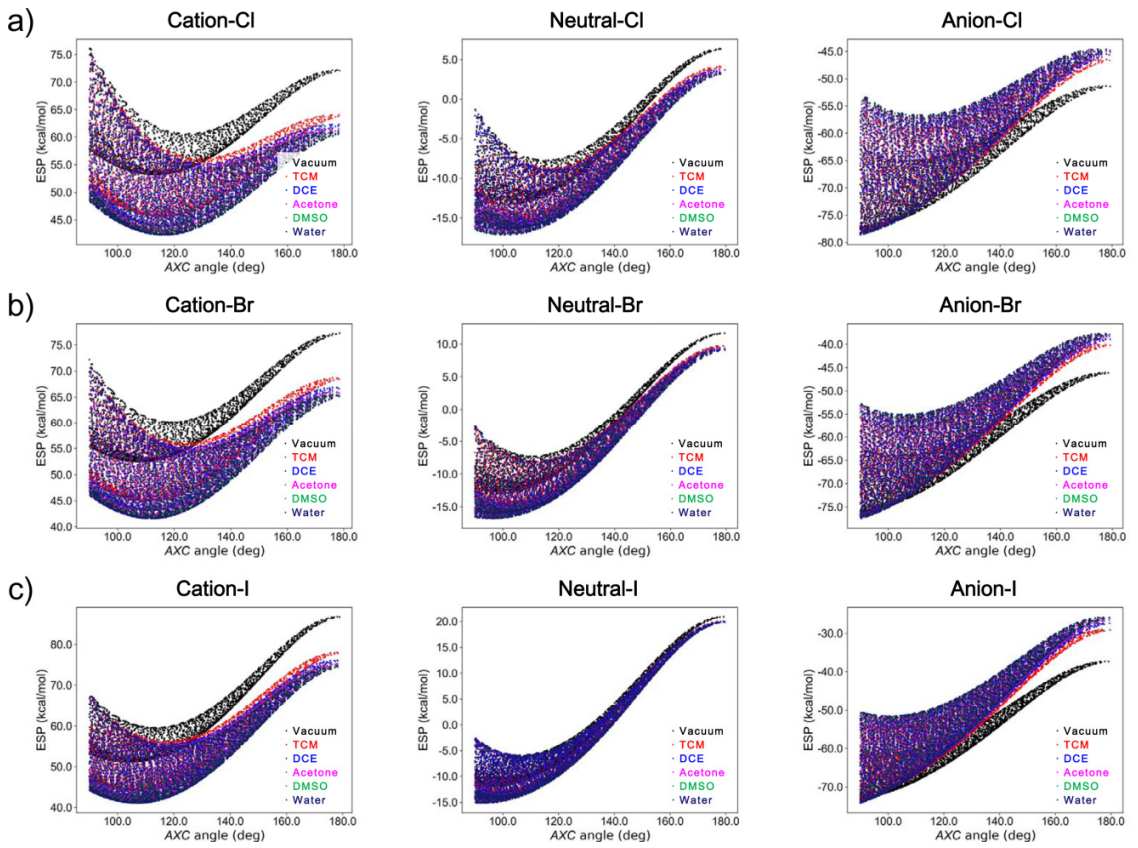

Figure S15 Scatter diagrams of surface electrostatic potential versus *AXC* angle (Figure S14) of the halogen atom for differently charged (a) 3-amino-5-chlorobenzoic acid, (b) 3-amino-5-bromobenzoic acid and (c) 3-amino-5-iodobenzoic donors in environments including vacuum (black), TCM (red), DCE (blue), acetone (magenta), DMSO (green) and water (midnightblue). The scatter peaks for local surface ESP maxima ($V_{S,max}$) are found for all the cationic, neutral and anionic donors in all dielectric environments, when the *AXC* angle approaches to 180°, suggesting the commonly recognized anisotropic electron density distribution for the halogen atom and the existence of locally electron-depleted region, namely, the σ-hole. These scatter peaks vary with changes in solvent. In general, the absolute values for electrostatic potential of the scatters decrease with the increase of environmental polarity, leading the scatter peaks to move towards zero. For neutral donors, the threshold *AXC* angle around which surface ESPs change from positive to negative, is smaller in less polar environments, indicating that solvents are able to change both size and magnitude of the σ-hole. Similar trends are also observed in Figure S6 and Table S5 as well.

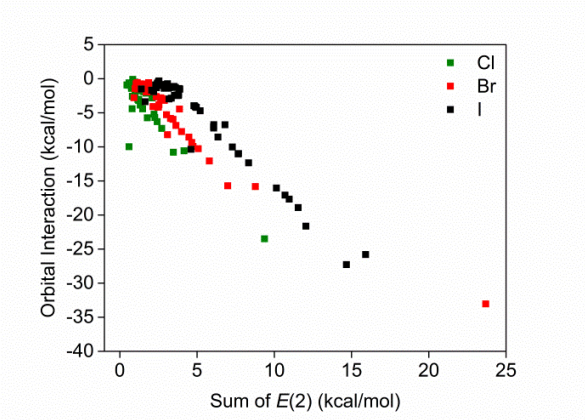

Figure S16. Orbital interaction versus the sum of second-order stabilization energy (*E*(2)) for all charge transfers from n_O and $n_{O'}$ orbital to the $\sigma^*_{C\text{-}X}$ orbital in all types of complexes between differently charged 3-amino-5-halobenzoic acid (green for Cl, red for Br, black for I) and glycine.

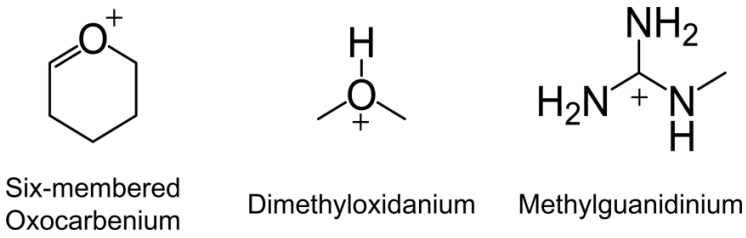

Figure S17. Schematic models of the six-membered oxocarbenium (left), dimethyloxidanium (middle) and methylguanidinium (right) cations.

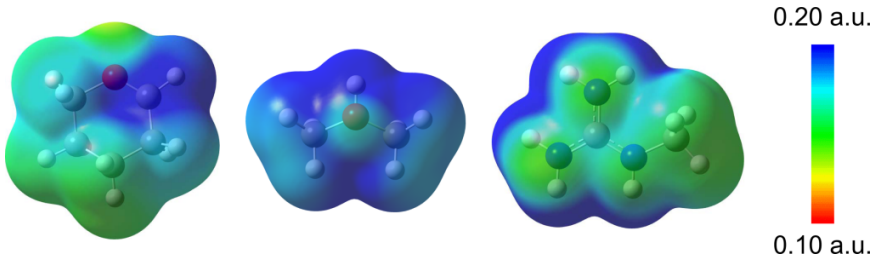

Figure S18. Electrostatic potentials (ESPs) mapped on the 0.001 electrons/Bohr^3 isosurface of electron density for the six-membered oxocarbenium (left), dimethyloxidanium (middle) and methylguanidinium (right) cations. ESP values range from 0.10 a.u. (red) to 0.20 a.u. (blue). All the three cationic acceptors have a locally less positively charged region that could form stable halogen bonds with organohalogens.

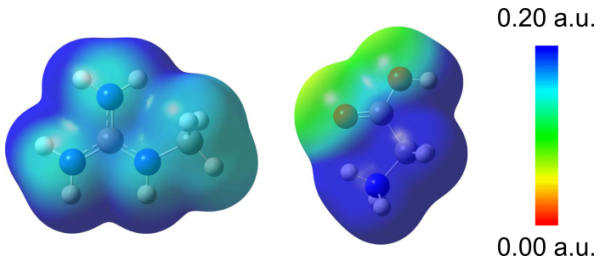

Figure S19. Electrostatic potentials (ESPs) mapped on the 0.001 electrons/Bohr^3 isosurface of electron density for cationic methylguanidinium (left) and cationic glycine (right) molecule. ESP values range from 0.00 a.u. (red) to 0.20 a.u. (blue). Surface electrostatic potential of the acceptor nitrogen that connecting the methyl group in the methylguanidinium cation is more positive than that of the carboxyl oxygen atom in the cationic glycine, which thus resulting in more repulsive electrostatic terms in halogen bonds.

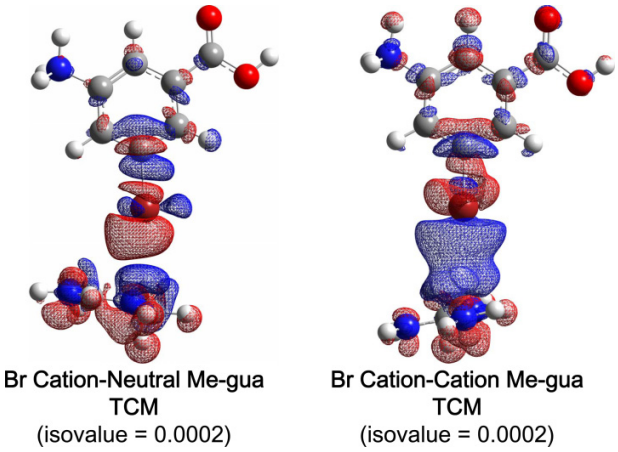

Figure S20. Electron density difference maps for complexes of the cationic 3-amino-5-bromobenzoic acid donor, and neutral (left) and cationic (right) methylguanidine acceptors. Electron transfer from the electron density decreases regions (red) to increased regions (blue). The corresponding isovalues are listed below the EDD maps. Intramolecular charge redistribution took place from the Br atom to the rest of the XB donor in cation-neutral complex while from the rest of XB donor to the Br atom in cation-cation complex, similar with that mentioned in manuscript, but based on optimized geometries without imaginary frequencies.

3. Tables

Table S1. Optimized halogen bonding interaction angles in complexes between differently charged 3-amino-5-halobenzoic acid and glycine.[a]

Environments	Cation-Anion			Cation-Neutral			Cation-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
Vacuum	178.3[b]	179.9[b]	179.1	178.8	176.7	177.5	174.2[c]	175.0[c]	177.0[c]
TCM	178.7[b]	178.8	176.6	177.0	176.0	176.9	174.2	175.0	177.0
DCE	176.9	176.3	176.0	175.6	175.4	176.5	176.0	175.5	176.2
Acetone	176.5	177.0	175.6	175.1	175.0	176.2	175.9	175.2	176.6
DMSO	176.3	176.2	175.5	174.8	174.4	175.9	174.4	174.9	176.5
Water	176.3	175.9	175.5	174.7	174.3	175.8	174.3	174.9	176.5
Environments	Neutral-Anion			Neutral-Neutral			Neutral-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
Vacuum	178.7[b]	178.5	176.6	175.5[b]	176.7[b]	177.2	173.3[c]	173.9[c]	176.2[c]
TCM	179.1	176.2	176.4	176.3	174.8	176.7	173.3	173.9	176.2
DCE	175.4	175.9	176.7	176.3	174.7	176.6	174.1	174.7	176.5
Acetone	175.6	175.8	176.8	176.3	174.6	175.8	174.6	174.3	176.6
DMSO	177.0	176.6	176.6	176.4	175.4	177.1	174.7	174.7	176.7
Water	175.8	176.0	177.0	176.4	175.2	176.3	174.8	174.7	176.7
Environments	Anion-Anion			Anion-Neutral			Anion-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
Vacuum	173.3[c]	176.8[c]	178.5	177.4[c]	176.5[c]	175.6[b]	175.6[c]	173.6[c]	175.2[c]
TCM	173.3	176.8	177.7	177.4[b]	176.5[b]	178.3	175.6[b]	173.6	175.2
DCE	177.8	178.2	177.7	176.8	176.9[b]	176.8	173.9	174.6	175.9
Acetone	177.7	177.7	177.5	175.7	177.0	177.7	174.2	174.9	176.1
DMSO	177.3	177.5	177.4	175.2	176.4	177.5	174.6	175.8	176.1

Water	176.6	177.4	177.3	176.0	176.2	176.8	174.6	175.9	176.3

[a]All values are in degree. [b]The complex geometry is obtained by constrained optimization. [c]The complex geometry is the optimized structure in TCM.

Table S2. Electronic properties at the bond critical points for complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine.[a]

Complex	Environment	ρ^b	$\nabla^2\rho^c$	H^d	V^e	G^f	$\lvert V\rvert/G$	$\lvert\lambda_1\rvert/\lambda_3{}^g$
Cl Cation-Anion	Vacuum[h]	0.0290	0.1087	0.0019	-0.0234	0.0253	0.9242	0.1680
	TCM[h]	0.0171	0.0644	0.0014	-0.0133	0.0147	0.9039	0.1509
	DCE	0.0148	0.0570	0.0014	-0.0114	0.0128	0.8896	0.1441
	Acetone	0.0139	0.0534	0.0014	-0.0106	0.0120	0.8862	0.1427
	DMSO	0.0135	0.0516	0.0013	-0.0102	0.0116	0.8836	0.1416
	Water	0.0133	0.0508	0.0013	-0.0100	0.0114	0.8829	0.1413
Cl Neutral-Anion	Vacuum[h]	0.0182	0.0685	0.0015	-0.0141	0.0156	0.9050	0.1537
	TCM	0.0114	0.0436	0.0013	-0.0084	0.0096	0.8702	0.1391
	DCE	0.0105	0.0400	0.0012	-0.0076	0.0088	0.8670	0.1389
	Acetone	0.0099	0.0373	0.0011	-0.0071	0.0082	0.8622	0.1379
	DMSO	0.0099	0.0379	0.0012	-0.0071	0.0083	0.8600	0.1361
	Water	0.0093	0.0351	0.0011	-0.0066	0.0077	0.8568	0.1369
Cl Anion-Anion	Vacuum[i]	0.0073	0.0298	0.0012	-0.0051	0.0063	0.8107	0.1273
	TCM	0.0076	0.0302	0.0011	-0.0053	0.0064	0.8216	0.1283
	DCE	0.0095	0.0362	0.0011	-0.0068	0.0079	0.8567	0.1363
	Acetone	0.0093	0.0350	0.0011	-0.0065	0.0076	0.8549	0.1358
	DMSO	0.0078	0.0293	0.0010	-0.0053	0.0063	0.8372	0.1336
	Water	0.0083	0.0312	0.0011	-0.0057	0.0068	0.8439	0.1342

Cl Cation-Neutral	Vacuum	0.0141	0.0606	0.0020	-0.0111	0.0131	0.8462	0.1356
	TCM	0.0123	0.0506	0.0016	-0.0094	0.0110	0.8510	0.1361
	DCE	0.0116	0.0468	0.0015	-0.0087	0.0102	0.8519	0.1368
	Acetone	0.0110	0.0444	0.0014	-0.0082	0.0097	0.8502	0.1365
	DMSO	0.0107	0.0427	0.0014	-0.0079	0.0093	0.8484	0.1361
	Water	0.0106	0.0427	0.0014	-0.0079	0.0093	0.8485	0.1361
Cl Neutral-Neutral	Vacuum[h]	0.0089	0.0363	0.0013	-0.0064	0.0078	0.8283	0.1334
	TCM	0.0087	0.0355	0.0013	-0.0063	0.0076	0.8268	0.1315
	DCE	0.0086	0.0349	0.0013	-0.0061	0.0074	0.8271	0.1314
	Acetone	0.0086	0.0345	0.0013	-0.0061	0.0074	0.8273	0.1313
	DMSO	0.0085	0.0342	0.0013	-0.0060	0.0073	0.8270	0.1312
	Water	0.0084	0.0340	0.0013	-0.0060	0.0072	0.8266	0.1311
Cl Anion-Neutral	Vacuum[i]	0.0062	0.0254	0.0011	-0.0042	0.0052	0.7918	0.1265
	TCM[h]	0.0064	0.0256	0.0011	-0.0043	0.0053	0.7997	0.1282
	DCE	0.0067	0.0266	0.0011	-0.0045	0.0056	0.8072	0.1295
	Acetone	0.0070	0.0278	0.0011	-0.0048	0.0059	0.8145	0.1308
	DMSO	0.0073	0.0287	0.0011	-0.0050	0.0061	0.8196	0.1317
	Water	0.0076	0.0301	0.0011	-0.0053	0.0064	0.8233	0.1320
Cl Cation-Cation	Vacuum[i]	0.0080	0.0339	0.0013	-0.0058	0.0071	0.8135	0.1316
	TCM	0.0083	0.0342	0.0013	-0.0060	0.0073	0.8225	0.1327
	DCE	0.0091	0.0376	0.0014	-0.0067	0.0080	0.8294	0.1330
	Acetone	0.0093	0.0382	0.0014	-0.0068	0.0082	0.8319	0.1333
	DMSO	0.0093	0.0380	0.0013	-0.0068	0.0082	0.8356	0.1346
	Water	0.0094	0.0381	0.0013	-0.0068	0.0082	0.8362	0.1347
Cl Neutral-Cation	Vacuum[i]	0.0074	0.0305	0.0012	-0.0052	0.0064	0.8118	0.1303

	TCM	0.0076	0.0307	0.0012	-0.0053	0.0065	0.8203	0.1320
	DCE	0.0077	0.0308	0.0012	-0.0054	0.0066	0.8234	0.1324
	Acetone	0.0078	0.0311	0.0012	-0.0055	0.0066	0.8252	0.1327
	DMSO	0.0078	0.0312	0.0012	-0.0055	0.0066	0.8261	0.1328
	Water	0.0078	0.0312	0.0012	-0.0055	0.0066	0.8264	0.1328
Cl Anion-Cation	Vacuum[i]	0.0082	0.0343	0.0014	-0.0059	0.0072	0.8125	0.1297
	TCM[h]	0.0084	0.0343	0.0013	-0.0060	0.0073	0.8220	0.1312
	DCE	0.0080	0.0325	0.0012	-0.0056	0.0069	0.8198	0.1312
	Acetone	0.0078	0.0318	0.0012	-0.0055	0.0067	0.8184	0.1309
	DMSO	0.0073	0.0292	0.0011	-0.0051	0.0062	0.8185	0.1314
	Water	0.0073	0.0291	0.0011	-0.0050	0.0062	0.8184	0.1314

[a]All values are given in atomic units except $|V|/G$ and $|\lambda_1|/\lambda_3$, which are dimensionless. [b]Electron density. [c]Laplacian of electron density. [d]Total energy density. [e]Potential energy density. [f]Kinetic energy density. [g]Ratio of the absolute value of the first eigenvalue of the Hessian matrix and the corresponding third eigenvalue. [h]Results from constrained optimizations. [i]Results from single-point energy calculations using the TCM-optimized geometries. Electronic properties at the bond critical points (BCP), e.g., the positive total energy density (H) and Laplacian of electron density ($\nabla^2\rho$) values, and smaller the ratio of $|\lambda_1|/\lambda_3$ than 1, classify these interactions as closed shell.[27]

Table S3. Electronic properties at the bond critical points for complexes between differently charged 3-amino-5-bromobenzoic acid and glycine.[a]

Complex	Environment	ρ^b	$\nabla^2\rho^c$	H^d	V^e	G^f	$\|V\|/G$	$\|\lambda_1\|/\lambda_3{}^g$
Br Cation-Anion	Vacuum[h]	0.0420	0.1310	-0.0004	-0.0336	0.0332	1.0128	0.1953
	TCM	0.0212	0.0743	0.0013	-0.0159	0.0172	0.9232	0.1584
	DCE	0.0193	0.0687	0.0014	-0.0144	0.0158	0.9125	0.1519

	Acetone	0.0180	0.0645	0.0014	-0.0133	0.0147	0.9054	0.1484
	DMSO	0.0171	0.0614	0.0014	-0.0126	0.0140	0.9025	0.1469
	Water	0.0168	0.0606	0.0014	-0.0124	0.0138	0.8990	0.1455
Br Neutral-Anion	Vacuum	0.0236	0.0821	0.0014	-0.0178	0.0191	0.9281	0.1627
	TCM	0.0173	0.0617	0.0014	-0.0127	0.0141	0.9034	0.1479
	DCE	0.0160	0.0567	0.0013	-0.0116	0.0129	0.9018	0.1469
	Acetone	0.0151	0.0540	0.0013	-0.0110	0.0122	0.8965	0.1443
	DMSO	0.0142	0.0508	0.0013	-0.0102	0.0114	0.8904	0.1430
	Water	0.0147	0.0524	0.0012	-0.0106	0.0119	0.8950	0.1433
Br Anion-Anion	Vacuum[i]	0.0130	0.0469	0.0013	-0.0092	0.0105	0.8783	0.1439
	TCM	0.0134	0.0476	0.0012	-0.0095	0.0107	0.8865	0.1430
	DCE	0.0109	0.0379	0.0010	-0.0074	0.0084	0.8780	0.1407
	Acetone	0.0119	0.0416	0.0011	-0.0083	0.0093	0.8855	0.1421
	DMSO	0.0121	0.0422	0.0011	-0.0084	0.0095	0.8866	0.1420
	Water	0.0122	0.0426	0.0011	-0.0085	0.0096	0.8870	0.1420
Br Cation-Neutral	Vacuum	0.0162	0.0632	0.0019	-0.0121	0.0139	0.8654	0.1410
	TCM	0.0139	0.0531	0.0016	-0.0101	0.0117	0.8641	0.1392
	DCE	0.0135	0.0511	0.0015	-0.0097	0.0113	0.8654	0.1393
	Acetone	0.0133	0.0500	0.0015	-0.0096	0.0110	0.8660	0.1394
	DMSO	0.0126	0.0465	0.0013	-0.0089	0.0103	0.8703	0.1415
	Water	0.0125	0.0461	0.0013	-0.0089	0.0102	0.8703	0.1415
Br Neutral-Neutral	Vacuum[h]	0.0114	0.0436	0.0014	-0.0081	0.0095	0.8510	0.1369
	TCM	0.0112	0.0418	0.0013	-0.0079	0.0092	0.8586	0.1381
	DCE	0.0112	0.0416	0.0013	-0.0078	0.0091	0.8602	0.1381
	Acetone	0.0109	0.0401	0.0012	-0.0076	0.0088	0.8602	0.1382
	DMSO	0.0106	0.0384	0.0012	-0.0073	0.0084	0.8621	0.1389

Br Anion-Neutral	Water	0.0105	0.0382	0.0012	-0.0072	0.0084	0.8621	0.1389
	Vacuum[i]	0.0082	0.0306	0.0011	-0.0055	0.0066	0.8370	0.1333
	TCM[h]	0.0084	0.0307	0.0010	-0.0056	0.0066	0.8436	0.1350
	DCE[h]	0.0088	0.0321	0.0010	-0.0059	0.0070	0.8493	0.1360
	Acetone	0.0092	0.0332	0.0011	-0.0062	0.0072	0.8526	0.1366
	DMSO	0.0093	0.0335	0.0011	-0.0062	0.0073	0.8540	0.1369
	Water	0.0093	0.0337	0.0011	-0.0063	0.0074	0.8545	0.1370
Br Cation-Cation	Vacuum[i]	0.0109	0.0424	0.0014	-0.0077	0.0092	0.8436	0.1364
	TCM	0.0112	0.0426	0.0014	-0.0079	0.0093	0.8522	0.1376
	DCE	0.0119	0.0455	0.0014	-0.0085	0.0099	0.8559	0.1377
	Acetone	0.0117	0.0443	0.0014	-0.0083	0.0097	0.8581	0.1384
	DMSO	0.0118	0.0446	0.0014	-0.0084	0.0098	0.8592	0.1386
	Water	0.0119	0.0449	0.0014	-0.0085	0.0098	0.8599	0.1387
Br Neutral-Cation	Vacuum[i]	0.0093	0.0358	0.0013	-0.0064	0.0077	0.8348	0.1332
	TCM	0.0095	0.0357	0.0012	-0.0065	0.0077	0.8430	0.1350
	DCE	0.0096	0.0360	0.0012	-0.0066	0.0078	0.8450	0.1352
	Acetone	0.0100	0.0375	0.0012	-0.0069	0.0081	0.8495	0.1360
	DMSO	0.0103	0.0385	0.0012	-0.0071	0.0084	0.8517	0.1362
	Water	0.0103	0.0386	0.0012	-0.0072	0.0084	0.8519	0.1362
Br Anion-Cation	Vacuum[i]	0.0091	0.0348	0.0012	-0.0062	0.0075	0.8350	0.1324
	TCM	0.0091	0.0344	0.0012	-0.0062	0.0074	0.8412	0.1341
	DCE	0.0090	0.0339	0.0012	-0.0062	0.0073	0.8416	0.1340
	Acetone	0.0091	0.0341	0.0012	-0.0062	0.0074	0.8431	0.1342
	DMSO	0.0088	0.0327	0.0011	-0.0059	0.0071	0.8421	0.1343
	Water	0.0086	0.0314	0.0011	-0.0057	0.0068	0.8450	0.1350

[a]All values are given in atomic units except $|V|/G$ and $|\lambda_1|/\lambda_3$, which are dimensionless. [b]Electron density.

[c]Laplacian of electron density. [d]Total energy density. [e]Potential energy density. [f]Kinetic energy density. [g]Ratio of the absolute value of the first eigenvalue of the Hessian matrix and the corresponding third eigenvalue. [h]Results from constrained optimizations. [i]Results from single-point energy calculations using the TCM-optimized geometries. Electronic properties at most of the bond critical points (BCP), e.g., the positive total energy density (H) and Laplacian of electron density ($\nabla^2\rho$) values, and smaller the ratio of $|\lambda_1|/\lambda_3$ than 1, classify these interactions as closed shell,[27] while the cation-anion organobromine complex has revealed more covalent characteristics in vacuum, namely, higher electron density (ρ), larger Laplacian value ($\nabla^2\rho$) and negative total energy density (H), which is in line with the stronger orbital terms in energy decomposition results as mentioned in the manuscript.

Table S4. Electronic properties at the bond critical points for complexes between differently charged 3-amino-5-iodobenzoic acid and glycine.[a]

Complex	Environment	ρ^b	$\nabla^2\rho^c$	H^d	V^e	G^f	$\|V\|/G$	$\|\lambda_1\|/\lambda_3{}^g$
I Cation-Anion	Vacuum	0.0504	0.1502	-0.0061	-0.0428	0.0367	1.1673	0.1892
	TCM	0.0304	0.1013	-0.0006	-0.0248	0.0242	1.0244	0.1622
	DCE	0.0271	0.0916	-0.0001	-0.0218	0.0217	1.0024	0.1571
	Acetone	0.0249	0.0848	0.0002	-0.0197	0.0200	0.9885	0.1540
	DMSO	0.0242	0.0828	0.0003	-0.0191	0.0195	0.9832	0.1524
	Water	0.0239	0.0820	0.0004	-0.0189	0.0192	0.9814	0.1520
I Neutral-Anion	Vacuum	0.0319	0.1052	-0.0008	-0.0260	0.0252	1.0332	0.1650
	TCM	0.0232	0.0796	0.0005	-0.0182	0.0186	0.9757	0.1514
	DCE	0.0211	0.0726	0.0006	-0.0163	0.0169	0.9629	0.1482
	Acetone	0.0200	0.0693	0.0007	-0.0153	0.0161	0.9545	0.1456
	DMSO	0.0201	0.0693	0.0007	-0.0154	0.0161	0.9574	0.1469
	Water	0.0194	0.0674	0.0008	-0.0148	0.0156	0.9511	0.1448

I Anion-Anion	Vacuum	0.0149	0.0565	0.0014	-0.0111	0.0125	0.8907	0.1270
	TCM	0.0179	0.0619	0.0009	-0.0134	0.0142	0.9398	0.1433
	DCE	0.0177	0.0612	0.0008	-0.0132	0.0141	0.9395	0.1429
	Acetone	0.0176	0.0610	0.0008	-0.0132	0.0140	0.9398	0.1428
	DMSO	0.0176	0.0611	0.0008	-0.0132	0.0141	0.9398	0.1426
	Water	0.0176	0.0611	0.0008	-0.0132	0.0140	0.9397	0.1425
I Cation-Neutral	Vacuum	0.0188	0.0704	0.0013	-0.0145	0.0158	0.9188	0.1389
	TCM	0.0164	0.0606	0.0013	-0.0123	0.0135	0.9068	0.1371
	DCE	0.0160	0.0589	0.0012	-0.0119	0.0131	0.9060	0.1371
	Acetone	0.0158	0.0580	0.0012	-0.0117	0.0130	0.9059	0.1372
	DMSO	0.0157	0.0575	0.0012	-0.0116	0.0128	0.9056	0.1371
	Water	0.0157	0.0573	0.0012	-0.0116	0.0128	0.9052	0.1370
I Neutral-Neutral	Vacuum	0.0133	0.0492	0.0013	-0.0095	0.0108	0.8808	0.1340
	TCM	0.0138	0.0508	0.0012	-0.0100	0.0112	0.8888	0.1346
	DCE	0.0137	0.0494	0.0012	-0.0098	0.0110	0.8943	0.1368
	Acetone	0.0140	0.0505	0.0012	-0.0101	0.0112	0.8955	0.1364
	DMSO	0.0140	0.0506	0.0012	-0.0101	0.0112	0.8951	0.1359
	Water	0.0137	0.0492	0.0011	-0.0098	0.0109	0.8967	0.1371
I Anion-Neutral	Vacuum[h]	0.0081	0.0285	0.0010	-0.0051	0.0061	0.8391	0.1292
	TCM	0.0113	0.0402	0.0011	-0.0077	0.0088	0.8752	0.1342
	DCE	0.0122	0.0436	0.0011	-0.0085	0.0096	0.8808	0.1343
	Acetone	0.0126	0.0452	0.0012	-0.0088	0.0100	0.8844	0.1344
	DMSO	0.0128	0.0458	0.0012	-0.0090	0.0101	0.8862	0.1347
	Water	0.0125	0.0441	0.0011	-0.0087	0.0098	0.8880	0.1361
I Cation-Cation	Vacuum[i]	0.0132	0.0499	0.0013	-0.0096	0.0109	0.8764	0.1330

	TCM	0.0135	0.0499	0.0013	-0.0097	0.0110	0.8842	0.1343
	DCE	0.0138	0.0505	0.0012	-0.0100	0.0112	0.8902	0.1357
	Acetone	0.0142	0.0523	0.0013	-0.0103	0.0116	0.8912	0.1352
	DMSO	0.0143	0.0526	0.0013	-0.0104	0.0116	0.8922	0.1353
	Water	0.0143	0.0526	0.0013	-0.0104	0.0116	0.8924	0.1353
I Neutral-Cation	Vacuum[i]	0.0117	0.0437	0.0013	-0.0082	0.0095	0.8623	0.1309
	TCM	0.0118	0.0433	0.0012	-0.0082	0.0095	0.8710	0.1325
	DCE	0.0123	0.0452	0.0012	-0.0087	0.0099	0.8765	0.1332
	Acetone	0.0126	0.0461	0.0012	-0.0089	0.0101	0.8791	0.1335
	DMSO	0.0127	0.0466	0.0012	-0.0090	0.0102	0.8805	0.1337
	Water	0.0128	0.0467	0.0012	-0.0091	0.0103	0.8809	0.1337
I Anion-Cation	Vacuum[i]	0.0108	0.0394	0.0012	-0.0073	0.0085	0.8569	0.1309
	TCM	0.0107	0.0387	0.0011	-0.0073	0.0084	0.8635	0.1321
	DCE	0.0111	0.0403	0.0012	-0.0077	0.0088	0.8692	0.1328
	Acetone	0.0113	0.0410	0.0012	-0.0078	0.0090	0.8717	0.1331
	DMSO	0.0114	0.0411	0.0011	-0.0078	0.0090	0.8724	0.1332
	Water	0.0115	0.0417	0.0012	-0.0080	0.0091	0.8737	0.1334

[a]All values are given in atomic units except $|V|/G$ and $|\lambda_1|/\lambda_3$, which are dimensionless. [b]Electron density. [c]Laplacian of electron density. [d]Total energy density. [e]Potential energy density. [f]Kinetic energy density. [g]Ratio of the absolute value of the first eigenvalue of the Hessian matrix and the corresponding third eigenvalue. [h]Results from constrained optimizations. [i]Results from single-point energy calculations using the TCM-optimized geometries. Electronic properties at most of the bond critical points (BCP), e.g., the positive total energy density (H) and Laplacian of electron density ($\nabla^2\rho$) values, and smaller the ratio of $|\lambda_1|/\lambda_3$ than 1, classify these interactions as closed shell,[27] while the cation-anion and neutral-anion organoiodine complex have revealed more covalent characteristics especially in less polar environments, namely, higher electron density (ρ), larger Laplacian value ($\nabla^2\rho$) and negative total energy

density (*H*), which is in line with the stronger orbital terms in energy decomposition results as mentioned in the manuscript.

Table S5. Local surface electrostatic potential maxima ($V_{S,max}$) for differently charged 3-amino-5-halobenzoic acid donors.[a]

Charge state of the XB donor	X	Environment					
		Vacuum	TCM	DCE	Acetone	DMSO	Water
Cation	Cl	72.19	64.02	62.32	61.50	61.04	60.89
	Br	77.26	68.65	66.86	66.02	65.54	65.38
	I	86.78	78.00	76.17	75.31	74.81	74.65
Neutral	Cl	6.40	4.14	3.72	3.48	3.35	3.32
	Br	11.67	9.71	9.40	9.24	9.14	9.11
	I	20.92	20.05	19.94	19.94	19.92	19.91
Anion	Cl	-51.33	-46.44	-45.40	-44.90	-44.62	-44.53
	Br	-46.05	-40.06	-38.80	-38.18	-37.83	-37.71
	I	-37.32	-29.08	-27.29	-26.43	-25.94	-25.77

[a]All values are in kcal/mol.

Table S6. The ratios of axial and radial distance (r_{ax}/r_{rad}) from the halogen atom to molecular surface for differently charged 3-amino-5-halobenzoic acid donors.[a]

Charge state of the XB donor	X	Environment					
		Vacuum	TCM	DCE	Acetone	DMSO	Water
Cation	Cl	0.8947	0.8968	0.8970	0.8975	0.8976	0.8976
	Br	0.8925	0.8941	0.8947	0.8944	0.8944	0.8949
	I	0.8665	0.8686	0.8689	0.8690	0.8694	0.8694
Neutral	Cl	0.9020	0.9008	0.9000	0.9005	0.9005	0.9005
	Br	0.9012	0.8989	0.8985	0.8981	0.8981	0.8981
	I	0.8794	0.8768	0.8757	0.8749	0.8745	0.8745
Anion	Cl	0.9121	0.9050	0.9036	0.9027	0.9027	0.9022
	Br	0.9126	0.9045	0.9019	0.9015	0.9010	0.9006
	I	0.8978	0.8837	0.8813	0.8797	0.8789	0.8789

[a]As shown in the table, the r_{ax}/r_{rad} values of iodine atoms in differently charged organoiodine donors are obviously much smaller than that of organobromine and organochlorine, reflecting the flatter shape and larger σ-hole region of heavier halogens which may lead to stronger σ-hole interactions and probably less Pauli repulsion.[28] In general, the shape of heavier halogen atoms is always more easily affected by the environmental dielectric constants, especially when the molecule is neutral or negatively charged, indicating that heavier halogens have a stronger ability to modify the corresponding atomic electron distribution for stronger binding strength with changes in solvent and charge state, and thus are better in deformability, which are also suggested by the amount of electron redistributed within the XB donor in the complexes (Table S17-S19 and Table S20-S22). Unsurprisingly, r_{ax}/r_{rad} values always follow the trend of cationic < neutral < anionic donors in all types of solvents, which is in agreement with the fact that complexes involving cationic organoiodine form the strongest XBs while those involving anionic organochlorine form the weakest. This observation demonstrates that the strong binding energies in charge-assisted complexes with cationic XB donors originate not only from background electrostatic

interaction, but also from the deformation of the halogen atom that may reshape the σ-hole, induced by the positively charged substituent group.

Table S7. Axial distances (r_{ax}) from the halogen atom to the molecular surface for differently charged 3-amino-5-halobenzoic acid donors.[a]

Charge state of the XB donor	X	Environment					
		Vacuum	TCM	DCE	Acetone	DMSO	Water
Cation	Cl	1.887	1.904	1.907	1.909	1.910	1.910
	Br	1.992	2.010	2.014	2.015	2.016	2.017
	I	2.116	2.136	2.140	2.142	2.144	2.144
Neutral	Cl	1.924	1.926	1.926	1.927	1.927	1.927
	Br	2.035	2.036	2.035	2.035	2.035	2.035
	I	2.172	2.170	2.169	2.168	2.168	2.168
Anion	Cl	1.961	1.943	1.940	1.938	1.938	1.937
	Br	2.078	2.056	2.051	2.049	2.048	2.047
	I	2.231	2.196	2.190	2.186	2.184	2.184

[a]All values are in angstrom.

Table S8. Radial distances (r_{rad}) from the halogen atom to the molecular surface for differently charged 3-amino-5-halobenzoic acid donors.[a]

Charge state of the XB donor	X	Environment					
		Vacuum	TCM	DCE	Acetone	DMSO	Water
Cation	Cl	2.109	2.123	2.126	2.127	2.128	2.128
	Br	2.232	2.248	2.251	2.253	2.254	2.254
	I	2.442	2.459	2.463	2.465	2.466	2.466
Neutral	Cl	2.133	2.138	2.140	2.140	2.140	2.140
	Br	2.258	2.265	2.265	2.266	2.266	2.266
	I	2.470	2.475	2.477	2.478	2.479	2.479
Anion	Cl	2.150	2.147	2.147	2.147	2.147	2.147
	Br	2.277	2.273	2.274	2.273	2.273	2.273
	I	2.485	2.485	2.485	2.485	2.485	2.485

[a]All values are in angstrom.

Table S9. Net binding energies (E_{bind_X}) between the halogen atom and acceptor for complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine at the optimized distance.[a]

Complex	Environment					
	Vacuum	TCM	DCE	Acetone	DMSO	Water
Cl Cation-Anion	-9.66[b]	-1.16[b]	-0.74	-0.62	-0.60	-0.60
Cl Neutral-Anion	-4.74[b]	-0.39	-0.16	-0.14	-0.14	-0.16
Cl Anion-Anion	-0.34[c]	0.17	0.08	0.08	0.05	0.04
Cl Cation-Neutral	-2.23	-0.70	-0.60	-0.58	-0.57	-0.57
Cl Neutral-Neutral	-0.70[b]	-0.40	-0.37	-0.36	-0.36	-0.36
Cl Anion-Neutral	-0.01[c]	-0.32[b]	-0.30	-0.28	-0.27	-0.27
Cl Cation-Cation	-1.19[c]	-0.78	-0.65	-0.59	-0.57	-0.56
Cl Neutral-Cation	-1.70[c]	-0.63	-0.51	-0.46	-0.43	-0.42
Cl Anion-Cation	-2.37[c]	-0.51[b]	-0.37	-0.32	-0.33	-0.32

[a]All values are in kcal/mol. [b]The complex geometry is obtained by constrained optimization. [c]The complex geometry is the optimized structure in TCM.

Table S10. Net binding energies (E_{bind_X}) between the halogen atom and acceptor for complexes between differently charged 3-amino-5-iodobenzoic acid and glycine at the optimized distance.[a]

Complex	Environment					
	Vacuum	TCM	DCE	Acetone	DMSO	Water
I Cation-Anion	-29.92	-8.32	-6.23	-5.44	-5.03	-4.91
I Neutral-Anion	-15.82	-5.45	-4.14	-3.67	-3.46	-3.38
I Anion-Anion	-5.59	-3.75	-3.09	-2.82	-2.67	-2.62
I Cation-Neutral	-6.29	-3.26	-2.89	-2.73	-2.65	-2.62
I Neutral-Neutral	-2.86	-2.26	-2.08	-2.02	-1.98	-1.96
I Anion-Neutral	-1.17[b]	-1.68	-1.66	-1.62	-1.60	-1.58
I Cation-Cation	-1.47[c]	-2.26	-2.18	-2.17	-2.14	-2.13
I Neutral-Cation	-2.01[c]	-1.72	-1.68	-1.65	-1.63	-1.62
I Anion-Cation	-3.05[c]	-1.42	-1.38	-1.35	-1.34	-1.33

[a]All values are in kcal/mol. [b]The complex geometry is obtained by constrained optimization. [c]The complex geometry is the optimized structure in TCM.

Table S11. ETS-NOCV based energy decomposition results for complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine.[a]

Complex	Environment	E_{elest}[b]	E_{Pauli}[c]	E_{orb}[d]	E_{disp}[e]	E_{solv}[f]	E_{bind}[g]
Cl Cation-Anion	Vacuum[h]	-65.84	23.21	-23.50	-1.39	-	-67.52
	TCM[h]	-52.65	8.15	-10.80	-1.03	42.81	-13.52
	DCE	-48.54	5.85	-7.30	-0.86	48.39	-2.46
	Acetone	-47.63	5.17	-6.31	-0.83	49.53	-0.07
	DMSO	-47.10	4.83	-5.70	-0.81	50.05	1.27
	Water	-46.68	4.68	-5.21	-0.80	49.17	1.16
Cl Neutral-Anion	Vacuum[h]	-4.28	9.43	-10.59	-1.07	-	-6.51
	TCM	-0.14	3.54	-5.74	-0.76	4.34	1.24
	DCE	0.79	3.06	-4.43	-0.75	3.54	2.21
	Acetone	1.16	2.70	-3.88	-0.73	3.14	2.39
	DMSO	1.29	2.68	-3.57	-0.70	2.74	2.44
	Water	1.55	2.39	-3.03	-0.72	1.63	1.82
Cl Anion-Anion	Vacuum[i]	40.96	1.48	-4.41	-0.61	-	37.42
	TCM	38.47	1.54	-2.58	-0.61	-24.42	12.40
	DCE	39.41	2.52	-3.18	-0.71	-32.14	5.90
	Acetone	39.49	2.38	-3.05	-0.70	-33.81	4.31
	DMSO	39.81	1.73	-2.76	-0.67	-34.67	3.44
	Water	39.78	1.91	-2.35	-0.67	-36.35	2.32
Cl Cation-Neutral	Vacuum	-7.68	4.44	-2.82	-0.83	-	-6.89
	TCM	-7.43	3.57	-2.13	-0.82	5.00	-1.81
	DCE	-7.07	3.24	-1.92	-0.83	6.03	-0.55
	Acetone	-6.84	2.97	-1.79	-0.82	6.21	-0.27
	DMSO	-6.68	2.77	-1.67	-0.81	6.28	-0.11

Cl Neutral-Neutral	Water	-6.60	2.76	-1.59	-0.81	6.09	-0.15
	Vacuum[h]	-1.11	2.05	-1.09	-0.84	-	-0.99
	TCM	-0.95	1.85	-1.09	-0.73	0.67	-0.25
	DCE	-0.84	1.80	-1.08	-0.72	0.81	-0.03
	Acetone	-0.80	1.76	-1.06	-0.72	0.83	0.01
	DMSO	-0.76	1.73	-1.04	-0.71	0.84	0.06
	Water	-0.72	1.71	-0.91	-0.71	0.59	-0.04
Cl Anion-Neutral	Vacuum[i]	3.62	1.09	-0.92	-0.73	-	3.06
	TCM[h]	3.94	1.10	-0.95	-0.73	-2.54	0.82
	DCE	4.33	1.20	-0.92	-0.75	-3.66	0.20
	Acetone	4.46	1.33	-0.94	-0.76	-4.04	0.05
	DMSO	4.49	1.44	-0.92	-0.77	-4.30	-0.06
	Water	4.35	1.52	-0.84	-0.75	-4.44	-0.16
Cl Cation-Cation	Vacuum[i]	29.26	1.46	-1.22	-0.79	-	28.71
	TCM	26.67	1.59	-0.10	-0.79	-20.25	7.12
	DCE	25.57	1.91	-0.50	-0.79	-24.19	2.00
	Acetone	25.30	1.98	-0.66	-0.79	-25.04	0.79
	DMSO	25.37	2.03	-0.77	-0.82	-25.77	0.04
	Water	25.30	2.05	-0.75	-0.82	-26.01	-0.23
Cl Neutral-Cation	Vacuum[i]	-2.69	1.46	-0.96	-0.85	-	-3.04
	TCM	-3.04	1.55	-0.63	-0.85	1.60	-1.37
	DCE	-3.13	1.60	-0.65	-0.86	2.14	-0.90
	Acetone	-3.16	1.62	-0.69	-0.86	2.30	-0.79
	DMSO	-3.18	1.63	-0.70	-0.86	2.41	-0.70
	Water	-3.19	1.63	-0.64	-0.86	2.31	-0.75

Cl Anion-Cation	Vacuum[i]	-33.26	1.65	-9.99	-0.76	-	-42.36
	TCM[h]	-31.30	1.66	-1.42	-0.76	22.50	-9.32
	DCE	-30.60	1.50	-0.92	-0.76	27.25	-3.53
	Acetone	-30.28	1.43	-0.78	-0.75	28.24	-2.14
	DMSO	-29.65	1.41	-0.72	-0.83	28.40	-1.39
	Water	-29.58	1.41	-0.61	-0.83	28.42	-1.19

[a]All values are in kcal/mol. [b]Electrostatic interaction term. [c]Pauli repulsion term. [d]Orbital interaction term. [e]Dispersion term. [f]Solvation energy term. [g]Overall binding energy calculated using ETS-NOCV scheme with ADF program package. [h]Results based on constrained optimizations. [i]Results based on TCM-optimized geometries.

Table S12. ETS-NOCV based energy decomposition results for complexes between differently charged 3-amino-5-bromobenzoic acid and glycine.[a]

Complex	Environment	E_{elest}[b]	E_{Pauli}[c]	E_{orb}[d]	E_{disp}[e]	E_{solv}[f]	E_{bind}[g]
Br Cation-Anion	Vacuum[h]	-76.22	37.61	-33.06	-1.45	-	-73.12
	TCM	-57.79	12.29	-15.72	-1.20	46.67	-15.75
	DCE	-53.64	9.82	-12.07	-1.07	53.34	-3.62
	Acetone	-51.87	8.44	-10.28	-1.02	53.85	-0.88
	DMSO	-51.04	7.69	-9.36	-0.99	54.45	0.75
	Water	-50.06	7.34	-8.58	-0.98	53.01	0.73
Br Neutral-Anion	Vacuum	-9.28	14.97	-15.84	-1.22	-	-11.37
	TCM	-4.90	8.07	-9.95	-0.99	7.35	-0.42
	DCE	-4.00	6.95	-7.77	-0.98	7.26	1.46
	Acetone	-3.40	6.20	-6.87	-0.93	6.88	1.88
	DMSO	-2.77	5.38	-5.83	-0.94	6.42	2.26

	Water	-3.01	5.84	-5.97	-0.92	5.67	1.61
Br Anion-Anion	Vacuum[i]	40.23	4.90	-8.22	-0.92	-	35.99
	TCM	36.51	4.95	-5.29	-0.92	-23.83	11.42
	DCE	36.62	3.36	-4.10	-0.84	-29.74	5.30
	Acetone	36.09	3.98	-4.19	-0.88	-31.23	3.77
	DMSO	35.92	4.08	-4.15	-0.88	-32.04	2.93
	Water	35.84	4.13	-3.82	-0.88	-33.19	2.08
Br Cation-Neutral	Vacuum	-9.37	6.21	-4.45	-1.01	-	-8.62
	TCM	-8.99	4.78	-3.19	-0.97	5.70	-2.67
	DCE	-8.96	4.57	-2.92	-0.97	7.07	-1.21
	Acetone	-8.83	4.43	-2.81	-0.97	7.30	-0.88
	DMSO	-8.23	4.21	-2.68	-1.03	7.01	-0.72
	Water	-8.12	4.17	-2.62	-1.03	6.89	-0.71
Br Neutral-Neutral	Vacuum[h]	-2.42	3.45	-1.94	-0.94	-	-1.85
	TCM	-2.42	3.36	-1.81	-0.95	0.88	-0.94
	DCE	-2.42	3.35	-1.79	-0.94	1.18	-0.62
	Acetone	-2.29	3.17	-1.73	-0.94	1.21	-0.58
	DMSO	-2.24	3.11	-1.64	-0.98	1.19	-0.56
	Water	-2.18	3.09	-1.62	-0.98	1.09	-0.60
Br Anion-Neutral	Vacuum[i]	2.49	2.27	-1.44	-0.94	-	2.38
	TCM[h]	2.44	2.19	-1.18	-0.94	-2.34	0.17
	DCE[h]	2.40	2.36	-1.15	-0.94	-3.00	-0.33
	Acetone	2.36	2.48	-1.17	-0.95	-3.17	-0.45
	DMSO	2.39	2.53	-1.18	-0.94	-3.33	-0.53
	Water	2.43	2.55	-1.10	-0.94	-3.57	-0.63

Br Cation-Cation	Vacuum[i]	28.31	2.82	-1.95	-0.97	-	28.21
	TCM	25.32	3.05	-0.59	-0.97	-20.40	6.41
	DCE	23.98	3.48	-0.97	-0.97	-24.34	1.18
	Acetone	24.09	3.39	-1.07	-0.99	-25.48	-0.06
	DMSO	23.90	3.44	-1.16	-0.99	-25.95	-0.76
	Water	23.76	3.49	-1.19	-0.99	-26.10	-1.03
Br Neutral-Cation	Vacuum[i]	-3.42	2.17	-1.29	-0.92	-	-3.46
	TCM	-3.95	2.27	-0.78	-0.92	1.35	-2.03
	DCE	-4.09	2.33	-0.76	-0.94	1.82	-1.64
	Acetone	-4.37	2.54	-0.78	-0.93	2.01	-1.53
	DMSO	-4.46	2.70	-0.82	-0.93	2.09	-1.42
	Water	-4.50	2.71	-0.77	-0.93	2.05	-1.44
Br Anion-Cation	Vacuum[i]	-33.81	2.29	-2.79	-0.89	-	-35.20
	TCM	-31.73	2.20	-1.53	-0.89	22.01	-9.94
	DCE	-30.85	2.14	-0.93	-0.89	26.31	-4.22
	Acetone	-30.53	2.16	-0.77	-0.89	27.15	-2.88
	DMSO	-31.14	2.02	-0.75	-0.93	28.83	-1.97
	Water	-29.92	2.14	-0.58	-0.96	27.40	-1.92

[a]All values are in kcal/mol. [b]Electrostatic interaction term. [c]Pauli repulsion term. [d]Orbital interaction term. [e]Dispersion term. [f]Solvation energy term. [g]Overall binding energy calculated using ETS-NOCV scheme with ADF program package. [h]Results based on constrained optimizations. [i]Results based on TCM-optimized geometries.

Table S13. ETS-NOCV based energy decomposition results for complexes between differently charged 3-amino-5-iodobenzoic acid and glycine.[a]

Complex	Environment	E_{elest}[b]	E_{Pauli}[c]	E_{orb}[d]	E_{disp}[e]	E_{solv}[f]	E_{bind}[g]
I Cation-Anion	Vacuum	-95.09	61.48	-48.33	-1.63	-	-83.57
	TCM	-71.25	27.00	-27.28	-1.45	51.86	-21.12
	DCE	-67.10	22.03	-21.64	-1.40	60.72	-7.39
	Acetone	-64.10	18.85	-18.91	-1.36	61.39	-4.13
	DMSO	-63.21	17.80	-17.67	-1.34	62.04	-2.38
	Water	-62.52	17.44	-17.09	-1.34	61.53	-1.98
I Neutral-Anion	Vacuum	-21.92	30.04	-25.81	-1.44	-	-19.13
	TCM	-14.93	16.98	-16.04	-1.31	10.89	-4.41
	DCE	-13.26	14.12	-12.35	-1.28	11.62	-1.15
	Acetone	-12.32	12.70	-11.05	-1.23	11.45	-0.45
	DMSO	-12.60	12.96	-10.99	-1.25	11.78	-0.10
	Water	-11.80	12.04	-10.02	-1.22	10.73	-0.27
I Anion-Anion	Vacuum	35.30	7.97	-10.36	-1.04	-	31.87
	TCM	29.48	10.67	-8.56	-1.17	-21.85	8.57
	DCE	28.08	10.35	-7.24	-1.17	-26.86	3.16
	Acetone	27.72	10.30	-7.07	-1.17	-27.93	1.85
	DMSO	27.43	10.30	-6.99	-1.17	-28.47	1.10
	Water	27.39	10.28	-6.75	-1.16	-29.14	0.62
I Cation-Neutral	Vacuum	-12.76	10.12	-6.76	-1.24	-	-10.64
	TCM	-12.61	8.04	-4.71	-1.20	6.71	-3.77
	DCE	-12.75	7.78	-4.22	-1.20	8.41	-1.98
	Acetone	-12.68	7.63	-4.13	-1.21	8.69	-1.70
	DMSO	-12.60	7.54	-3.98	-1.20	8.93	-1.31
	Water	-12.50	7.49	-3.97	-1.20	8.97	-1.21
I Neutral-Neutral	Vacuum	-4.59	5.75	-2.86	-1.15	-	-2.85

	TCM	-5.59	6.10	-2.48	-1.14	1.50	-1.61
	DCE	-5.89	6.24	-2.45	-1.22	2.06	-1.26
	Acetone	-6.05	6.37	-2.47	-1.18	2.23	-1.10
	DMSO	-6.16	6.32	-2.34	-1.17	2.27	-1.08
	Water	-6.00	6.28	-2.39	-1.21	2.28	-1.04
I Anion-Neutral	Vacuum[h]	1.12	2.82	-1.50	-1.07	-	1.37
	TCM	-0.50	4.56	-1.33	-1.16	-1.94	-0.37
	DCE	-0.57	5.03	-1.41	-1.12	-2.69	-0.76
	Acetone	-1.00	5.33	-1.38	-1.12	-2.71	-0.88
	DMSO	-1.12	5.47	-1.41	-1.13	-2.76	-0.95
	Water	-0.96	5.41	-1.38	-1.17	-2.87	-0.97
I Cation-Cation	Vacuum[i]	26.79	5.08	-2.97	-1.18	-	27.72
	TCM	23.11	5.43	-1.14	-1.18	-20.16	6.06
	DCE	22.09	5.80	-1.29	-1.22	-24.45	0.93
	Acetone	21.26	6.07	-1.45	-1.20	-24.98	-0.30
	DMSO	20.98	6.16	-1.54	-1.20	-25.40	-1.00
	Water	20.87	6.16	-1.53	-1.20	-25.51	-1.21
I Neutral-Cation	Vacuum[i]	-4.58	4.29	-1.92	-1.13	-	-3.34
	TCM	-5.47	4.40	-1.02	-1.13	1.10	-2.12
	DCE	-6.05	4.82	-0.86	-1.14	1.49	-1.74
	Acetone	-6.28	5.01	-0.85	-1.14	1.56	-1.70
	DMSO	-6.40	5.11	-0.83	-1.15	1.63	-1.64
	Water	-6.46	5.14	-0.74	-1.15	1.71	-1.50
I Anion-Cation	Vacuum[i]	-34.62	4.20	-3.38	-1.10	-	-34.90
	TCM	-32.31	3.88	-1.68	-1.10	21.39	-9.82
	DCE	-31.83	4.17	-0.90	-1.12	25.41	-4.27

Acetone	-31.77	4.30	-0.67	-1.12	26.24	-3.02
DMSO	-31.58	4.31	-0.49	-1.12	26.65	-2.23
Water	-31.75	4.42	-0.32	-1.13	26.79	-1.99

[a]All values are in kcal/mol. [b]Electrostatic interaction term. [c]Pauli repulsion term. [d]Orbital interaction term. [e]Dispersion term. [f]Solvation energy term. [g]Overall binding energy calculated using ETS-NOCV scheme with ADF program package. [h]Results based on constrained optimizations. [i]Results based on TCM-optimized geometries.

Table S14. Natural bond orbitals and the *E*(2) results involved in electron transfer from lone pair electron orbitals of the oxygen atom to $\sigma^*_{C\text{-}X}$ for complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine.

Complex	Environment	$E(2)_{Sum}$[a]	$E(2)$[b]	Electron donor orbtial[c]	Electron acceptor orbtial[d]
Cl Cation-Anion	Vacuum[f]	9.37	7.50	53.LP(2)O7	420.BD*(1)C10-Cl19
			1.64	52.LP(1)O7	420.BD*(1)C10-Cl19
			0.23	56.LP(2)O9[e]	420.BD*(1)C10-Cl19
	TCM[f]	3.47	2.48	54.LP(2)O7	419.BD*(1)C10-Cl19
			0.99	53.LP(1)O7	419.BD*(1)C10-Cl19
	DCE	2.72	1.72	54.LP(2)O7	419.BD*(1)C10-Cl19
			1.00	53.LP(1)O7	419.BD*(1)C10-Cl19
	Acetone	2.42	1.53	54.LP(2)O7	419.BD*(1)C10-Cl19
			0.89	53.LP(1)O7	419.BD*(1)C10-Cl19
	DMSO	2.27	1.41	54.LP(2)O7	419.BD*(1)C10-Cl19
			0.86	53.LP(1)O7	419.BD*(1)C10-Cl19
	Water	2.22	1.38	54.LP(2)O7	419.BD*(1)C10-Cl19
			0.84	53.LP(1)O7	419.BD*(1)C10-Cl19
Cl Neutral-Anion	Vacuum[f]	4.16	3.07	53.LP(2)O7	413.BD*(1)C10-Cl19
			1.04	52.LP(1)O7	413.BD*(1)C10-Cl19
			0.05	56.LP(2)O9[e]	413.BD*(1)C10-Cl19
	TCM	1.78	1.06	52.LP(2)O7	414.BD*(1)C10-Cl19
			0.66	51.LP(1)O7	414.BD*(1)C10-Cl19
			0.06	53.LP(3)O7	414.BD*(1)C10-Cl19
	DCE	1.48	0.95	52.LP(2)O7	414.BD*(1)C10-Cl19
			0.53	51.LP(1)O7	414.BD*(1)C10-Cl19

	Acetone	1.32	0.86	52.LP(2)O7	414.BD*(1)C10-Cl19
			0.46	51.LP(1)O7	414.BD*(1)C10-Cl19
	DMSO	1.34	0.82	52.LP(2)O7	414.BD*(1)C10-Cl19
			0.52	51.LP(1)O7	414.BD*(1)C10-Cl19
	Water	1.23	0.78	52.LP(2)O7	414.BD*(1)C10-Cl19
			0.40	51.LP(1)O7	414.BD*(1)C10-Cl19
			0.05	53.LP(3)O7	414.BD*(1)C10-Cl19
Cl Anion-Anion	Vacuum[g]	0.80	0.39	51.LP(1)O7	407.BD*(1)C10-Cl19
			0.25	52.LP(2)O7	407.BD*(1)C10-Cl19
			0.16	53.LP(3)O7	407.BD*(1)C10-Cl19
	TCM	0.81	0.39	50.LP(1)O7	408.BD*(1)C10-Cl19
			0.26	51.LP(2)O7	408.BD*(1)C10-Cl19
			0.16	52.LP(3)O7	408.BD*(1)C10-Cl19
	DCE	1.22	0.77	51.LP(2)O7	408.BD*(1)C10-Cl19
			0.45	50.LP(1)O7	408.BD*(1)C10-Cl19
	Acetone	1.17	0.75	51.LP(2)O7	408.BD*(1)C10-Cl19
			0.42	50.LP(1)O7	408.BD*(1)C10-Cl19
	DMSO	0.90	0.63	51.LP(2)O7	408.BD*(1)C10-Cl19
			0.27	50.LP(1)O7	408.BD*(1)C10-Cl19
	Water	0.99	0.67	51.LP(2)O7	408.BD*(1)C10-Cl19
			0.32	50.LP(1)O7	408.BD*(1)C10-Cl19
Cl Cation-Neutral	Vacuum	2.09	1.29	54.LP(1)O7	426.BD*(1)C10-Cl19
			0.80	55.LP(2)O7	426.BD*(1)C10-Cl19
	TCM	1.71	0.90	55.LP(2)O7	426.BD*(1)C10-Cl19
			0.81	54.LP(1)O7	426.BD*(1)C10-Cl19
	DCE	1.55	0.90	55.LP(2)O7	426.BD*(1)C10-Cl19

			0.65	54.LP(1)O7	426.BD*(1)C10-Cl19
	Acetone	1.43	0.85	55.LP(2)O7	426.BD*(1)C10-Cl19
			0.58	54.LP(1)O7	426.BD*(1)C10-Cl19
	DMSO	1.35	0.81	55.LP(2)O7	426.BD*(1)C10-Cl19
			0.54	54.LP(1)O7	426.BD*(1)C10-Cl19
	Water	1.34	0.81	55.LP(2)O7	426.BD*(1)C10-Cl19
			0.53	54.LP(1)O7	426.BD*(1)C10-Cl19
Cl Neutral-Neutral	Vacuum[f]	0.85	0.51	54.LP(2)O7	420.BD*(1)C10-Cl19
			0.34	53.LP(1)O7	420.BD*(1)C10-Cl19
	TCM	0.95	0.54	54.LP(2)O7	420.BD*(1)C10-Cl19
			0.41	53.LP(1)O7	420.BD*(1)C10-Cl19
	DCE	0.92	0.53	54.LP(2)O7	420.BD*(1)C10-Cl19
			0.39	53.LP(1)O7	420.BD*(1)C10-Cl19
	Acetone	0.92	0.53	54.LP(2)O7	420.BD*(1)C10-Cl19
			0.39	53.LP(1)O7	420.BD*(1)C10-Cl19
	DMSO	0.90	0.52	54.LP(2)O7	420.BD*(1)C10-Cl19
			0.38	53.LP(1)O7	420.BD*(1)C10-Cl19
	Water	0.90	0.52	54.LP(2)O7	420.BD*(1)C10-Cl19
			0.38	53.LP(1)O7	420.BD*(1)C10-Cl19
Cl Anion-Neutral	Vacuum[g]	0.46	0.31	53.LP(2)O7	414.BD*(1)C10-Cl19
			0.15	52.LP(1)O7	414.BD*(1)C10-Cl19
	TCM[f]	0.53	0.37	52.LP(2)O7	415.BD*(1)C10-Cl19
			0.16	51.LP(1)O7	415.BD*(1)C10-Cl19
	DCE	0.57	0.40	52.LP(2)O7	415.BD*(1)C10-Cl19
			0.17	51.LP(1)O7	415.BD*(1)C10-Cl19
	Acetone	0.63	0.44	52.LP(2)O7	415.BD*(1)C10-Cl19

			0.19	51.LP(1)O7	415.BD*(1)C10-Cl19
	DMSO	0.67	0.47	52.LP(2)O7	415.BD*(1)C10-Cl19
			0.20	51.LP(1)O7	415.BD*(1)C10-Cl19
	Water	0.74	0.50	52.LP(2)O7	415.BD*(1)C10-Cl19
			0.24	51.LP(1)O7	415.BD*(1)C10-Cl19
Cl Cation-Cation	Vacuum[g]	0.75	0.48	55.LP(2)O7	433.BD*(1)C10-Cl19
			0.27	54.LP(1)O7	433.BD*(1)C10-Cl19
	TCM	0.84	0.54	55.LP(2)O7	433.BD*(1)C10-Cl19
			0.30	54.LP(1)O7	433.BD*(1)C10-Cl19
	DCE	0.98	0.58	55.LP(2)O7	433.BD*(1)C10-Cl19
			0.40	54.LP(1)O7	433.BD*(1)C10-Cl19
	Acetone	1.02	0.60	55.LP(2)O7	433.BD*(1)C10-Cl19
			0.42	54.LP(1)O7	433.BD*(1)C10-Cl19
	DMSO	1.01	0.63	55.LP(2)O7	433.BD*(1)C10-Cl19
			0.38	54.LP(1)O7	433.BD*(1)C10-Cl19
	Water	1.01	0.63	55.LP(2)O7	433.BD*(1)C10-Cl19
			0.38	54.LP(1)O7	433.BD*(1)C10-Cl19
Cl Neutral-Cation	Vacuum[g]	0.53	0.37	54.LP(2)O7	427.BD*(1)C10-Cl19
			0.16	53.LP(1)O7	427.BD*(1)C10-Cl19
	TCM	0.64	0.46	54.LP(2)O7	427.BD*(1)C10-Cl19
			0.18	53.LP(1)O7	427.BD*(1)C10-Cl19
	DCE	0.67	0.48	54.LP(2)O7	427.BD*(1)C10-Cl19
			0.19	53.LP(1)O7	427.BD*(1)C10-Cl19
	Acetone	0.70	0.50	54.LP(2)O7	427.BD*(1)C10-Cl19
			0.20	53.LP(1)O7	427.BD*(1)C10-Cl19
	DMSO	0.70	0.50	54.LP(2)O7	427.BD*(1)C10-Cl19

			0.20	53.LP(1)O7	427.BD*(1)C10-Cl19
	Water	0.70	0.50	54.LP(2)O7	427.BD*(1)C10-Cl19
			0.20	53.LP(1)O7	427.BD*(1)C10-Cl19
Cl Anion-Cation	Vacuum[g]	0.60	0.32	53.LP(2)O7	421.BD*(1)C10-Cl19
			0.28	52.LP(1)O7	421.BD*(1)C10-Cl19
	TCM[f]	0.76	0.44	52.LP(2)O7	422.BD*(1)C10-Cl19
			0.32	51.LP(1)O7	422.BD*(1)C10-Cl19
	DCE	0.72	0.44	52.LP(2)O7	422.BD*(1)C10-Cl19
			0.28	51.LP(1)O7	422.BD*(1)C10-Cl19
	Acetone	0.71	0.27	51.LP(1)O7	422.BD*(1)C10-Cl19
			0.44	52.LP(2)O7	422.BD*(1)C10-Cl19
	DMSO	0.60	0.42	52.LP(2)O7	422.BD*(1)C10-Cl19
			0.18	51.LP(1)O7	422.BD*(1)C10-Cl19
	Water	0.60	0.42	52.LP(2)O7	422.BD*(1)C10-Cl19
			0.18	51.LP(1)O7	422.BD*(1)C10-Cl19

[a]Sum of *b* in each molecular system. Values are in kcal/mol. [b]The corresponding second-order perturbation stabilization energy for each intermolecular electron transfer. Values are in kcal/mol. [c]The natural bond orbitals that donate electrons. For instance, 53.LP(2)O7, refers to one of the orbitals for lone pair of electrons on the acceptor oxygen atom, where 53 is the serial number of this orbital; LP means lone pair; 2 in the brackets is the serial number of lone pair electron orbital for O7, O stands for oxygen and 7 is the serial number of this oxygen atom in the complex geometry. [d]The natural bond orbitals that accept electrons. Similar with c, BD* stands for antibonding molecular orbital. [e]The lone pair electron orbital for the other oxygen (O9) in the acceptor's carboxyl group, indicating the existence of the multiple halogen bonding. [f]Results based on constrained optimizations. [g]Results based on TCM-optimized geometries.

Table S15. Natural bond orbitals and the *E*(2) results involved in electron transfer from lone pair electron orbitals of the oxygen atom to $\sigma^*_{C\text{-}X}$ for complexes between differently charged 3-amino-5-bromobenzoic acid and glycine.

Complex	Environment	$E(2)_{Sum}$[a]	$E(2)$[b]	Electron donor orbtial[c]	Electron acceptor orbtial[d]
Br Cation-Anion	Vacuum[f]	23.69	19.74	63.LP(2)O7	437.BD*(1)C10-Br27
			3.63	62.LP(1)O7	437.BD*(1)C10-Br27
			0.24	66.LP(2)O9[e]	437.BD*(1)C10-Br27
			0.08	65.LP(1)O9[e]	437.BD*(1)C10-Br27
	TCM	6.99	4.86	63.LP(2)O7	437.BD*(1)C10-Br27
			1.96	62.LP(1)O7	437.BD*(1)C10-Br27
			0.11	64.LP(3)O7	437.BD*(1)C10-Br27
			0.06	66.LP(2)O9[e]	437.BD*(1)C10-Br27
	DCE	5.80	3.86	63.LP(2)O7	437.BD*(1)C10-Br27
			1.94	62.LP(1)O7	437.BD*(1)C10-Br27
	Acetone	5.08	3.05	63.LP(2)O7	437.BD*(1)C10-Br27
			1.87	62.LP(1)O7	437.BD*(1)C10-Br27
			0.16	64.LP(3)O7	437.BD*(1)C10-Br27
	DMSO	4.66	2.84	63.LP(2)O7	437.BD*(1)C10-Br27
			1.76	62.LP(1)O7	437.BD*(1)C10-Br27
			0.06	64.LP(3)O7	437.BD*(1)C10-Br27
	Water	4.48	2.47	63.LP(2)O7	437.BD*(1)C10-Br27
			1.77	62.LP(1)O7	437.BD*(1)C10-Br27
			0.24	64.LP(3)O7	437.BD*(1)C10-Br27
Br Neutral-Anion	Vacuum	8.78	6.49	62.LP(2)O7	431.BD*(1)C10-Br26
			2.22	61.LP(1)O7	431.BD*(1)C10-Br26

			0.07	65.LP(2)O9[e]	431.BD*(1)C10-Br26
	TCM	4.74	3.03	62.LP(2)O7	431.BD*(1)C10-Br26
			1.71	61.LP(1)O7	431.BD*(1)C10-Br26
	DCE	4.00	2.48	62.LP(2)O7	431.BD*(1)C10-Br26
			1.52	61.LP(1)O7	431.BD*(1)C10-Br26
	Acetone	3.64	2.16	62.LP(2)O7	431.BD*(1)C10-Br26
			1.48	61.LP(1)O7	431.BD*(1)C10-Br26
	DMSO	3.29	1.35	62.LP(2)O7	431.BD*(1)C10-Br26
			1.33	61.LP(1)O7	431.BD*(1)C10-Br26
			0.61	63.LP(3)O7	431.BD*(1)C10-Br26
	Water	3.45	2.03	62.LP(2)O7	431.BD*(1)C10-Br26
			1.42	61.LP(1)O7	431.BD*(1)C10-Br26
Br Anion-Anion	Vacuum[g]	3.09	1.25	61.LP(2)O7	425.BD*(1)C10-Br25
			1.21	60.LP(1)O7	425.BD*(1)C10-Br25
			0.63	62.LP(3)O7	425.BD*(1)C10-Br25
	TCM	3.03	1.23	60.LP(2)O7	426.BD*(1)C10-Br25
			1.19	59.LP(1)O7	426.BD*(1)C10-Br25
			0.61	61.LP(3)O7	426.BD*(1)C10-Br25
	DCE	2.15	1.24	60.LP(2)O7	426.BD*(1)C10-Br25
			0.84	59.LP(1)O7	426.BD*(1)C10-Br25
			0.07	61.LP(3)O7	426.BD*(1)C10-Br25
	Acetone	2.46	1.28	60.LP(2)O7	426.BD*(1)C10-Br25
			0.94	59.LP(1)O7	426.BD*(1)C10-Br25
			0.24	61.LP(3)O7	426.BD*(1)C10-Br25
	DMSO	2.51	1.30	60.LP(2)O7	426.BD*(1)C10-Br25
			0.96	59.LP(1)O7	426.BD*(1)C10-Br25

			0.25	61.LP(3)O7	426.BD*(1)C10-Br25
	Water	2.54	1.30	60.LP(2)O7	426.BD*(1)C10-Br25
			0.98	59.LP(1)O7	426.BD*(1)C10-Br25
			0.26	61.LP(3)O7	426.BD*(1)C10-Br25
Br Cation-Neutral	Vacuum	3.87	1.96	63.LP(1)O7	444.BD*(1)C10-Br28
			1.91	64.LP(2)O7	444.BD*(1)C10-Br28
	TCM	2.89	1.52	64.LP(2)O7	444.BD*(1)C10-Br28
			1.37	63.LP(1)O7	444.BD*(1)C10-Br28
	DCE	2.74	1.49	64.LP(2)O7	444.BD*(1)C10-Br28
			1.25	63.LP(1)O7	444.BD*(1)C10-Br28
	Acetone	2.65	1.46	64.LP(2)O7	444.BD*(1)C10-Br28
			1.19	63.LP(1)O7	444.BD*(1)C10-Br28
	DMSO	2.37	1.45	64.LP(2)O7	444.BD*(1)C10-Br28
			0.92	63.LP(1)O7	444.BD*(1)C10-Br28
	Water	2.35	1.44	64.LP(2)O7	444.BD*(1)C10-Br28
			0.91	63.LP(1)O7	444.BD*(1)C10-Br28
Br Neutral-Neutral	Vacuum[f]	1.93	1.00	63.LP(2)O7	438.BD*(1)C10-Br27
			0.93	62.LP(1)O7	438.BD*(1)C10-Br27
	TCM	1.92	1.09	63.LP(2)O7	438.BD*(1)C10-Br27
			0.83	62.LP(1)O7	438.BD*(1)C10-Br27
	DCE	1.91	1.09	63.LP(2)O7	438.BD*(1)C10-Br27
			0.82	62.LP(1)O7	438.BD*(1)C10-Br27
	Acetone	1.83	1.07	63.LP(2)O7	438.BD*(1)C10-Br27
			0.76	62.LP(1)O7	438.BD*(1)C10-Br27
	DMSO	1.71	1.05	63.LP(2)O7	438.BD*(1)C10-Br27
			0.66	62.LP(1)O7	438.BD*(1)C10-Br27

	Water	1.70	1.05	63.LP(2)O7	438.BD*(1)C10-Br27
			0.65	62.LP(1)O7	438.BD*(1)C10-Br27
Br Anion-Neutral	Vacuum[g]	0.99	0.59	62.LP(2)O7	432.BD*(1)C10-Br26
			0.40	61.LP(1)O7	432.BD*(1)C10-Br26
	TCM[f]	1.11	0.70	61.LP(2)O7	433.BD*(1)C10-Br26
			0.41	60.LP(1)O7	433.BD*(1)C10-Br26
	DCE[f]	1.23	0.77	61.LP(2)O7	433.BD*(1)C10-Br26
			0.46	60.LP(1)O7	433.BD*(1)C10-Br26
	Acetone	1.31	0.81	61.LP(2)O7	433.BD*(1)C10-Br26
			0.50	60.LP(1)O7	433.BD*(1)C10-Br26
	DMSO	1.35	0.84	61.LP(2)O7	433.BD*(1)C10-Br26
			0.51	60.LP(1)O7	433.BD*(1)C10-Br26
	Water	1.37	0.85	61.LP(2)O7	433.BD*(1)C10-Br26
			0.52	60.LP(1)O7	433.BD*(1)C10-Br26
Br Cation-Cation	Vacuum[g]	1.70	0.93	64.LP(2)O7	451.BD*(1)C10-Br29
			0.77	63.LP(1)O7	451.BD*(1)C10-Br29
	TCM	1.87	1.05	64.LP(2)O7	451.BD*(1)C10-Br29
			0.82	63.LP(1)O7	451.BD*(1)C10-Br29
	DCE	2.08	1.13	64.LP(2)O7	451.BD*(1)C10-Br29
			0.95	63.LP(1)O7	451.BD*(1)C10-Br29
	Acetone	2.01	1.13	64.LP(2)O7	451.BD*(1)C10-Br29
			0.88	63.LP(1)O7	451.BD*(1)C10-Br29
	DMSO	2.03	1.15	64.LP(2)O7	451.BD*(1)C10-Br29
			0.88	63.LP(1)O7	451.BD*(1)C10-Br29
	Water	2.05	1.16	64.LP(2)O7	451.BD*(1)C10-Br29
			0.89	63.LP(1)O7	451.BD*(1)C10-Br29

Br Neutral-Cation	Vacuum[g]	1.09	0.57	63.LP(2)O7	445.BD*(1)C10-Br28
			0.52	62.LP(1)O7	445.BD*(1)C10-Br28
	TCM	1.31	0.73	63.LP(2)O7	445.BD*(1)C10-Br28
			0.58	62.LP(1)O7	445.BD*(1)C10-Br28
	DCE	1.29	0.70	63.LP(2)O7	445.BD*(1)C10-Br28
			0.59	62.LP(1)O7	445.BD*(1)C10-Br28
	Acetone	1.49	0.84	63.LP(2)O7	445.BD*(1)C10-Br28
			0.65	62.LP(1)O7	445.BD*(1)C10-Br28
	DMSO	1.61	0.92	63.LP(2)O7	445.BD*(1)C10-Br28
			0.69	62.LP(1)O7	445.BD*(1)C10-Br28
	Water	1.62	0.92	63.LP(2)O7	445.BD*(1)C10-Br28
			0.70	62.LP(1)O7	445.BD*(1)C10-Br28
Br Anion-Cation	Vacuum[g]	0.92	0.48	61.LP(1)O7	439.BD*(1)C10-Br27
			0.44	62.LP(2)O7	439.BD*(1)C10-Br27
	TCM	1.16	0.62	61.LP(2)O7	440.BD*(1)C10-Br27
			0.54	60.LP(1)O7	440.BD*(1)C10-Br27
	DCE	1.22	0.67	61.LP(2)O7	440.BD*(1)C10-Br27
			0.55	60.LP(1)O7	440.BD*(1)C10-Br27
	Acetone	1.26	0.70	61.LP(2)O7	440.BD*(1)C10-Br27
			0.56	60.LP(1)O7	440.BD*(1)C10-Br27
	DMSO	1.05	0.56	61.LP(2)O7	440.BD*(1)C10-Br27
			0.49	60.LP(1)O7	440.BD*(1)C10-Br27
	Water	1.13	0.72	61.LP(2)O7	440.BD*(1)C10-Br27
			0.41	60.LP(1)O7	440.BD*(1)C10-Br27

[a]Sum of *b* in each molecular system. Values are in kcal/mol. [b]The corresponding second-order perturbation stabilization energy for each intermolecular electron transfer. Values are in kcal/mol. [c]The

natural bond orbitals that donate electrons. For instance, 53.LP(2)O7, refers to one of the orbitals for lone pair of electrons on the acceptor oxygen atom, where 53 is the serial number of this orbital; LP means lone pair; 2 in the brackets is the serial number of lone pair electron orbital for O7, O stands for oxygen and 7 is the serial number of this oxygen atom in the complex geometry. [d]The natural bond orbitals that accept electrons. Similar with c, BD* stands for antibonding molecular orbital. [e]The lone pair electron orbital for the other oxygen (O9) in the acceptor's carboxyl group, indicating the existence of the multiple halogen bonding. [f]Results based on constrained optimizations. [g]Results based on TCM-optimized geometries.

Table S16. Natural bond orbitals and the *E*(2) results involved in electron transfer from lone pair electron orbitals of the oxygen atom to $\sigma^*_{C\text{-}X}$ for complexes between differently charged 3-amino-5-iodobenzoic acid and glycine.

Complex	Environment	$E(2)_{Sum}$[a]	*E*(2)[b]	Electron donor orbtial[c]	Electron acceptor orbtial[d]
I Cation-Anion	Vacuum	34.46	27.49	48.LP(2)O7	400.BD*(1)C10-I27
			6.24	47.LP(1)O7	400.BD*(1)C10-I27
			0.38	51.LP(2)O9[e]	400.BD*(1)C10-I27
			0.24	50.LP(1)O9[e]	400.BD*(1)C10-I27
			0.11	49.LP(3)O7	400.BD*(1)C10-I27
	TCM	14.67	10.24	49.LP(2)O7	400.BD*(1)C10-I27
			4.13	48.LP(1)O7	400.BD*(1)C10-I27
			0.18	52.LP(2)O9[e]	400.BD*(1)C10-I27
			0.12	51.LP(1)O9[e]	400.BD*(1)C10-I27
	DCE	12.05	8.07	49.LP(2)O7	400.BD*(1)C10-I27
			3.75	48.LP(1)O7	400.BD*(1)C10-I27
			0.13	52.LP(2)O9[e]	400.BD*(1)C10-I27

			0.10	51.LP(1)O9[e]	400.BD*(1)C10-I27
	Acetone	11.55	7.79	49.LP(2)O7	400.BD*(1)C10-I27
			3.53	48.LP(1)O7	400.BD*(1)C10-I27
			0.10	52.LP(2)O9[e]	400.BD*(1)C10-I27
			0.07	50.LP(3)O7	400.BD*(1)C10-I27
			0.06	51.LP(1)O9[e]	400.BD*(1)C10-I27
	DMSO	10.97	7.27	49.LP(2)O7	400.BD*(1)C10-I27
			3.48	48.LP(1)O7	400.BD*(1)C10-I27
			0.09	50.LP(3)O7	400.BD*(1)C10-I27
			0.08	52.LP(2)O9[e]	400.BD*(1)C10-I27
			0.05	51.LP(1)O9[e]	400.BD*(1)C10-I27
	Water	10.70	7.09	49.LP(2)O7	400.BD*(1)C10-I27
			3.44	48.LP(1)O7	400.BD*(1)C10-I27
			0.09	50.LP(3)O7	400.BD*(1)C10-I27
			0.08	52.LP(2)O9[e]	400.BD*(1)C10-I27
I Neutral-Anion	Vacuum	15.91	11.36	48.LP(2)O7	394.BD*(1)C10-I26
			4.30	47.LP(1)O7	394.BD*(1)C10-I26
			0.13	51.LP(2)O9[e]	394.BD*(1)C10-I26
			0.12	50.LP(1)O9[e]	394.BD*(1)C10-I26
	TCM	10.14	6.66	48.LP(2)O7	394.BD*(1)C10-I26
			3.32	47.LP(1)O7	394.BD*(1)C10-I26
			0.10	49.LP(3)O7	394.BD*(1)C10-I26
			0.06	51.LP(2)O9[e]	394.BD*(1)C10-I26
	DCE	8.34	5.12	48.LP(2)O7	394.BD*(1)C10-I26
			3.12	47.LP(1)O7	394.BD*(1)C10-I26
			0.10	49.LP(3)O7	394.BD*(1)C10-I26
	Acetone	7.66	4.46	48.LP(2)O7	394.BD*(1)C10-I26

			3.03	47.LP(1)O7	394.BD*(1)C10-I26
			0.17	49.LP(3)O7	394.BD*(1)C10-I26
			4.72	48.LP(2)O7	394.BD*(1)C10-I26
	DMSO	7.69	2.90	47.LP(1)O7	394.BD*(1)C10-I26
			0.07	49.LP(3)O7	394.BD*(1)C10-I26
			4.17	48.LP(2)O7	394.BD*(1)C10-I26
	Water	7.29	2.92	47.LP(1)O7	394.BD*(1)C10-I26
			0.20	49.LP(3)O7	394.BD*(1)C10-I26
			3.54	46.LP(1)O7	388.BD*(1)C10-I25
	Vacuum	4.61	0.90	47.LP(2)O7	388.BD*(1)C10-I25
			0.17	48.LP(3)O7	388.BD*(1)C10-I25
			3.60	46.LP(2)O7	389.BD*(1)C10-I25
	TCM	6.36	2.67	45.LP(1)O7	389.BD*(1)C10-I25
			0.09	47.LP(3)O7	389.BD*(1)C10-I25
			3.35	46.LP(2)O7	389.BD*(1)C10-I25
	DCE	6.08	2.66	45.LP(1)O7	389.BD*(1)C10-I25
			0.07	47.LP(3)O7	389.BD*(1)C10-I25
I Anion-Anion			3.41	46.LP(2)O7	389.BD*(1)C10-I25
	Acetone	6.07	2.61	45.LP(1)O7	389.BD*(1)C10-I25
			0.05	47.LP(3)O7	389.BD*(1)C10-I25
			3.42	46.LP(2)O7	389.BD*(1)C10-I25
	DMSO	6.09	2.61	45.LP(1)O7	389.BD*(1)C10-I25
			0.06	47.LP(3)O7	389.BD*(1)C10-I25
			3.42	46.LP(2)O7	389.BD*(1)C10-I25
	Water	6.09	2.61	45.LP(1)O7	389.BD*(1)C10-I25
			0.06	47.LP(3)O7	389.BD*(1)C10-I25
I Cation-Neutral	Vacuum	6.81	3.64	49.LP(1)O7	407.BD*(1)C10-I28

			3.17	50.LP(2)O7	407.BD*(1)C10-I28
	TCM	5.21	2.72	49.LP(1)O7	407.BD*(1)C10-I28
			2.49	50.LP(2)O7	407.BD*(1)C10-I28
	DCE	4.96	2.53	49.LP(1)O7	407.BD*(1)C10-I28
			2.43	50.LP(2)O7	407.BD*(1)C10-I28
	Acetone	4.89	2.43	49.LP(1)O7	407.BD*(1)C10-I28
			2.41	50.LP(2)O7	407.BD*(1)C10-I28
			0.05	51.LP(1)O9[e]	407.BD*(1)C10-I28
	DMSO	4.83	2.39	50.LP(2)O7	407.BD*(1)C10-I28
			2.39	49.LP(1)O7	407.BD*(1)C10-I28
			0.05	51.LP(1)O9[e]	407.BD*(1)C10-I28
	Water	4.80	2.38	49.LP(1)O7	407.BD*(1)C10-I28
			2.37	50.LP(2)O7	407.BD*(1)C10-I28
			0.05	51.LP(1)O9[e]	407.BD*(1)C10-I28
I Neutral-Neutral	Vacuum	3.34	1.89	48.LP(1)O7	401.BD*(1)C10-I27
			1.45	49.LP(2)O7	401.BD*(1)C10-I27
	TCM	3.69	2.01	48.LP(1)O7	401.BD*(1)C10-I27
			1.68	49.LP(2)O7	401.BD*(1)C10-I27
	DCE	3.54	1.74	49.LP(2)O7	401.BD*(1)C10-I27
			1.73	48.LP(1)O7	401.BD*(1)C10-I27
			0.07	50.LP(1)O9[e]	401.BD*(1)C10-I27
	Acetone	3.80	1.89	49.LP(2)O7	401.BD*(1)C10-I27
			1.85	48.LP(1)O7	401.BD*(1)C10-I27
			0.06	50.LP(1)O9[e]	401.BD*(1)C10-I27
	DMSO	3.82	1.91	48.LP(1)O7	401.BD*(1)C10-I27
			1.86	49.LP(2)O7	401.BD*(1)C10-I27
			0.05	50.LP(1)O9[e]	401.BD*(1)C10-I27

	Water	3.69	1.89	49.LP(2)O7	401.BD*(1)C10-I27
			1.71	48.LP(1)O7	401.BD*(1)C10-I27
			0.09	50.LP(1)O9[e]	401.BD*(1)C10-I27
I Anion-Neutral	Vacuum[f]	1.39	0.70	48.LP(2)O7	395.BD*(1)C10-I26
			0.61	47.LP(1)O7	395.BD*(1)C10-I26
			0.08	49.LP(1)O9[e]	395.BD*(1)C10-I26
	TCM	2.38	1.21	46.LP(1)O7	396.BD*(1)C10-I26
			1.11	47.LP(2)O7	396.BD*(1)C10-I26
			0.06	48.LP(1)O9[e]	396.BD*(1)C10-I26
	DCE	2.88	1.49	46.LP(1)O7	396.BD*(1)C10-I26
			1.39	47.LP(2)O7	396.BD*(1)C10-I26
	Acetone	3.09	1.60	46.LP(1)O7	396.BD*(1)C10-I26
			1.49	47.LP(2)O7	396.BD*(1)C10-I26
	DMSO	3.17	1.63	46.LP(1)O7	396.BD*(1)C10-I26
			1.54	47.LP(2)O7	396.BD*(1)C10-I26
	Water	3.07	1.57	47.LP(2)O7	396.BD*(1)C10-I26
			1.42	46.LP(1)O7	396.BD*(1)C10-I26
			0.08	48.LP(1)O9[e]	396.BD*(1)C10-I26
I Cation-Cation	Vacuum[g]	3.19	1.74	49.LP(1)O7	414.BD*(1)C10-I29
			1.45	50.LP(2)O7	414.BD*(1)C10-I29
	TCM	3.51	1.85	49.LP(1)O7	414.BD*(1)C10-I29
			1.66	50.LP(2)O7	414.BD*(1)C10-I29
	DCE	3.61	1.80	49.LP(1)O7	414.BD*(1)C10-I29
			1.76	50.LP(2)O7	414.BD*(1)C10-I29
			0.05	51.LP(1)O9[e]	414.BD*(1)C10-I29
	Acetone	3.84	1.99	49.LP(1)O7	414.BD*(1)C10-I29

			1.85	50.LP(2)O7	414.BD*(1)C10-I29
	DMSO	3.89	2.01	49.LP(1)O7	414.BD*(1)C10-I29
			1.88	50.LP(2)O7	414.BD*(1)C10-I29
	Water	3.89	2.01	49.LP(1)O7	414.BD*(1)C10-I29
			1.88	50.LP(2)O7	414.BD*(1)C10-I29
I Neutral-Cation	Vacuum[g]	2.20	1.29	48.LP(1)O7	408.BD*(1)C10-I28
			0.91	49.LP(2)O7	408.BD*(1)C10-I28
	TCM	2.60	1.42	48.LP(1)O7	408.BD*(1)C10-I28
			1.18	49.LP(2)O7	408.BD*(1)C10-I28
	DCE	2.86	1.55	48.LP(1)O7	408.BD*(1)C10-I28
			1.31	49.LP(2)O7	408.BD*(1)C10-I28
	Acetone	3.00	1.62	48.LP(1)O7	408.BD*(1)C10-I28
			1.38	49.LP(2)O7	408.BD*(1)C10-I28
	DMSO	3.08	1.66	48.LP(1)O7	408.BD*(1)C10-I28
			1.42	49.LP(2)O7	408.BD*(1)C10-I28
	Water	3.09	1.66	48.LP(1)O7	408.BD*(1)C10-I28
			1.43	49.LP(2)O7	408.BD*(1)C10-I28
I Anion-Cation	Vacuum[g]	1.64	1.00	47.LP(1)O7	402.BD*(1)C10-I27
			0.64	48.LP(2)O7	402.BD*(1)C10-I27
	TCM	2.06	1.12	46.LP(1)O7	403.BD*(1)C10-I27
			0.94	47.LP(2)O7	403.BD*(1)C10-I27
	DCE	2.32	1.23	46.LP(1)O7	403.BD*(1)C10-I27
			1.09	47.LP(2)O7	403.BD*(1)C10-I27
	Acetone	2.43	1.28	46.LP(1)O7	403.BD*(1)C10-I27
			1.15	47.LP(2)O7	403.BD*(1)C10-I27
	DMSO	2.49	1.30	46.LP(1)O7	403.BD*(1)C10-I27

			1.19	47.LP(2)O7	403.BD*(1)C10-I27
	Water	2.54	1.33	46.LP(1)O7	403.BD*(1)C10-I27
			1.21	47.LP(2)O7	403.BD*(1)C10-I27

[a]Sum of *b* in each molecular system. Values are in kcal/mol. [b]The corresponding second-order perturbation stabilization energy for each intermolecular electron transfer. Values are in kcal/mol. [c]The natural bond orbitals that donate electrons. For instance, 53.LP(2)O7, refers to one of the orbitals for lone pair of electrons on the acceptor oxygen atom, where 53 is the serial number of this orbital; LP means lone pair; 2 in the brackets is the serial number of lone pair electron orbital for O7, O stands for oxygen and 7 is the serial number of this oxygen atom in the complex geometry. [d]The natural bond orbitals that accept electrons. Similar with c, BD* stands for antibonding molecular orbital. [e]The lone pair electron orbital for the other oxygen (O9) in the acceptor's carboxyl group, indicating the existence of the multiple halogen bonding. [f]Results based on constrained optimizations. [g]Results based on TCM-optimized geometries.

Table S17. Calculated atomic charge and electron transfer results from natural population analysis for complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
Cl Cation-Anion	Vacuum[g]	0.0529	0.0987	0.2192	0.1206	-0.1734
	TCM[g]	0.0193	0.0558	0.1051	0.0494	-0.0686
	DCE	0.0137	0.0469	0.0806	0.0336	-0.0473
	Acetone	0.0123	0.0427	0.0690	0.0264	-0.0387
	DMSO	0.0115	0.0403	0.0623	0.0221	-0.0336
	Water	0.0113	0.0395	0.0601	0.0206	-0.0319
Cl Neutral-Anion	Vacuum[g]	0.0233	0.0131	0.1222	0.1091	-0.1324
	TCM	0.0094	0.0019	0.0461	0.0442	-0.0536
	DCE	0.0086	0.0004	0.0289	0.0285	-0.0370
	Acetone	0.0080	-0.0011	0.0204	0.0215	-0.0295
	DMSO	0.0074	-0.0017	0.0172	0.0189	-0.0264
	Water	0.0076	-0.0018	0.0135	0.0154	-0.0229
Cl Anion-Anion	Vacuum[h]	0.0039	-0.0555	0.0299	0.0854	-0.0893
	TCM	0.0039	-0.0339	0.0039	0.0378	-0.0417
	DCE	0.0070	-0.0294	0.0002	0.0296	-0.0366
	Acetone	0.0069	-0.0272	-0.0048	0.0225	-0.0294
	DMSO	0.0065	-0.0260	-0.0106	0.0154	-0.0219
	Water	0.0065	-0.0256	-0.0105	0.0151	-0.0216
Cl Cation-Neutral	Vacuum	0.0070	0.0987	0.1333	0.0346	-0.0417
	TCM	0.0061	0.0558	0.0753	0.0195	-0.0257
	DCE	0.0061	0.0469	0.0620	0.0150	-0.0211
	Acetone	0.0058	0.0427	0.0553	0.0126	-0.0184
	DMSO	0.0056	0.0403	0.0513	0.0110	-0.0167

	Water	0.0056	0.0395	0.0500	0.0105	-0.0162
Cl Neutral-Neutral	Vacuum[g]	0.0038	0.0131	0.0380	0.0249	-0.0286
	TCM	0.0038	0.0019	0.0193	0.0174	-0.0212
	DCE	0.0039	0.0004	0.0135	0.0130	-0.0169
	Acetone	0.0039	-0.0011	0.0104	0.0115	-0.0154
	DMSO	0.0039	-0.0017	0.0085	0.0102	-0.0141
	Water	0.0039	-0.0018	0.0079	0.0098	-0.0136
Cl Anion-Neutral	Vacuum[h]	0.0015	-0.0555	-0.0277	0.0278	-0.0293
	TCM[g]	0.0030	-0.0339	-0.0182	0.0157	-0.0186
	DCE	0.0034	-0.0294	-0.0178	0.0116	-0.0150
	Acetone	0.0037	-0.0272	-0.0174	0.0098	-0.0135
	DMSO	0.0039	-0.0260	-0.0172	0.0088	-0.0127
	Water	0.0039	-0.0256	-0.0167	0.0089	-0.0128
Cl Cation-Cation	Vacuum[h]	0.0026	0.0987	0.0720	-0.0267	0.0240
	TCM	0.0035	0.0558	0.0567	0.0009	-0.0045
	DCE	0.0038	0.0469	0.0522	0.0053	-0.0091
	Acetone	0.0040	0.0427	0.0492	0.0065	-0.0105
	DMSO	0.0043	0.0403	0.0469	0.0067	-0.0109
	Water	0.0043	0.0395	0.0463	0.0068	-0.0111
Cl Neutral-Cation	Vacuum[h]	0.0012	0.0131	-0.0098	-0.0229	0.0218
	TCM	0.0031	0.0019	0.0041	0.0021	-0.0053
	DCE	0.0035	0.0004	0.0046	0.0042	-0.0077
	Acetone	0.0037	-0.0011	0.0045	0.0056	-0.0093
	DMSO	0.0038	-0.0017	0.0043	0.0060	-0.0098
	Water	0.0039	-0.0018	0.0042	0.0061	-0.0099

Cl Anion-Cation	Vacuum[h]	-0.0012	-0.0555	-0.0701	-0.0146	0.0159
	TCM[g]	0.0023	-0.0339	-0.0296	0.0043	-0.0065
	DCE	0.0027	-0.0294	-0.0228	0.0067	-0.0093
	Acetone	0.0029	-0.0272	-0.0202	0.0070	-0.0099
	DMSO	0.0033	-0.0260	-0.0200	0.0060	-0.0093
	Water	0.0033	-0.0256	-0.0196	0.0060	-0.0093

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from natural population analysis (NPA). [d]Atomic charge of the halogen atom in complex from NPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]The complex geometry is the optimized structure in TCM.

Table S18. Calculated atomic charge and charge transfer results from natural population analysis for complexes between differently charged 3-amino-5-bromobenzoic acid and glycine.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
Br Cation-Anion	Vacuum[g]	0.1119	0.1775	0.2852	0.1077	-0.2195
	TCM	0.0351	0.1289	0.1859	0.0570	-0.0920
	DCE	0.0282	0.1188	0.1612	0.0423	-0.0705
	Acetone	0.0239	0.1141	0.1486	0.0345	-0.0584
	DMSO	0.0222	0.1113	0.1412	0.0299	-0.0520
	Water	0.0208	0.1105	0.1386	0.0282	-0.0489
Br Neutral-Anion	Vacuum	0.0438	0.0780	0.1969	0.1190	-0.1628
	TCM	0.0228	0.0667	0.1241	0.0574	-0.0802
	DCE	0.0197	0.0651	0.1075	0.0424	-0.0621

	Acetone	0.0176	0.0642	0.0989	0.0347	-0.0523
	DMSO	0.0151	0.0636	0.0923	0.0286	-0.0437
	Water	0.0167	0.0635	0.0924	0.0289	-0.0455
Br Anion-Anion	Vacuum[h]	0.0143	-0.0044	0.1066	0.1110	-0.1253
	TCM	0.0139	0.0247	0.0786	0.0539	-0.0679
	DCE	0.0121	0.0308	0.0672	0.0364	-0.0484
	Acetone	0.0130	0.0337	0.0647	0.0310	-0.0440
	DMSO	0.0130	0.0354	0.0626	0.0272	-0.0403
	Water	0.0131	0.0359	0.0620	0.0261	-0.0392
Br Cation-Neutral	Vacuum	0.0144	0.1775	0.2160	0.0385	-0.0529
	TCM	0.0112	0.1289	0.1519	0.0230	-0.0342
	DCE	0.0109	0.1188	0.1378	0.0189	-0.0298
	Acetone	0.0107	0.1141	0.1307	0.0166	-0.0273
	DMSO	0.0110	0.1113	0.1252	0.0139	-0.0248
	Water	0.0109	0.1105	0.1239	0.0134	-0.0243
Br Neutral-Neutral	Vacuum[g]	0.0071	0.0780	0.1101	0.0321	-0.0392
	TCM	0.0081	0.0667	0.0895	0.0228	-0.0310
	DCE	0.0083	0.0651	0.0837	0.0187	-0.0270
	Acetone	0.0083	0.0642	0.0802	0.0160	-0.0243
	DMSO	0.0085	0.0636	0.0777	0.0140	-0.0225
	Water	0.0085	0.0635	0.0770	0.0135	-0.0220
Br Anion-Neutral	Vacuum[h]	0.0037	-0.0044	0.0297	0.0341	-0.0378
	TCM[g]	0.0060	0.0247	0.0450	0.0203	-0.0263
	DCE[g]	0.0066	0.0308	0.0475	0.0167	-0.0233
	Acetone	0.0070	0.0337	0.0484	0.0147	-0.0217
	DMSO	0.0072	0.0354	0.0489	0.0135	-0.0207

Br Cation-Cation	Water	0.0073	0.0359	0.0490	0.0132	-0.0204
	Vacuum[h]	0.0056	0.1775	0.1483	-0.0292	0.0236
	TCM	0.0073	0.1289	0.1319	0.0030	-0.0103
	DCE	0.0079	0.1188	0.1266	0.0078	-0.0156
	Acetone	0.0081	0.1141	0.1227	0.0087	-0.0167
	DMSO	0.0082	0.1113	0.1208	0.0094	-0.0177
	Water	0.0083	0.1105	0.1202	0.0097	-0.0180
Br Neutral-Cation	Vacuum[h]	0.0022	0.0780	0.0529	-0.0250	0.0228
	TCM	0.0052	0.0667	0.0710	0.0043	-0.0095
	DCE	0.0056	0.0651	0.0716	0.0065	-0.0121
	Acetone	0.0062	0.0642	0.0733	0.0091	-0.0153
	DMSO	0.0066	0.0636	0.0739	0.0103	-0.0169
	Water	0.0066	0.0635	0.0740	0.0105	-0.0171
Br Anion-Cation	Vacuum[h]	-0.0011	-0.0044	-0.0200	-0.0156	0.0166
	TCM	0.0042	0.0247	0.0304	0.0057	-0.0099
	DCE	0.0048	0.0308	0.0394	0.0086	-0.0135
	Acetone	0.0052	0.0337	0.0433	0.0096	-0.0149
	DMSO	0.0051	0.0354	0.0432	0.0078	-0.0129
	Water	0.0059	0.0359	0.0446	0.0087	-0.0146

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from natural population analysis (NPA). [d]Atomic charge of the halogen atom in complex from NPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]The complex geometry is the optimized structure in TCM.

Table S19. Calculated atomic charge and charge transfer results from natural population analysis for complexes between differently charged 3-amino-5-iodobenzoic acid and glycine.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
I Cation-Anion	Vacuum	0.1723	0.3121	0.4009	0.0887	-0.2611
	TCM	0.0782	0.2580	0.3213	0.0633	-0.1415
	DCE	0.0642	0.2470	0.2990	0.0520	-0.1162
	Acetone	0.0562	0.2418	0.2888	0.0470	-0.1032
	DMSO	0.0530	0.2388	0.2820	0.0433	-0.0962
	Water	0.0520	0.2378	0.2798	0.0420	-0.0939
I Neutral-Anion	Vacuum	0.0861	0.1916	0.3203	0.1287	-0.2147
	TCM	0.0498	0.1842	0.2593	0.0752	-0.1250
	DCE	0.0411	0.1831	0.2436	0.0605	-0.1016
	Acetone	0.0372	0.1829	0.2351	0.0522	-0.0894
	DMSO	0.0383	0.1827	0.2310	0.0484	-0.0866
	Water	0.0355	0.1826	0.2286	0.0460	-0.0815
I Anion-Anion	Vacuum	0.0190	0.0878	0.2269	0.1392	-0.1582
	TCM	0.0313	0.1330	0.2096	0.0766	-0.1078
	DCE	0.0299	0.1422	0.2033	0.0611	-0.0909
	Acetone	0.0299	0.1467	0.1999	0.0533	-0.0832
	DMSO	0.0299	0.1492	0.1980	0.0488	-0.0787
	Water	0.0298	0.1500	0.1973	0.0473	-0.0771
I Cation-Neutral	Vacuum	0.0264	0.3121	0.3555	0.0434	-0.0698
	TCM	0.0209	0.2580	0.2890	0.0310	-0.0519
	DCE	0.0203	0.2470	0.2741	0.0271	-0.0474
	Acetone	0.0201	0.2418	0.2667	0.0249	-0.0450
	DMSO	0.0199	0.2388	0.2624	0.0236	-0.0435

	Water	0.0197	0.2378	0.2610	0.0232	-0.0429
I Neutral-Neutral	Vacuum	0.0126	0.1916	0.2335	0.0419	-0.0545
	TCM	0.0146	0.1842	0.2179	0.0337	-0.0483
	DCE	0.0155	0.1831	0.2111	0.0280	-0.0436
	Acetone	0.0161	0.1829	0.2099	0.0271	-0.0431
	DMSO	0.0159	0.1827	0.2085	0.0259	-0.0417
	Water	0.0163	0.1826	0.2070	0.0244	-0.0406
I Anion-Neutral	Vacuum[g]	0.0055	0.0878	0.1246	0.0368	-0.0422
	TCM	0.0107	0.1330	0.1632	0.0302	-0.0409
	DCE	0.0123	0.1422	0.1712	0.0290	-0.0412
	Acetone	0.0130	0.1467	0.1738	0.0272	-0.0401
	DMSO	0.0134	0.1492	0.1751	0.0259	-0.0393
	Water	0.0139	0.1500	0.1741	0.0241	-0.0379
I Cation-Cation	Vacuum[h]	0.0101	0.3121	0.2817	-0.0304	0.0203
	TCM	0.0133	0.2580	0.2655	0.0075	-0.0208
	DCE	0.0144	0.2470	0.2591	0.0122	-0.0266
	Acetone	0.0148	0.2418	0.2574	0.0156	-0.0305
	DMSO	0.0151	0.2388	0.2556	0.0168	-0.0319
	Water	0.0151	0.2378	0.2550	0.0172	-0.0323
I Neutral-Cation	Vacuum[h]	0.0036	0.1916	0.1682	-0.0234	0.0198
	TCM	0.0093	0.1842	0.1947	0.0105	-0.0198
	DCE	0.0107	0.1831	0.1989	0.0158	-0.0265
	Acetone	0.0113	0.1829	0.2007	0.0179	-0.0292
	DMSO	0.0117	0.1827	0.2016	0.0190	-0.0307
	Water	0.0118	0.1826	0.2019	0.0193	-0.0311

I Anion-Cation	Vacuum[h]	-0.0030	0.0878	0.0773	-0.0104	0.0134
	TCM	0.0071	0.1330	0.1443	0.0113	-0.0184
	DCE	0.0088	0.1422	0.1582	0.0159	-0.0247
	Acetone	0.0096	0.1467	0.1641	0.0175	-0.0270
	DMSO	0.0099	0.1492	0.1673	0.0181	-0.0281
	Water	0.0102	0.1500	0.1685	0.0184	-0.0286

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from natural population analysis (NPA). [d]Atomic charge of the halogen atom in complex from NPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]The complex geometry is the optimized structure in TCM.

Table S20. Calculated atomic charge and electron transfer results from Hirshfeld population analysis for complexes between differently charged 3-amino-5-chlorobenzoic acid and glycine.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
Cl Cation-Anion	Vacuum[g]	0.1507	0.0267	0.0546	0.0279	-0.1786
	TCM[g]	0.0777	-0.0137	-0.0199	-0.0062	-0.0715
	DCE	0.0653	-0.0222	-0.0380	-0.0158	-0.0495
	Acetone	0.0614	-0.0262	-0.0468	-0.0206	-0.0408
	DMSO	0.0593	-0.0285	-0.0521	-0.0236	-0.0357
	Water	0.0586	-0.0293	-0.0538	-0.0245	-0.0340
Cl Neutral-Anion	Vacuum[g]	0.0858	-0.0565	-0.0088	0.0477	-0.1335
	TCM	0.0518	-0.0675	-0.0651	0.0025	-0.0542
	DCE	0.0477	-0.0693	-0.0785	-0.0092	-0.0385
	Acetone	0.0455	-0.0707	-0.0853	-0.0146	-0.0309
	DMSO	0.0453	-0.0713	-0.0889	-0.0176	-0.0277
	Water	0.0435	-0.0714	-0.0906	-0.0191	-0.0244
Cl Anion-Anion	Vacuum[h]	0.0337	-0.1256	-0.0695	0.0560	-0.0898
	TCM	0.0338	-0.1044	-0.0960	0.0084	-0.0422
	DCE	0.0422	-0.1001	-0.1048	-0.0047	-0.0375
	Acetone	0.0417	-0.0980	-0.1093	-0.0113	-0.0304
	DMSO	0.0383	-0.0968	-0.1122	-0.0154	-0.0228
	Water	0.0394	-0.0964	-0.1131	-0.0167	-0.0227
Cl Cation-Neutral	Vacuum	0.0407	0.0267	0.0289	0.0022	-0.0430
	TCM	0.0336	-0.0137	-0.0202	-0.0064	-0.0271
	DCE	0.0317	-0.0222	-0.0313	-0.0091	-0.0226
	Acetone	0.0305	-0.0262	-0.0369	-0.0106	-0.0198
	DMSO	0.0296	-0.0285	-0.0401	-0.0115	-0.0181

Cl Neutral-Neutral	Water	0.0295	-0.0293	-0.0412	-0.0119	-0.0176
	Vacuum[g]	0.0194	-0.0565	-0.0467	0.0098	-0.0292
	TCM	0.0225	-0.0675	-0.0683	-0.0007	-0.0218
	DCE	0.0227	-0.0693	-0.0742	-0.0049	-0.0178
	Acetone	0.0228	-0.0707	-0.0773	-0.0066	-0.0162
	DMSO	0.0228	-0.0713	-0.0791	-0.0078	-0.0149
	Water	0.0227	-0.0714	-0.0797	-0.0083	-0.0144
Cl Anion-Neutral	Vacuum[h]	0.0090	-0.1256	-0.1058	0.0197	-0.0287
	TCM[g]	0.0147	-0.1044	-0.1001	0.0043	-0.0191
	DCE	0.0163	-0.1001	-0.1007	-0.0006	-0.0157
	Acetone	0.0175	-0.0980	-0.1012	-0.0032	-0.0142
	DMSO	0.0183	-0.0968	-0.1016	-0.0048	-0.0135
	Water	0.0193	-0.0964	-0.1020	-0.0056	-0.0137
Cl Cation-Cation	Vacuum[h]	0.0153	0.0267	-0.0088	-0.0355	0.0202
	TCM	0.0189	-0.0137	-0.0269	-0.0131	-0.0057
	DCE	0.0213	-0.0222	-0.0333	-0.0111	-0.0102
	Acetone	0.0219	-0.0262	-0.0366	-0.0103	-0.0115
	DMSO	0.0218	-0.0285	-0.0384	-0.0098	-0.0120
	Water	0.0219	-0.0293	-0.0390	-0.0097	-0.0122
Cl Neutral-Cation	Vacuum[h]	0.0050	-0.0565	-0.0819	-0.0254	0.0204
	TCM	0.0135	-0.0675	-0.0747	-0.0072	-0.0063
	DCE	0.0151	-0.0693	-0.0755	-0.0062	-0.0089
	Acetone	0.0160	-0.0707	-0.0763	-0.0056	-0.0104
	DMSO	0.0164	-0.0713	-0.0768	-0.0055	-0.0109
	Water	0.0165	-0.0714	-0.0770	-0.0056	-0.0110

Cl Anion-Cation	Vacuum[h]	-0.0013	-0.1256	-0.1417	-0.0162	0.0174
	TCM[g]	0.0124	-0.1044	-0.1095	-0.0050	-0.0073
	DCE	0.0139	-0.1001	-0.1040	-0.0039	-0.0100
	Acetone	0.0147	-0.0980	-0.1021	-0.0041	-0.0106
	DMSO	0.0136	-0.0968	-0.1003	-0.0035	-0.0101
	Water	0.0138	-0.0964	-0.1000	-0.0036	-0.0102

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from Hirshfeld population analysis (HPA). [d]Atomic charge of the halogen atom in complex from HPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]The complex geometry is the optimized structure in TCM.

Table S21. Calculated atomic charge and charge transfer results from Hirshfeld population analysis for complexes between differently charged 3-amino-5-bromobenzoic acid and glycine.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
Br Cation-Anion	Vacuum[g]	0.2384	0.0573	0.0459	-0.0115	-0.2269
	TCM	0.1136	0.0118	-0.0083	-0.0201	-0.0935
	DCE	0.1002	0.0023	-0.0267	-0.0290	-0.0713
	Acetone	0.0918	-0.0022	-0.0352	-0.0329	-0.0588
	DMSO	0.0879	-0.0048	-0.0403	-0.0355	-0.0524
	Water	0.0854	-0.0057	-0.0416	-0.0359	-0.0495
Br Neutral-Anion	Vacuum	0.1283	-0.0391	-0.0046	0.0345	-0.1628
	TCM	0.0883	-0.0503	-0.0590	-0.0087	-0.0796
	DCE	0.0802	-0.0521	-0.0706	-0.0185	-0.0617

	Acetone	0.0760	-0.0531	-0.0772	-0.0241	-0.0519
	DMSO	0.0693	-0.0536	-0.0795	-0.0258	-0.0435
	Water	0.0740	-0.0538	-0.0825	-0.0287	-0.0453
Br Anion-Anion	Vacuum[h]	0.0654	-0.1212	-0.0634	0.0579	-0.1233
	TCM	0.0650	-0.0933	-0.0915	0.0018	-0.0667
	DCE	0.0580	-0.0875	-0.0984	-0.0109	-0.0471
	Acetone	0.0610	-0.0848	-0.1027	-0.0179	-0.0431
	DMSO	0.0615	-0.0832	-0.1053	-0.0221	-0.0395
	Water	0.0618	-0.0827	-0.1061	-0.0234	-0.0384
Br Cation-Neutral	Vacuum	0.0591	0.0573	0.0510	-0.0063	-0.0529
	TCM	0.0480	0.0118	-0.0017	-0.0135	-0.0344
	DCE	0.0464	0.0023	-0.0140	-0.0163	-0.0301
	Acetone	0.0456	-0.0022	-0.0201	-0.0179	-0.0277
	DMSO	0.0438	-0.0048	-0.0232	-0.0183	-0.0255
	Water	0.0436	-0.0057	-0.0243	-0.0186	-0.0249
Br Neutral-Neutral	Vacuum[g]	0.0328	-0.0391	-0.0332	0.0060	-0.0388
	TCM	0.0353	-0.0503	-0.0549	-0.0047	-0.0306
	DCE	0.0359	-0.0521	-0.0612	-0.0090	-0.0268
	Acetone	0.0354	-0.0531	-0.0642	-0.0112	-0.0243
	DMSO	0.0347	-0.0536	-0.0658	-0.0121	-0.0226
	Water	0.0347	-0.0538	-0.0664	-0.0126	-0.0221
Br Anion-Neutral	Vacuum[h]	0.0160	-0.1212	-0.1015	0.0197	-0.0357
	TCM[g]	0.0244	-0.0933	-0.0918	0.0015	-0.0258
	DCE[g]	0.0271	-0.0875	-0.0915	-0.0040	-0.0230
	Acetone	0.0285	-0.0848	-0.0919	-0.0071	-0.0214
	DMSO	0.0294	-0.0832	-0.0921	-0.0089	-0.0205

Br Cation-Cation	Water	0.0297	-0.0827	-0.0922	-0.0095	-0.0202
	Vacuum[h]	0.0268	0.0573	0.0113	-0.0460	0.0192
	TCM	0.0321	0.0118	-0.0090	-0.0209	-0.0112
	DCE	0.0348	0.0023	-0.0162	-0.0185	-0.0162
	Acetone	0.0345	-0.0022	-0.0194	-0.0172	-0.0173
	DMSO	0.0349	-0.0048	-0.0216	-0.0167	-0.0182
	Water	0.0351	-0.0057	-0.0223	-0.0167	-0.0185
Br Neutral-Cation	Vacuum[h]	0.0121	-0.0391	-0.0733	-0.0341	0.0220
	TCM	0.0230	-0.0503	-0.0637	-0.0134	-0.0095
	DCE	0.0245	-0.0521	-0.0642	-0.0121	-0.0124
	Acetone	0.0269	-0.0531	-0.0647	-0.0116	-0.0154
	DMSO	0.0287	-0.0536	-0.0653	-0.0117	-0.0170
	Water	0.0289	-0.0538	-0.0655	-0.0117	-0.0172
Br Anion-Cation	Vacuum[h]	0.0007	-0.1212	-0.1421	-0.0209	0.0202
	TCM	0.0186	-0.0933	-0.1023	-0.0090	-0.0095
	DCE	0.0214	-0.0875	-0.0958	-0.0083	-0.0131
	Acetone	0.0229	-0.0848	-0.0932	-0.0084	-0.0145
	DMSO	0.0212	-0.0832	-0.0916	-0.0084	-0.0128
	Water	0.0226	-0.0827	-0.0907	-0.0080	-0.0145

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from Hirshfeld population analysis (HPA). [d]Atomic charge of the halogen atom in complex from HPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]The complex geometry is the optimized structure in TCM.

Table S22. Calculated atomic charge and charge transfer results from Hirshfeld population analysis for complexes between differently charged 3-amino-5-iodobenzoic acid and glycine.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
I Cation-Anion	Vacuum	0.3419	0.1131	0.0580	-0.0552	-0.2867
	TCM	0.1968	0.0627	0.0138	-0.0489	-0.1479
	DCE	0.1729	0.0523	-0.0003	-0.0526	-0.1203
	Acetone	0.1586	0.0474	-0.0070	-0.0543	-0.1042
	DMSO	0.1530	0.0445	-0.0116	-0.0561	-0.0969
	Water	0.1511	0.0436	-0.0131	-0.0567	-0.0944
I Neutral-Anion	Vacuum	0.2083	-0.0024	0.0092	0.0115	-0.2199
	TCM	0.1465	-0.0102	-0.0338	-0.0236	-0.1229
	DCE	0.1300	-0.0115	-0.0427	-0.0312	-0.0988
	Acetone	0.1228	-0.0118	-0.0485	-0.0366	-0.0862
	DMSO	0.1242	-0.0121	-0.0528	-0.0407	-0.0836
	Water	0.1194	-0.0122	-0.0533	-0.0411	-0.0782
I Anion-Anion	Vacuum	0.0926	-0.1033	-0.0435	0.0597	-0.1523
	TCM	0.1100	-0.0620	-0.0685	-0.0065	-0.1034
	DCE	0.1067	-0.0535	-0.0734	-0.0199	-0.0868
	Acetone	0.1069	-0.0495	-0.0772	-0.0277	-0.0792
	DMSO	0.1070	-0.0472	-0.0795	-0.0322	-0.0748
	Water	0.1070	-0.0465	-0.0802	-0.0338	-0.0733
I Cation-Neutral	Vacuum	0.0888	0.1131	0.0943	-0.0188	-0.0699
	TCM	0.0741	0.0627	0.0395	-0.0232	-0.0509
	DCE	0.0720	0.0523	0.0266	-0.0257	-0.0463
	Acetone	0.0711	0.0474	0.0201	-0.0272	-0.0438
	DMSO	0.0705	0.0445	0.0164	-0.0282	-0.0423

	Water	0.0701	0.0436	0.0152	-0.0285	-0.0417
I Neutral-Neutral	Vacuum	0.0501	-0.0024	-0.0009	0.0014	-0.0515
	TCM	0.0563	-0.0102	-0.0212	-0.0110	-0.0454
	DCE	0.0563	-0.0115	-0.0269	-0.0154	-0.0409
	Acetone	0.0585	-0.0118	-0.0299	-0.0181	-0.0404
	DMSO	0.0588	-0.0121	-0.0319	-0.0198	-0.0391
	Water	0.0582	-0.0122	-0.0323	-0.0201	-0.0381
I Anion-Neutral	Vacuum[g]	0.0223	-0.1033	-0.0862	0.0170	-0.0393
	TCM	0.0410	-0.0620	-0.0644	-0.0025	-0.0385
	DCE	0.0475	-0.0535	-0.0623	-0.0088	-0.0387
	Acetone	0.0502	-0.0495	-0.0621	-0.0126	-0.0377
	DMSO	0.0515	-0.0472	-0.0619	-0.0147	-0.0369
	Water	0.0508	-0.0465	-0.0614	-0.0150	-0.0358
I Cation-Cation	Vacuum[h]	0.0434	0.1131	0.0539	-0.0592	0.0158
	TCM	0.0516	0.0627	0.0318	-0.0309	-0.0207
	DCE	0.0532	0.0523	0.0251	-0.0272	-0.0260
	Acetone	0.0557	0.0474	0.0213	-0.0261	-0.0296
	DMSO	0.0563	0.0445	0.0191	-0.0254	-0.0309
	Water	0.0564	0.0436	0.0184	-0.0252	-0.0313
I Neutral-Cation	Vacuum[h]	0.0221	-0.0024	-0.0449	-0.0425	0.0204
	TCM	0.0385	-0.0102	-0.0308	-0.0206	-0.0179
	DCE	0.0428	-0.0115	-0.0300	-0.0185	-0.0243
	Acetone	0.0449	-0.0118	-0.0299	-0.0180	-0.0269
	DMSO	0.0460	-0.0121	-0.0299	-0.0177	-0.0283
	Water	0.0464	-0.0122	-0.0299	-0.0177	-0.0287

I Anion-Cation	Vacuum[h]	0.0025	-0.1033	-0.1256	-0.0224	0.0199
	TCM	0.0297	-0.0620	-0.0751	-0.0132	-0.0165
	DCE	0.0353	-0.0535	-0.0660	-0.0125	-0.0228
	Acetone	0.0378	-0.0495	-0.0622	-0.0126	-0.0252
	DMSO	0.0390	-0.0472	-0.0600	-0.0128	-0.0262
	Water	0.0398	-0.0465	-0.0594	-0.0130	-0.0268

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from Hirshfeld population analysis (HPA). [d]Atomic charge of the halogen atom in complex from HPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]The complex geometry is the optimized structure in TCM.

Table S23. Calculated binding energies and geometrical parameters for complexes between the neutral 3-amino-5-halobenzoic acid donors, and six-membered oxocarbenium, dimethyloxidanium, methylguanidinium cation acceptors in dichloroethane.

Complex	E_{bind}[a]	d[b]	θ[c]
Cl Neutral-Cation oxocarbenium^{+} [d]	-0.84	3.13	173.1
Br Neutral-Cation oxocarbenium^{+}	-0.96	3.24	174.2
I Neutral-Cation oxocarbenium^{+}	-0.98	3.33	175.6
Cl Neutral-Cation dimethyloxidanium^{+} [e]	-1.03	3.12	177.3
Br Neutral-Cation dimethyloxidanium^{+}	-1.27	3.20	166.3
I Neutral-Cation dimethyloxidanium^{+}	-1.28	3.39	156.0
Cl Neutral-Cation Me-gua^{+} [f]	-1.70	3.16	171.1
Br Neutral-Cation Me-gua^{+}	-1.78	3.26	172.5
I Neutral-Cation Me-gua^{+}	-1.91	3.38	169.7

[a]Calculated binding energies, values are in kcal/mol. [b]The interaction distance, values are in angstrom. [c]The interaction angle, values are in degree. [d]Complex formed between neutral 3-amino-5-halobenzoic acid and six-membered oxocarbenium cation. [e]Complex formed between neutral 3-amino-5-halobenzoic acid and dimethyloxidanium cation. [e]Complex formed between neutral 3-amino-5-halobenzoic acid and methylguanidinium (Me-gua^{+}) cation. Calculation results reveal that all the three cations could form stable halogen bonds with favorable binding energies in solvents.

Table S24. Calculated atomic charge and charge transfer results from natural population analysis for complexes of the cationic 3-amino-5-halobenzoic acid donors, and neutral and cationic methylguanidine acceptors.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
Cl Cation-Neutral Me-gua [h]	TCM[g]	0.0075	0.0558	0.0599	0.0041	-0.0116
	DCE	0.0069	0.0469	0.0489	0.0020	-0.0089
	Acetone	0.0062	0.0427	0.0440	0.0013	-0.0075
	DMSO	0.0061	0.0403	0.0415	0.0012	-0.0073
	Water	0.0061	0.0395	0.0405	0.0010	-0.0071
Br Cation-Neutral Me-gua	TCM	0.0135	0.1289	0.1332	0.0043	-0.0178
	DCE	0.0131	0.1188	0.1228	0.0039	-0.0171
	Acetone	0.0121	0.1141	0.1179	0.0038	-0.0158
	DMSO	0.0118	0.1113	0.1151	0.0037	-0.0156
	Water	0.0117	0.1105	0.1141	0.0036	-0.0153
I Cation-Neutral Me-gua	TCM	0.0283	0.2580	0.2674	0.0094	-0.0378
	DCE	0.0265	0.2470	0.2569	0.0099	-0.0364
	Acetone	0.0268	0.2418	0.2496	0.0079	-0.0347
	DMSO	0.0256	0.2388	0.2462	0.0074	-0.0331
	Water	0.0253	0.2378	0.2453	0.0075	-0.0329
Cl Cation-Cation Me-gua^{+} [i]	TCM	0.0015	0.0558	0.0298	-0.0260	0.0245
	DCE	0.0014	0.0469	0.0266	-0.0203	0.0190
	Acetone	0.0015	0.0427	0.0267	-0.0160	0.0145
	DMSO	0.0016	0.0403	0.0281	-0.0121	0.0106
	Water	0.0016	0.0395	0.0282	-0.0113	0.0098
Br Cation-Cation	TCM	0.0034	0.1289	0.0988	-0.0301	0.0267

Me-gua$^+$	DCE	0.0040	0.1188	0.0984	-0.0204	0.0164
	Acetone	0.0033	0.1141	0.0975	-0.0166	0.0133
	DMSO	0.0033	0.1113	0.0981	-0.0132	0.0099
	Water	0.0033	0.1105	0.0982	-0.0123	0.0090
I Cation-Cation Me-gua$^+$	TCM	0.0066	0.2580	0.2264	-0.0316	0.0250
	DCE	0.0071	0.2470	0.2265	-0.0205	0.0134
	Acetone	0.0072	0.2418	0.2265	-0.0152	0.0080
	DMSO	0.0073	0.2388	0.2265	-0.0122	0.0050
	Water	0.0073	0.2378	0.2265	-0.0113	0.0040

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from natural population analysis (NPA). [d]Atomic charge of the halogen atom in complex from NPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]Complex formed between cationic 3-amino-5-halobenzoic acid and neutral methylguanidine (Me-gua) acceptor. [i]Complex formed between cationic 3-amino-5-halobenzoic acid and cationic methylguanidinium (Me-gua$^+$) acceptor. Once we switch the cationic glycine XB acceptor to the cationic methylguanidinium ion, negative $\Delta q(X)$ and positive $\Delta Q_{CT}X$ values are presented in all cation-cation organohalogen complexes for all various solvents, suggesting the wide existence of intramolecular electron flows from the rest of the donor to the halogen atom in these systems, which simply results from the more positive surface electrostatic potential of methylguanidinium cation. These results further demonstrate the charge state based intramolecular electron redistribution tendencies to be valid.

Table S25. Calculated atomic charge and charge transfer results in Hirshfeld population analysis for complexes of the cationic 3-amino-5-halobenzoic acid donors, and neutral and cationic methylguanidine acceptors.[a]

Complex	Environment	Q_{CT}[b]	$q(X)_{monomer}$[c]	$q(X)_{complex}$[d]	$\Delta q(X)$[e]	$\Delta Q_{CT}X$[f]
Cl Cation-Neutral Me-gua [h]	TCM[g]	0.0111	-0.0137	-0.0089	0.0048	-0.0159
	DCE	0.0076	-0.0222	-0.0156	0.0065	-0.0141
	Acetone	0.0030	-0.0262	-0.0171	0.0092	-0.0122
	DMSO	0.0031	-0.0285	-0.0206	0.0080	-0.0111
	Water	0.0029	-0.0293	-0.0213	0.0080	-0.0109
Br Cation-Neutral Me-gua	TCM	0.0251	0.0118	0.0087	-0.0032	-0.0219
	DCE	0.0212	0.0023	0.0018	-0.0006	-0.0206
	Acetone	0.0184	-0.0022	-0.0014	0.0008	-0.0192
	DMSO	0.0188	-0.0048	-0.0050	-0.0001	-0.0187
	Water	0.0176	-0.0057	-0.0051	0.0006	-0.0182
I Cation-Neutral Me-gua	TCM	0.0554	0.0627	0.0486	-0.0141	-0.0413
	DCE	0.0507	0.0523	0.0408	-0.0115	-0.0392
	Acetone	0.0470	0.0474	0.0375	-0.0099	-0.0371
	DMSO	0.0426	0.0445	0.0374	-0.0071	-0.0355
	Water	0.0420	0.0436	0.0368	-0.0068	-0.0352
Cl Cation-Cation Me-gua^{+} [i]	TCM	-0.0177	-0.0137	-0.0176	-0.0038	0.0215
	DCE	-0.0189	-0.0222	-0.0187	0.0035	0.0154
	Acetone	-0.0192	-0.0262	-0.0182	0.0081	0.0112
	DMSO	-0.0217	-0.0285	-0.0145	0.0140	0.0077
	Water	-0.0222	-0.0293	-0.0140	0.0152	0.0069
Br Cation-Cation	TCM	-0.0111	0.0118	0.0000	-0.0118	0.0230

Me-gua$^+$	DCE	-0.0113	0.0023	0.0005	-0.0018	0.0131
	Acetone	-0.0146	-0.0022	0.0025	0.0048	0.0098
	DMSO	-0.0166	-0.0048	0.0050	0.0098	0.0068
	Water	-0.0169	-0.0057	0.0054	0.0110	0.0059
I Cation-Cation Me-gua$^+$	TCM	-0.0052	0.0627	0.0467	-0.0160	0.0212
	DCE	-0.0043	0.0523	0.0462	-0.0061	0.0104
	Acetone	-0.0038	0.0474	0.0459	-0.0014	0.0053
	DMSO	-0.0036	0.0445	0.0458	0.0012	0.0024
	Water	-0.0036	0.0436	0.0457	0.0021	0.0015

[a]All values are in atomic units. [b]Amount of electron transferred from the XB acceptor to donor. [c]Atomic charge of the halogen atom in monomer from Hirshfeld population analysis (HPA). [d]Atomic charge of the halogen atom in complex from HPA. [e]Difference of *d* and *c*. [f]$\Delta Q_{CT}X = -Q_{CT} - \Delta q(X)$, negative $\Delta Q_{CT}X$ value means electron transfer from the halogen atom to the rest of the XB donor molecule, and vice versa. [g]The complex geometry is obtained by constrained optimization. [h]Complex formed between cationic 3-amino-5-halobenzoic acid and neutral methylguanidine (Me-gua) acceptor. [i]Complex formed between cationic 3-amino-5-halobenzoic acid and cationic methylguanidinium (Me-gua$^+$) acceptor.

Table S26. Products and characteristics of the electron transfer reaction according to the Marcus theory with differently charged glycine and neutral and cationic methylguanidine as electron donors, and differently charged 3-amino-5-bromobenzoic acid as electron acceptors.[a]

Complex	Reactants[b]	Products[c]	Environment	ΔG^{o} [d]	λ [e]	w_p [f]	ΔG^{*} [g]
Br Cation-Anion	$R\text{-}Br^+$ Gly^-	R-Br· CH_2NH_2· CO_2	TCM	34.61	202.45	-8.74	64.38
			DCE	47.55	207.14	-4.07	75.81
			Acetone	53.23	211.78	-2.01	81.66
			DMSO	56.35	209.60	-0.88	83.81
			Water	57.33	214.31	-0.53	85.74
Br Neutral-Anion	R-Br Gly^-	$[R\text{-}Br\cdot]^-$ CH_2NH_2· CO_2	TCM	60.20	192.20	0.00	82.86
			DCE	63.53	192.14	0.00	85.05
			Acetone	65.02	192.09	0.00	86.03
			DMSO	65.83	192.17	0.00	86.60
			Water	66.09	192.07	0.00	86.75
Br Anion-Anion	$R\text{-}Br^-$ Gly^-	$[R\cdot]^-$ Br^- CH_2NH_2· CO_2	TCM	52.85	182.96	-2.83	74.17
			DCE	53.37	178.17	-1.32	74.37
			Acetone	53.64	173.46	-0.65	73.91
			DMSO	53.80	175.80	-0.28	74.78
			Water	53.86	170.95	-0.17	73.80
Br Cation-Neutral	$R\text{-}Br^+$ Gly	R-Br· $[Gly\cdot]^+$	TCM	77.50	118.38	0.00	81.03
			DCE	72.27	118.34	0.00	76.76
			Acetone	69.88	118.29	0.00	74.83
			DMSO	68.54	118.31	0.00	73.77
			Water	68.12	118.26	0.00	73.43
Br Neutral-Neutral	R-Br	$[R\text{-}Br\cdot]^-$	TCM	103.09	118.92	8.77	111.96

	Gly	$[Gly\cdot]^+$	DCE	88.26	118.92	4.08	93.83
			Acetone	81.66	118.92	2.02	86.29
			DMSO	78.02	118.92	0.88	82.27
			Water	76.88	118.92	0.53	81.03
Br Anion-Neutral	$R\text{-}Br^-$ Gly	$[R\cdot]^-$ Br^- $[Gly\cdot]^+$	TCM[h]	95.74	120.66	10.64	106.80
			DCE[h]	78.09	120.70	4.95	85.98
			Acetone	70.29	120.74	2.45	77.50
			DMSO	65.99	120.72	1.07	73.02
			Water	64.64	120.76	0.64	71.65
Br Cation-Cation	$R\text{-}Br^+$ Gly^+	$R\text{-}Br\cdot$ $[Gly\cdot]^{2+}$	TCM	131.01	100.54	8.79	143.63
			DCE	113.18	95.69	4.09	118.48
			Acetone	105.26	90.92	2.02	108.02
			DMSO	100.89	93.29	0.88	101.97
			Water	99.52	88.38	0.53	100.43
Br Neutral-Cation	R-Br Gly^+	$[R\text{-}Br\cdot]^-$ $[Gly\cdot]^{2+}$	TCM	156.60	112.30	17.56	182.67
			DCE	129.16	112.34	8.17	138.72
			Acetone	117.04	112.38	4.04	121.24
			DMSO	110.37	112.37	1.77	112.14
			Water	108.28	112.40	1.06	109.36
Br Anion-Cation	$R\text{-}Br^-$ Gly^+	$[R\cdot]^-$ Br^- $[Gly\cdot]^{2+}$	TCM	149.25	125.27	24.13	178.00
			DCE	118.99	130.16	0.88	120.08
			Acetone	105.66	134.98	0.44	107.64
			DMSO	98.34	132.59	0.19	100.72
			Water	96.05	137.57	0.11	99.28
Br Cation-Neutral	$R\text{-}Br^+$	$R\text{-}Br\cdot$	TCM	61.78	101.95	0.00	65.73

Me-gua[i]	Me-gua	[Me-gua·]$^+$	DCE	59.14	101.89	0.00	63.62
			Acetone	57.93	101.85	0.00	62.67
			DMSO	57.25	101.89	0.00	62.14
			Water	57.04	101.83	0.00	61.96
Br Cation-Cation Me-gua$^+$[j]	R-Br$^+$ Me-gua$^+$	R-Br· [Me-gua·]$^{2+}$	TCM	105.10	85.59	8.67	116.09
			DCE	86.20	80.84	4.04	90.50
			Acetone	77.80	76.16	1.99	79.84
			DMSO	73.17	78.49	0.87	74.10
			Water	71.71	73.67	0.52	72.24

[a]All values are in kcal/mol. [b]Reactants of the electron transfer reaction, R and Gly refer to the 3-amino-benzoic acid and glycine groups respectively with different charge states. [c]Products of the electron transfer reaction, all free radical and ionic products are labeled properly. [d]The free energy that drives the electron transfer reaction in solvents. [e]The total reorganization energy that has considered the contribution of the carbon-halogen bond dissociation energies[21, 24], which are 81.73, 82.14, 83.81 kcal/mol for cationic, neutral and anionic 3-amino-5-bromobenzoic acid respectively. Intramolecular reorganization energies of electron donors are 30.10, 36.78, 110.30, 20.37, 14.94 kcal/mol for cationic, neutral, anionic glycine and neutral, cationic methylguanidine respectively. [f]The work term of bring the ionic reactants and products together, evaluated via the Coulomb formula. [g]The outer-sphere electron transfer activation barrier from the Marcus theory. [h]The complex geometry is obtained by constrained optimization. [i]Complex formed between cationic 3-amino-5-bromobenzoic acid and neutral methylguanidine (Me-gua) acceptor. [j]Complex formed between cationic 3-amino-5-bromobenzoic acid and cationic methylguanidinium (Me-gua$^+$) acceptor.

Table S27. Calculated binding energies in solvents for halogen-bonded complexes between differently charged 3-amino-5-halobenzoic acid and glycine with the IEFPCM model using UA0 radii.[a]

Environment	Cation-Anion			Cation-Neutral			Cation-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	-10.57	-12.73	-17.29	-1.83	-2.76	-4.32	4.64	4.01	3.03
DCE	-4.91	-6.67	-10.39	-1.16	-2.04	-3.45	1.75	1.11	0.22
Acetone	-2.73	-4.31	-7.56	-0.90	-1.73	-3.07	0.54	-0.07	-1.02
DMSO	-1.60	-3.09	-6.07	-0.76	-1.56	-2.87	-0.11	-0.71	-1.65
Water	-1.25	-2.69	-5.61	-0.72	-1.51	-2.80	-0.31	-0.91	-1.85
Environment	Neutral-Anion			Neutral-Neutral			Neutral-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	0.32	-1.39	-4.75	-0.24	-0.88	-2.10	-0.84	-1.31	-1.96
DCE	0.26	-1.08	-3.74	-0.29	-0.89	-1.99	-0.63	-1.05	-1.77
Acetone	0.07	-1.12	-3.45	-0.33	-0.92	-1.97	-0.54	-0.97	-1.68
DMSO	-0.07	-1.18	-3.34	-0.36	-0.95	-1.96	-0.49	-0.91	-1.62
Water	-0.14	-1.19	-3.31	-0.37	-0.96	-1.96	-0.48	-0.89	-1.60
Environment	Anion-Anion			Anion-Neutral			Anion-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	8.08	7.00	4.34	0.97	0.36	-0.73	-6.01	-6.37	-6.75
DCE	4.04	2.93	0.76	0.40	-0.18	-1.06	-2.88	-3.24	-3.75
Acetone	2.03	1.04	-0.90	0.08	-0.46	-1.33	-1.56	-1.92	-2.50
DMSO	0.86	0.00	-1.81	-0.12	-0.62	-1.46	-0.87	-1.26	-1.82
Water	0.52	-0.33	-2.10	-0.18	-0.67	-1.50	-0.66	-1.03	-1.61

[a]All values are in kcal/mol. The binding energies are obtained based on single-point energy calculations utilizing the structures optimized with the IEFPCM model using the default UFF radii.

Table S28. Calculated binding energies in solvents for halogen-bonded complexes between differently charged 3-amino-5-halobenzoic acid and glycine with the IEFPCM model using UAHF radii.[a]

Environment	Cation-Anion			Cation-Neutral			Cation-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	-9.13	-10.70	-13.75	-1.55	-2.46	-4.07	4.55	3.87	2.70
DCE	-3.54	-4.65	-6.87	-0.81	-1.62	-3.05	1.84	1.19	0.10
Acetone	-1.50	-2.42	-4.28	-0.51	-1.26	-2.59	0.72	0.12	-1.01
DMSO	-0.46	-1.26	-2.87	-0.37	-1.08	-2.34	0.14	-0.46	-1.56
Water	-0.15	-0.93	-2.45	-0.32	-1.03	-2.27	-0.05	-0.64	-1.73
Environment	Neutral-Anion			Neutral-Neutral			Neutral-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	1.25	0.05	-2.48	-0.02	-0.62	-1.89	-0.73	-1.25	-2.04
DCE	0.92	0.26	-1.47	-0.04	-0.59	-1.70	-0.47	-0.93	-1.78
Acetone	0.59	0.15	-1.23	-0.09	-0.61	-1.64	-0.36	-0.81	-1.64
DMSO	0.46	-0.09	-1.15	-0.12	-0.66	-1.62	-0.30	-0.72	-1.56
Water	0.24	-0.01	-1.13	-0.13	-0.66	-1.59	-0.28	-0.69	-1.53
Environment	Anion-Anion			Anion-Neutral			Anion-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	8.27	7.67	5.72	1.16	0.54	-0.61	-5.74	-6.15	-6.64
DCE	4.33	3.57	2.31	0.58	0.02	-0.87	-2.67	-3.06	-3.70
Acetone	2.29	1.75	0.74	0.26	-0.26	-1.12	-1.37	-1.76	-2.46
DMSO	0.97	0.71	-0.12	0.06	-0.42	-1.24	-0.70	-1.13	-1.78
Water	0.67	0.39	-0.40	-0.03	-0.47	-1.26	-0.50	-0.91	-1.58

[a]All values are in kcal/mol. The binding energies are obtained based on single-point energy calculations utilizing the structures optimized with the IEFPCM model using the default UFF radii.

Table S29. Calculated binding energies in solvents for halogen-bonded complexes between differently charged 3-amino-5-halobenzoic acid and glycine with the IEFPCM model using UAKS radii.[a]

Environment	Cation-Anion			Cation-Neutral			Cation-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	-9.14	-10.71	-13.76	-1.47	-2.35	-3.92	4.61	3.95	2.79
DCE	-3.54	-4.66	-6.89	-0.70	-1.48	-2.87	1.90	1.28	0.22
Acetone	-1.51	-2.43	-4.29	-0.40	-1.11	-2.40	0.80	0.22	-0.87
DMSO	-0.46	-1.26	-2.88	-0.26	-0.95	-2.14	0.21	-0.35	-1.41
Water	-0.15	-0.93	-2.45	-0.21	-0.89	-2.06	0.02	-0.53	-1.57
Environment	Neutral-Anion			Neutral-Neutral			Neutral-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	1.26	0.08	-2.45	0.05	-0.51	-1.75	-0.70	-1.20	-1.96
DCE	0.94	0.28	-1.44	0.03	-0.45	-1.54	-0.43	-0.86	-1.67
Acetone	0.61	0.17	-1.20	-0.01	-0.48	-1.45	-0.31	-0.72	-1.51
DMSO	0.47	-0.08	-1.12	-0.04	-0.55	-1.41	-0.25	-0.62	-1.40
Water	0.25	0.01	-1.10	-0.05	-0.55	-1.39	-0.23	-0.59	-1.37
Environment	Anion-Anion			Anion-Neutral			Anion-Cation		
	Cl	Br	I	Cl	Br	I	Cl	Br	I
TCM	8.29	7.70	5.76	1.20	0.61	-0.51	-5.74	-6.13	-6.60
DCE	4.35	3.59	2.35	0.62	0.10	-0.70	-2.63	-3.01	-3.61
Acetone	2.31	1.77	0.77	0.31	-0.17	-0.94	-1.33	-1.69	-2.34
DMSO	0.99	0.73	-0.09	0.11	-0.33	-1.05	-0.67	-1.07	-1.65
Water	0.68	0.40	-0.37	0.04	-0.38	-1.07	-0.46	-0.83	-1.44

[a]All values are in kcal/mol. The binding energies are obtained based on single-point energy calculations utilizing the structures optimized with the IEFPCM model using the default UFF radii.

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5. Cartesian Coordinates of All Optimized Geometries.

Detailed Cartesian coordinates of all optimized geometries in this research are listed below. Constraint optimization and single-point energy calculation cases are labeled with "ModRedundant" and "SP" in the title of the Cartesian coordinates, respectively. Information for the fixed plane angles and dihedral angles in constraint optimizations are provided in the corresponding annotations as their original formats in the input gjf files. For instance, "A 7 10 15 120.0 F" refers to fix the angle among atoms with serial number of 7, 10 and 12 to 120.0°, while A stands for "angle". Similarly, "D 15 10 7 4 0.0 F" refers to fix the dihedral angle among atoms with serial number of 15, 10, 7 and 4 to 0.0°, while D stands for "dihedral".

HOOC-phCl-NH_3^+ Vacuum

C	2.23311200	4.50590500	-0.53109700
C	3.60184500	4.24902400	-0.52797800
C	4.50138200	5.30451400	-0.59599700
C	4.05686500	6.62409200	-0.66862400
C	2.69259800	6.83164200	-0.66988300
C	1.75792700	5.81115200	-0.60349200
H	3.97771700	3.23362300	-0.47149100
H	4.77477900	7.43522300	-0.72150900
H	0.69016900	6.00137400	-0.60564900
Cl	1.10974100	3.20654000	-0.44224300
N	2.18712300	8.22889900	-0.75885300
H	2.95796700	8.89912800	-0.67206400
H	1.72324900	8.40597000	-1.65734000
C	5.96734500	4.97610500	-0.58825700
O	6.38891000	3.86131800	-0.53342000
O	6.72313800	6.07949900	-0.65003800
H	7.65511300	5.81545500	-0.64147200
H	1.51516200	8.43406600	-0.01101900

HOOC-phCl-NH_3^+ TCM

C	2.24212500	4.51283000	-0.44670300
C	3.60285500	4.24769700	-0.48278000
C	4.49937600	5.30482900	-0.60719200
C	4.05133000	6.61891200	-0.69677300
C	2.68605200	6.83692200	-0.65850700
C	1.76160600	5.81531600	-0.53384900
H	3.97558400	3.23304900	-0.41695700
H	4.75655500	7.43536100	-0.79409600
H	0.69573300	6.00695000	-0.50535600
Cl	1.11241400	3.21042500	-0.29575400
N	2.19587000	8.22706100	-0.76023300
H	2.55227800	8.80889200	0.00572000
H	2.48461000	8.66453800	-1.64226200

C	5.96035500	4.97880100	-0.64597200
O	6.39381800	3.86275300	-0.56876400
O	6.72037100	6.06915700	-0.77723900
H	7.65003700	5.79816800	-0.79983900
H	1.17317600	8.27186500	-0.72387100

HOOC-phCl-NH_3^+ DCE

C	2.24325800	4.51386000	-0.44665400
C	3.60296400	4.24694300	-0.48275200
C	4.49942500	5.30444300	-0.60683300
C	4.05095400	6.61826500	-0.69600600
C	2.68564700	6.83821000	-0.65829400
C	1.76198700	5.81571500	-0.53369600
H	3.97428900	3.23197100	-0.41738100
H	4.75484800	7.43559200	-0.79264000
H	0.69640100	6.00821000	-0.50533100
Cl	1.11255700	3.20923100	-0.29531800
N	2.19633900	8.22617800	-0.76035800
H	2.55147900	8.80886000	0.00542300
H	2.48542600	8.66396700	-1.64199600
C	5.95957800	4.97977200	-0.64617500
O	6.39534000	3.86287300	-0.56945100
O	6.71994900	6.06865400	-0.77730900
H	7.64985700	5.79847200	-0.80052700
H	1.17384300	8.27231000	-0.72512800

HOOC-phCl-NH_3^+ Acetone

C	2.24391100	4.51443700	-0.44564900
C	3.60300700	4.24657800	-0.48216400
C	4.49947600	5.30426000	-0.60713800
C	4.05081700	6.61783400	-0.69661200
C	2.68541900	6.83884900	-0.65873100
C	1.76226000	5.81604100	-0.53324700
H	3.97379400	3.23152900	-0.41657900
H	4.75395400	7.43562600	-0.79343300
H	0.69679400	6.00888900	-0.50454700
Cl	1.11255400	3.20901300	-0.29273000
N	2.19654600	8.22581600	-0.76042000
H	2.54455900	8.80645300	0.01014000
H	2.49245300	8.66686200	-1.63810000
C	5.95922000	4.98022900	-0.64719900
O	6.39589700	3.86270400	-0.57164600
O	6.71978800	6.06831900	-0.77742100
H	7.64981900	5.79856200	-0.80123400
H	1.17387200	8.27152500	-0.73371800

HOOC-phCl-NH_3^+ DMSO

C	2.24427100	4.51492600	-0.44400800
C	3.60309200	4.24650300	-0.48109700
C	4.49951400	5.30411000	-0.60742600
C	4.05071700	6.61758800	-0.69763200
C	2.68537600	6.83914000	-0.65945900
C	1.76240300	5.81626600	-0.53252600
H	3.97344700	3.23137800	-0.41500000

H	4.75342100	7.43556400	-0.79506200
H	0.69706900	6.00953200	-0.50323700
Cl	1.11276300	3.20901700	-0.28890000
N	2.19671100	8.22555900	-0.76039600
H	2.53113200	8.80163800	0.01955800
H	2.50602700	8.67297500	-1.63015800
C	5.95898100	4.98033900	-0.64839800
O	6.39625900	3.86256500	-0.57265200
O	6.71955300	6.06792100	-0.77970600
H	7.64966000	5.79846300	-0.80426500
H	1.17374700	8.27004600	-0.75006400

HOOC-phCl-NH_3^+ Water

C	2.24440500	4.51511300	-0.44306500
C	3.60312500	4.24649400	-0.48049400
C	4.49951800	5.30405200	-0.60764000
C	4.05065700	6.61746900	-0.69828400
C	2.68534000	6.83920900	-0.65986400
C	1.76244900	5.81635400	-0.53209800
H	3.97336200	3.23136200	-0.41408500
H	4.75317000	7.43551300	-0.79617600
H	0.69716500	6.00976800	-0.50246200
Cl	1.11285300	3.20909300	-0.28681000
N	2.19678500	8.22548200	-0.76037300
H	2.52359100	8.79885400	0.02480300
H	2.51368700	8.67643400	-1.62554800
C	5.95889100	4.98036400	-0.64906400
O	6.39636900	3.86251900	-0.57312000
O	6.71944300	6.06775400	-0.78101700
H	7.64957300	5.79839100	-0.80589400
H	1.17375900	8.26930000	-0.75923400

HOOC-phBr-NH_3^+ Vacuum

C	2.23873000	4.51004900	-0.40894600
C	3.60425800	4.25292900	-0.46171800
C	4.50059500	5.30556300	-0.61902800
C	4.05503900	6.62006000	-0.72594500
C	2.69029000	6.82930000	-0.66938500
C	1.76214500	5.81510300	-0.51380800
H	3.98870700	3.24244100	-0.38517900
H	4.76804400	7.42768600	-0.84812500
H	0.69596500	6.00976600	-0.47350200
N	2.19016300	8.22932800	-0.75414800
H	2.24465500	8.70724800	0.15314700
H	2.73444300	8.77560100	-1.43039600
C	5.96484700	4.97334400	-0.67522400
O	6.38719800	3.85985400	-0.60059200
O	6.71784500	6.07115100	-0.81741700
H	7.64826000	5.80383400	-0.85038400
H	1.21175700	8.25290900	-1.05966300
Br	1.01236200	3.10536700	-0.19638500

HOOC-phBr-NH_3^+ TCM

C	2.24090400	4.51161100	-0.44738100

C	3.60199300	4.24717800	-0.48507300
C	4.49923100	5.30451600	-0.61051700
C	4.05123200	6.61841300	-0.69911000
C	2.68588700	6.83651100	-0.66140800
C	1.76102900	5.81476600	-0.53674500
H	3.97934600	3.23455500	-0.41815600
H	4.75646400	7.43508400	-0.79493800
H	0.69594100	6.01173100	-0.50928100
N	2.19641900	8.22728300	-0.76007500
H	2.55047800	8.80605200	0.00932300
H	2.48795000	8.66812700	-1.63948700
C	5.96032400	4.97861100	-0.64841700
O	6.39370700	3.86216300	-0.57650900
O	6.72053200	6.06975400	-0.77162100
H	7.65032400	5.79916100	-0.79334800
H	1.17361700	8.27201500	-0.72661600
Br	1.00992300	3.09400400	-0.26733600

HOOC-phBr-NH_3^+ DCE

C	2.24210600	4.51263200	-0.44719700
C	3.60214600	4.24622200	-0.48503400
C	4.49926700	5.30397900	-0.61028600
C	4.05089800	6.61763700	-0.69853400
C	2.68557300	6.83779700	-0.66115200
C	1.76152600	5.81519600	-0.53629900
H	3.97814900	3.23328200	-0.41853600
H	4.75483400	7.43513700	-0.79389300
H	0.69681500	6.01311000	-0.50854800
N	2.19686800	8.22631600	-0.76035400
H	2.54919000	8.80596600	0.00905800
H	2.48906300	8.66751200	-1.63924700
C	5.95958800	4.97955200	-0.64885400
O	6.39530900	3.86220300	-0.57842200
O	6.71999300	6.06941200	-0.77082500
H	7.65010000	5.79986700	-0.79325000
H	1.17424500	8.27222600	-0.72849300
Br	1.00963300	3.09348700	-0.26683200

HOOC-phBr-NH_3^+ Acetone

C	2.24280800	4.51328800	-0.44566200
C	3.60226500	4.24585600	-0.48406300
C	4.49932700	5.30374200	-0.61058700
C	4.05079000	6.61718700	-0.69956800
C	2.68545000	6.83838200	-0.66189700
C	1.76188700	5.81557200	-0.53551600
H	3.97768200	3.23282200	-0.41712900
H	4.75405400	7.43503500	-0.79536000
H	0.69737900	6.01395700	-0.50690100
N	2.19702800	8.22585100	-0.76037800
H	2.53590600	8.80128200	0.01817600
H	2.50217600	8.67331200	-1.63162000
C	5.95923100	4.97990900	-0.65004800
O	6.39597900	3.86209100	-0.57975400
O	6.71977100	6.06893700	-0.77274100

H	7.65001000	5.79985100	-0.79592300
H	1.17407500	8.27063900	-0.74461000
Br	1.00948600	3.09382000	-0.26311700

HOOC-phBr-NH_3^+ DMSO

C	2.24320200	4.51382900	-0.44350300
C	3.60238300	4.24574200	-0.48258900
C	4.49935700	5.30351900	-0.61094900
C	4.05069300	6.61687600	-0.70095700
C	2.68546900	6.83864400	-0.66273800
C	1.76208900	5.81582400	-0.53447500
H	3.97738200	3.23263900	-0.41497500
H	4.75350900	7.43486900	-0.79778800
H	0.69776200	6.01472500	-0.50505800
N	2.19719100	8.22553000	-0.76034100
H	2.51829700	8.79490400	0.03013100
H	2.51972700	8.68113300	-1.62098500
C	5.95899100	4.97998500	-0.65155000
O	6.39642600	3.86196900	-0.58092800
O	6.71944200	6.06855300	-0.77568200
H	7.64977600	5.79984200	-0.79982500
H	1.17412000	8.26875000	-0.76583800
Br	1.00948800	3.09420200	-0.25864700

HOOC-phBr-NH_3^+ Water

C	2.24333200	4.51400400	-0.44265100
C	3.60242100	4.24570400	-0.48201400
C	4.49935900	5.30343300	-0.61114700
C	4.05062900	6.61673700	-0.70161700
C	2.68544800	6.83870900	-0.66308300
C	1.76213900	5.81590100	-0.53404600
H	3.97729900	3.23259300	-0.41406800
H	4.75325300	7.43479500	-0.79894800
H	0.69787200	6.01496600	-0.50429900
N	2.19726700	8.22544200	-0.76030300
H	2.51113500	8.79225700	0.03491200
H	2.52690100	8.68429200	-1.61649100
C	5.95891200	4.98001800	-0.65216800
O	6.39657000	3.86193500	-0.58140200
O	6.71931000	6.06842700	-0.77684400
H	7.64968100	5.79986000	-0.80130500
H	1.17427400	8.26811600	-0.77443400
Br	1.00950200	3.09434400	-0.25679000

HOOC-phI-NH_3^+ Vacuum

C	2.23992900	4.51621600	-0.35025800
C	3.60673700	4.25924100	-0.43826100
C	4.50174600	5.30529200	-0.63042600
C	4.05457400	6.62079400	-0.73886500
C	2.69440700	6.83319000	-0.64757700
C	1.76688700	5.82053000	-0.45641900
H	3.99789100	3.25127500	-0.35959900
H	4.76717300	7.42452000	-0.88855400
H	0.70455300	6.03103000	-0.39074400

N	2.18465800	8.22758400	-0.76555300
H	1.62931200	8.49579700	0.05442200
H	2.96181600	8.89171000	-0.84129900
C	5.96309300	4.97064800	-0.71902500
O	6.38866400	3.85892200	-0.63480800
O	6.71320800	6.06497700	-0.90285300
H	7.64197700	5.79553600	-0.95594700
H	1.59576600	8.34500400	-1.59796000
I	0.87771800	2.93740900	-0.05558300

HOOC-phI-NH_3^+ TCM

C	2.23835200	4.51006900	-0.44694500
C	3.60083000	4.24914300	-0.48536900
C	4.49987000	5.30609200	-0.61002800
C	4.05257500	6.61991500	-0.69865600
C	2.68744800	6.83766500	-0.66057300
C	1.76243200	5.81512300	-0.53547600
H	3.98598200	3.23911600	-0.42080800
H	4.75784400	7.43661000	-0.79475600
H	0.69903300	6.02219000	-0.50862600
N	2.19842500	8.22891400	-0.76058500
H	2.55412700	8.80911900	0.00687200
H	2.48816600	8.66799100	-1.64140700
C	5.96069400	4.97995600	-0.64767300
O	6.39481100	3.86374600	-0.57419300
O	6.72135500	6.07089100	-0.77261200
H	7.65094400	5.79965500	-0.79394200
H	1.17574700	8.27410900	-0.72513000
I	0.86147000	2.91937400	-0.24940100

HOOC-phI-NH_3^+ DCE

C	2.23960800	4.51108200	-0.44676500
C	3.60106300	4.24803400	-0.48551500
C	4.49986900	5.30543900	-0.60981600
C	4.05221700	6.61912900	-0.69781300
C	2.68718900	6.83884500	-0.66038000
C	1.76282900	5.81548200	-0.53525600
H	3.98477700	3.23758200	-0.42163800
H	4.75624500	7.43664000	-0.79324300
H	0.69978100	6.02330900	-0.50837800
N	2.19895500	8.22780100	-0.76090600
H	2.55316000	8.80900200	0.00637700
H	2.48915400	8.66723300	-1.64128300
C	5.95992200	4.98080600	-0.64826200
O	6.39650200	3.86374500	-0.57672500
O	6.72057400	6.07069700	-0.77146000
H	7.65057800	5.80080200	-0.79349000
H	1.17647300	8.27436600	-0.72678600
I	0.86121000	2.91968400	-0.24796900

HOOC-phI-NH_3^+ Acetone

C	2.24041400	4.51167100	-0.44532800
C	3.60124900	4.24757600	-0.48479600
C	4.49997200	5.30519600	-0.61036000

C	4.05211600	6.61863500	-0.69888300
C	2.68701900	6.83949300	-0.66117900
C	1.76328100	5.81586000	-0.53462300
H	3.98430100	3.23699700	-0.42063200
H	4.75539500	7.43656500	-0.79465100
H	0.70037400	6.02389100	-0.50693000
N	2.19900000	8.22738900	-0.76093600
H	2.54044800	8.80452200	0.01515200
H	2.50152800	8.67276600	-1.63410300
C	5.95963700	4.98125200	-0.64963000
O	6.39713100	3.86361200	-0.57901300
O	6.72056900	6.07029700	-0.77245700
H	7.65063800	5.80065200	-0.79525900
H	1.17614500	8.27263700	-0.74212100
I	0.86088900	2.92066500	-0.24355700

HOOC-phI-NH_3^+ DMSO

C	2.24082800	4.51219500	-0.44352300
C	3.60138500	4.24742100	-0.48368100
C	4.50000700	5.30497100	-0.61077700
C	4.05201700	6.61834700	-0.70013200
C	2.68702600	6.83975500	-0.66205300
C	1.76344400	5.81608900	-0.53387500
H	3.98400200	3.23675100	-0.41895800
H	4.75485200	7.43644500	-0.79666600
H	0.70069900	6.02453700	-0.50547500
N	2.19913500	8.22706600	-0.76087500
H	2.52457400	8.79872900	0.02608100
H	2.51734000	8.67992100	-1.62452700
C	5.95941700	4.98131600	-0.65105100
O	6.39753400	3.86343300	-0.58037200
O	6.72028800	6.06990900	-0.77485100
H	7.65047200	5.80068400	-0.79845800
H	1.17610600	8.27087400	-0.76121800
I	0.86098000	2.92123400	-0.23889600

HOOC-phI-NH_3^+ Water

C	2.24097900	4.51237600	-0.44258800
C	3.60143200	4.24737900	-0.48307200
C	4.50001200	5.30488800	-0.61101600
C	4.05195300	6.61820400	-0.70083900
C	2.68699600	6.83981200	-0.66248400
C	1.76349400	5.81617200	-0.53349100
H	3.98392500	3.23669700	-0.41800800
H	4.75458400	7.43637500	-0.79787100
H	0.70080000	6.02473100	-0.50476000
N	2.19920600	8.22697500	-0.76080600
H	2.51633800	8.79565000	0.03170200
H	2.52561600	8.68362900	-1.61935300
C	5.95933700	4.98134400	-0.65175300
O	6.39767300	3.86339900	-0.58084900
O	6.72015900	6.06976300	-0.77623600
H	7.65037500	5.80066500	-0.80018800
H	1.17621900	8.27011000	-0.77110400

I	0.86100800	2.92150700	-0.23659000

HOOC-phCl-NH_2 Vacuum

C	2.27201100	4.56623000	-0.53113300
C	3.61960700	4.24692500	-0.53702000
C	4.53221000	5.29868000	-0.58597400
C	4.11566500	6.62342100	-0.62847000
C	2.75007200	6.92578300	-0.62334200
C	1.82500000	5.87836000	-0.57153500
H	3.96554300	3.22269900	-0.50582400
H	4.84977600	7.41881500	-0.66231100
H	0.76147200	6.08507400	-0.55921200
Cl	1.09062100	3.28458800	-0.47377800
N	2.31706100	8.24569400	-0.61134100
H	2.97264000	8.92571900	-0.96453800
H	1.37631100	8.40575400	-0.93719300
C	5.98095900	4.94647200	-0.59319300
O	6.41231100	3.82679400	-0.55789100
O	6.78359300	6.02769200	-0.64497600
H	7.69375800	5.70377500	-0.64334700

HOOC-phCl-NH_2 TCM

C	2.27367900	4.56758500	-0.53112100
C	3.62048900	4.24518400	-0.53407600
C	4.53356100	5.29770300	-0.58496200
C	4.11642300	6.62227900	-0.62996900
C	2.74942300	6.92739200	-0.62462000
C	1.82366300	5.87806600	-0.57403800
H	3.96225700	3.21979700	-0.50021300
H	4.84812700	7.41942300	-0.66766100
H	0.76054100	6.08658400	-0.56740500
Cl	1.09136100	3.28152600	-0.47481400
N	2.31797900	8.24385600	-0.60975000
H	2.97034400	8.92642300	-0.96671100
H	1.37413100	8.40530800	-0.92880400
C	5.98341800	4.94832300	-0.59074300
O	6.41205300	3.82382500	-0.54755500
O	6.78212000	6.02393400	-0.65011600
H	7.69904100	5.71526700	-0.64852100

HOOC-phCl-NH_2 DCE

C	2.28009500	4.58163600	-0.37617700
C	3.62433500	4.25399900	-0.43551700
C	4.53130000	5.29360800	-0.63856000
C	4.11038100	6.61007000	-0.78043600
C	2.74546700	6.92034500	-0.72082100
C	1.82584700	5.88395800	-0.51467000
H	3.96879500	3.23474700	-0.32817000
H	4.83682600	7.39711300	-0.93896100
H	0.76483800	6.09710200	-0.46492500
Cl	1.10858700	3.31150600	-0.11504000
N	2.30522000	8.21776800	-0.92203000
H	1.38975100	8.43682000	-0.55720300
H	2.97968900	8.94616200	-0.73803000

C	5.97869800	4.93853000	-0.69906200
O	6.40784200	3.81772600	-0.58944400
O	6.77226700	6.00049100	-0.89024300
H	7.68867400	5.69089600	-0.92178700

HOOC-phCl-NH_2 Acetone

C	2.27356500	4.56851600	-0.53247100
C	3.62001900	4.24494200	-0.53478500
C	4.53390900	5.29746100	-0.58466800
C	4.11702500	6.62204400	-0.62889800
C	2.74943500	6.92825300	-0.62383900
C	1.82301800	5.87883900	-0.57475300
H	3.96009200	3.21900300	-0.50165500
H	4.84775000	7.42009700	-0.66675000
H	0.76014900	6.08853300	-0.57020500
Cl	1.09063900	3.28144900	-0.47784200
N	2.31917300	8.24408400	-0.60622200
H	2.97122400	8.92596400	-0.96619500
H	1.37538000	8.40570800	-0.92671600
C	5.98398400	4.94802600	-0.59037600
O	6.41052700	3.82136100	-0.54691200
O	6.78191000	6.02120400	-0.64951500
H	7.70081200	5.71698900	-0.64927700

HOOC-phCl-NH_2 DMSO

C	2.27351200	4.56878900	-0.53269400
C	3.62018700	4.24484600	-0.53525900
C	4.53394000	5.29720000	-0.58477100
C	4.11715100	6.62215300	-0.62843100
C	2.74971700	6.92852100	-0.62294400
C	1.82296600	5.87877500	-0.57430900
H	3.95982100	3.21876600	-0.50291600
H	4.84800000	7.42006100	-0.66668100
H	0.76023000	6.08907800	-0.56985500
Cl	1.09072800	3.28112900	-0.47923000
N	2.31884000	8.24375300	-0.60546500
H	2.97094200	8.92659500	-0.96353200
H	1.37508900	8.40518000	-0.92623100
C	5.98416200	4.94808000	-0.59077100
O	6.41052300	3.82103800	-0.54744500
O	6.78175000	6.02089600	-0.64991100
H	7.70105200	5.71761700	-0.65063000

HOOC-phCl-NH_2 Water

C	2.27360600	4.56870200	-0.53195700
C	3.62015100	4.24493800	-0.53423800
C	4.53400000	5.29744500	-0.58442100
C	4.11710300	6.62213400	-0.62906500
C	2.74945600	6.92843200	-0.62369200
C	1.82287000	5.87880500	-0.57430300
H	3.95990400	3.21890300	-0.50107200
H	4.84764800	7.42030300	-0.66802100
H	0.76007300	6.08882300	-0.56975000
Cl	1.09079400	3.28114400	-0.47745600

N	2.31900100	8.24385400	-0.60633400
H	2.97112300	8.92578500	-0.96629200
H	1.37538900	8.40516400	-0.92776400
C	5.98418200	4.94821400	-0.59003900
O	6.41044300	3.82114300	-0.54505100
O	6.78173200	6.02086900	-0.65078200
H	7.70113500	5.71781800	-0.65084000

HOOC-phBr-NH_2 Vacuum

C	2.27867600	4.57844400	-0.37726800
C	3.62447900	4.25528300	-0.43228400
C	4.53030400	5.29490300	-0.63597700
C	4.10911200	6.61093000	-0.78023500
C	2.74620700	6.91769000	-0.72005700
C	1.82693400	5.88225300	-0.51818300
H	3.97906600	3.23954000	-0.32419100
H	4.83825400	7.39491700	-0.94340700
H	0.76564500	6.09681600	-0.47726700
N	2.30391200	8.21980300	-0.91680000
H	1.39097500	8.43718500	-0.54783500
H	2.98040100	8.94511500	-0.73455000
C	5.97681900	4.93784100	-0.69634800
O	6.41133700	3.82474100	-0.58148300
O	6.77318000	6.00616800	-0.89742100
H	7.68183900	5.67936600	-0.92722000
Br	1.00263100	3.19948800	-0.10682200

HOOC-phBr-NH_2 TCM

C	2.27256900	4.56790900	-0.52980200
C	3.61942600	4.24504400	-0.53813500
C	4.53329000	5.29732900	-0.59143900
C	4.11645200	6.62181600	-0.63447800
C	2.74968800	6.92761600	-0.62779300
C	1.82239400	5.87879600	-0.57433600
H	3.96510400	3.22127700	-0.50322700
H	4.84834100	7.41892900	-0.67107100
H	0.76053600	6.09364700	-0.56437500
N	2.31979500	8.24451100	-0.61106300
H	2.97227300	8.92691700	-0.96815500
H	1.37531900	8.40772900	-0.92732200
C	5.98297900	4.94652500	-0.59637800
O	6.41011300	3.82109000	-0.56594600
O	6.78265600	6.02207900	-0.63758200
H	7.69937000	5.71276100	-0.63554900
Br	0.98946300	3.16651300	-0.44069800

HOOC-phBr-NH_2 DCE

C	2.28020600	4.58039900	-0.37688000
C	3.62488000	4.25334200	-0.43280600
C	4.53190000	5.29387900	-0.63494200
C	4.11048300	6.60985500	-0.77839200
C	2.74558000	6.91987500	-0.72028200
C	1.82531300	5.88301100	-0.51581900
H	3.97425000	3.23591500	-0.32576500

H	4.83673000	7.39705400	-0.93720500
H	0.76509900	6.10114700	-0.46978700
N	2.30522100	8.21696800	-0.92281800
H	1.38855800	8.43569800	-0.56081200
H	2.97873200	8.94599700	-0.73779300
C	5.97953000	4.93923000	-0.69561900
O	6.40959100	3.81953300	-0.57926600
O	6.77180400	6.00047600	-0.89613400
H	7.68839100	5.69143700	-0.92797700
Br	1.00350300	3.19666800	-0.10505200

HOOC-phBr-NH_2 Acetone

C	2.27989400	4.58084500	-0.37835000
C	3.62455400	4.25316200	-0.43443400
C	4.53194800	5.29361300	-0.63560700
C	4.11080800	6.60989000	-0.77809600
C	2.74590600	6.92038600	-0.71971900
C	1.82507400	5.88350000	-0.51614500
H	3.97309100	3.23540300	-0.32797500
H	4.83704100	7.39728900	-0.93572600
H	0.76510400	6.10255900	-0.46927200
N	2.30583500	8.21756100	-0.92158100
H	1.38962100	8.43557000	-0.55755700
H	2.97922600	8.94593200	-0.73273400
C	5.97951900	4.93879600	-0.69676900
O	6.40885800	3.81809000	-0.58240300
O	6.77154700	5.99940800	-0.89570400
H	7.68876800	5.69179200	-0.92808000
Br	1.00297800	3.19668800	-0.10719700

HOOC-phBr-NH_2 DMSO

C	2.28023000	4.58073400	-0.37702600
C	3.62489500	4.25309600	-0.43395500
C	4.53202900	5.29369200	-0.63610800
C	4.11065000	6.60990200	-0.77837900
C	2.74566300	6.92041700	-0.71891100
C	1.82502500	5.88321800	-0.51467500
H	3.97349900	3.23539000	-0.32740000
H	4.83657700	7.39750800	-0.93648800
H	0.76509900	6.10232600	-0.46723900
N	2.30543900	8.21719300	-0.91996400
H	1.38902400	8.43512100	-0.55623800
H	2.97895800	8.94591500	-0.73261300
C	5.97984100	4.93922700	-0.69819900
O	6.40917300	3.81859400	-0.58100000
O	6.77112600	5.99914500	-0.90107100
H	7.68887600	5.69285200	-0.93311000
Br	1.00366800	3.19615200	-0.10497400

HOOC-phBr-NH_2 Water

C	2.28018400	4.58056100	-0.37849400
C	3.62495800	4.25302800	-0.43438300
C	4.53214900	5.29374600	-0.63564700
C	4.11075100	6.60996300	-0.77802400

C	2.74566600	6.92037900	-0.71957100
C	1.82493800	5.88299200	-0.51626200
H	3.97341600	3.23530600	-0.32765900
H	4.83672600	7.39767900	-0.93534400
H	0.76498800	6.10211600	-0.46950200
N	2.30537800	8.21698700	-0.92076400
H	1.38843400	8.43460300	-0.55813400
H	2.97843300	8.94596100	-0.73266600
C	5.98008400	4.93952500	-0.69648800
O	6.40940800	3.81880900	-0.57915600
O	6.77135400	5.99949000	-0.89823500
H	7.68929400	5.69359700	-0.92966700
Br	1.00361200	3.19574100	-0.10735100

HOOC-phI-NH_2 Vacuum

C	2.27734700	4.57764000	-0.38439800
C	3.62365700	4.25544300	-0.43811600
C	4.53113900	5.29550400	-0.63755300
C	4.11116900	6.61194100	-0.77925000
C	2.74873800	6.91909200	-0.72090700
C	1.82842000	5.88273100	-0.52319100
H	3.98513400	3.24179800	-0.33247700
H	4.84107300	7.39602300	-0.93882000
H	0.76891300	6.10625800	-0.48488800
N	2.30686600	8.22209100	-0.91451000
H	1.39298000	8.43799800	-0.54695400
H	2.98267400	8.94660500	-0.72645300
C	5.97764200	4.93811200	-0.69548800
O	6.41188400	3.82448900	-0.58383300
O	6.77482400	6.00717800	-0.89018800
H	7.68349600	5.68029400	-0.91821900
I	0.84861900	3.03542900	-0.08471400

HOOC-phI-NH_2 TCM

C	2.27884800	4.57845100	-0.38142200
C	3.62466000	4.25388900	-0.43809700
C	4.53250700	5.29484800	-0.63739500
C	4.11179000	6.61129000	-0.77800300
C	2.74788200	6.92050700	-0.71985800
C	1.82735500	5.88267000	-0.51814600
H	3.98204500	3.23882000	-0.33439200
H	4.83893900	7.39807800	-0.93544100
H	0.76874600	6.10875800	-0.47389100
N	2.30676500	8.21922100	-0.91867400
H	1.39026700	8.43627900	-0.55577800
H	2.98002300	8.94732500	-0.73017900
C	5.97999300	4.94004800	-0.69776600
O	6.41135600	3.82111400	-0.58698100
O	6.77352500	6.00380900	-0.89149200
H	7.68872500	5.69161800	-0.92329400
I	0.85114900	3.03190100	-0.07915100

HOOC-phI-NH_2 DCE

C	2.27867400	4.57902500	-0.38112200

C	3.62435500	4.25360900	-0.43831800
C	4.53269800	5.29445300	-0.63770700
C	4.11229100	6.61104800	-0.77819800
C	2.74809700	6.92114200	-0.71981400
C	1.82714100	5.88324700	-0.51739100
H	3.98059700	3.23818400	-0.33464200
H	4.83912500	7.39824200	-0.93486900
H	0.76889600	6.11059000	-0.47148100
N	2.30753400	8.21908000	-0.91941500
H	1.39048100	8.43599900	-0.55712900
H	2.98041200	8.94743400	-0.72925400
C	5.98031500	4.93980500	-0.69811500
O	6.41070400	3.81972200	-0.58567300
O	6.77298000	6.00191500	-0.89351000
H	7.68960300	5.69297700	-0.92533700
I	0.85067100	3.03215600	-0.07798400

HOOC-phI-NH_2 Acetone

C	2.27211700	4.56691700	-0.52805900
C	3.62027400	4.24572900	-0.53783300
C	4.53495300	5.29854000	-0.59234900
C	4.11825200	6.62322700	-0.63521000
C	2.75157200	6.92898600	-0.62763000
C	1.82399900	5.87845700	-0.57293400
H	3.97276500	3.22412900	-0.50340000
H	4.84918200	7.42119400	-0.67363900
H	0.76422000	6.10272400	-0.56387500
N	2.32056600	8.24499100	-0.60964400
H	2.97053800	8.92649500	-0.97416300
H	1.37546700	8.40548400	-0.92688000
C	5.98507600	4.94894500	-0.59758900
O	6.41179500	3.82177800	-0.57114900
O	6.78338400	6.02304800	-0.63319900
H	7.70223600	5.71867500	-0.63241700
I	0.83817700	2.99930800	-0.41998800

HOOC-phI-NH_2 DMSO

C	2.27212400	4.56695100	-0.52797500
C	3.62030400	4.24570500	-0.53756100
C	4.53503400	5.29854800	-0.59214300
C	4.11830200	6.62322800	-0.63529000
C	2.75150600	6.92908900	-0.62763900
C	1.82388700	5.87844300	-0.57283900
H	3.97255000	3.22403700	-0.50311300
H	4.84900500	7.42137400	-0.67440800
H	0.76415300	6.10286300	-0.56393900
N	2.32051700	8.24482000	-0.60969300
H	2.97067900	8.92656500	-0.97359000
H	1.37550300	8.40541600	-0.92734100
C	5.98524100	4.94905200	-0.59738100
O	6.41165200	3.82151600	-0.57068300
O	6.78332100	6.02273300	-0.63318400
H	7.70254700	5.71921700	-0.63281800
I	0.83825100	2.99906900	-0.42036000

HOOC-phI-NH_2 Water

C	2.27212000	4.56697600	-0.52793400
C	3.62030600	4.24570100	-0.53751400
C	4.53505900	5.29855200	-0.59210900
C	4.11832500	6.62323600	-0.63529300
C	2.75148900	6.92912900	-0.62763200
C	1.82384400	5.87845000	-0.57279000
H	3.97247400	3.22400700	-0.50309000
H	4.84896000	7.42144100	-0.67456200
H	0.76412400	6.10292700	-0.56392900
N	2.32052400	8.24479200	-0.60967700
H	2.97069300	8.92652100	-0.97365500
H	1.37552500	8.40537300	-0.92744900
C	5.98529700	4.94907900	-0.59734900
O	6.41161000	3.82141500	-0.57069700
O	6.78330900	6.02262900	-0.63305100
H	7.70265600	5.71939000	-0.63283000
I	0.83826000	2.99900900	-0.42039800

$^{-}$OOC-phCl-NH_2 Vacuum

C	2.26314300	4.57062700	-0.53319500
C	3.60752100	4.24853000	-0.52920000
C	4.53779400	5.28972200	-0.55612700
C	4.09991800	6.60707700	-0.58618900
C	2.73880200	6.91408300	-0.59299800
C	1.80159200	5.88059300	-0.56092900
H	3.96668900	3.22757200	-0.50992700
H	4.85815900	7.38391300	-0.61095700
H	0.73813000	6.08912800	-0.55154600
Cl	1.05840000	3.27855700	-0.50431000
N	2.30227300	8.25793000	-0.58144400
H	3.00995500	8.89208900	-0.92583800
H	1.43445500	8.39799800	-1.07994700
C	6.06552200	4.97698100	-0.56712300
O	6.35073300	3.76737600	-0.54006800
O	6.80068800	5.98055700	-0.60413900

$^{-}$OOC-phCl-NH_2 TCM

C	2.26500600	4.57190900	-0.53406400
C	3.61048300	4.24635200	-0.52571700
C	4.54005900	5.28758300	-0.56023900
C	4.10740100	6.60632600	-0.59887400
C	2.74401100	6.91944900	-0.60796200
C	1.80792400	5.88144600	-0.57310800
H	3.95206800	3.22042200	-0.49611800
H	4.85515800	7.39082900	-0.62549200
H	0.74517800	6.09257500	-0.57453300
Cl	1.06968100	3.28073000	-0.49794100
N	2.31711700	8.25148100	-0.59239700
H	2.99369200	8.90492300	-0.96174900
H	1.40327700	8.40563700	-0.99502700
C	6.05132800	4.97455200	-0.56239200
O	6.35803500	3.76483600	-0.53600800

O	6.81335800	5.96368500	-0.59231800

$^{-}$OOC-phCl-NH_2 DCE

C	2.26562600	4.57242700	-0.53473400
C	3.61155500	4.24672300	-0.52607500
C	4.54097300	5.28803100	-0.56220700
C	4.10925400	6.60728700	-0.60321300
C	2.74497300	6.92098200	-0.61152300
C	1.80917900	5.88168500	-0.57532600
H	3.95078400	3.22025500	-0.49489000
H	4.85377100	7.39459900	-0.63133500
H	0.74661900	6.09347600	-0.57817200
Cl	1.07259500	3.28086200	-0.49690000
N	2.31892700	8.25006800	-0.59448900
H	2.98854900	8.90845900	-0.96772500
H	1.39659300	8.40639900	-0.97643500
C	6.04858400	4.97248400	-0.56040600
O	6.35764100	3.76223500	-0.52641500
O	6.81815200	5.95676100	-0.59409300

$^{-}$OOC-phCl-NH_2 Acetone

C	2.26634800	4.57210700	-0.53883800
C	3.61267600	4.24689100	-0.52884800
C	4.54163400	5.28860700	-0.56276900
C	4.10991400	6.60807600	-0.60295600
C	2.74508300	6.92153500	-0.61203600
C	1.80979200	5.88109900	-0.57843500
H	3.95097300	3.22017300	-0.49820000
H	4.85260000	7.39713500	-0.62924400
H	0.74726400	6.09293200	-0.58344200
Cl	1.07496200	3.27977800	-0.50404200
N	2.31867200	8.24894500	-0.59247200
H	2.98495900	8.91078500	-0.96558100
H	1.39262100	8.40644100	-0.96491200
C	6.04766700	4.97221500	-0.55821200
O	6.35796500	3.76167300	-0.52196100
O	6.82064900	5.95434200	-0.59198800

$^{-}$OOC-phCl-NH_2 DMSO

C	2.26651400	4.57231600	-0.53888100
C	3.61286700	4.24710700	-0.52844600
C	4.54191500	5.28891400	-0.56301700
C	4.11047700	6.60848900	-0.60441700
C	2.74523200	6.92197400	-0.61331400
C	1.81006300	5.88129900	-0.57908500
H	3.95079700	3.22036600	-0.49693900
H	4.85196500	7.39857600	-0.63166300
H	0.74757300	6.09311100	-0.58422200
Cl	1.07559300	3.28000300	-0.50309900
N	2.31906100	8.24859600	-0.59405500
H	2.98397700	8.91153300	-0.96768300
H	1.39126500	8.40659000	-0.96198000
C	6.04676800	4.97138600	-0.55702900
O	6.35746000	3.76060200	-0.51942000

O	6.82225000	5.95187100	-0.59068600

$^{-}$OOC-phCl-NH_2 Water

C	2.26674300	4.57242100	-0.53699900
C	3.61327200	4.24723300	-0.52867900
C	4.54210600	5.28900800	-0.56455000
C	4.11060100	6.60874000	-0.60528400
C	2.74540600	6.92210400	-0.61273400
C	1.81022800	5.88120600	-0.57697900
H	3.95086300	3.22033500	-0.49795000
H	4.85183400	7.39907800	-0.63309200
H	0.74775800	6.09318900	-0.58091000
Cl	1.07637700	3.27978700	-0.49966000
N	2.31912000	8.24841600	-0.59276800
H	2.98241800	8.91164900	-0.96874000
H	1.38986000	8.40590700	-0.95720800
C	6.04667700	4.97137900	-0.56042800
O	6.35798000	3.76068000	-0.52297000
O	6.82253400	5.95160300	-0.59498700

$^{-}$OOC-phBr-NH_2 Vacuum

C	2.27102000	4.58418800	-0.37821200
C	3.61175500	4.25413000	-0.44168900
C	4.53302200	5.28063600	-0.66519400
C	4.09015500	6.58743100	-0.81652700
C	2.73252000	6.90165900	-0.74512300
C	1.80214200	5.88370300	-0.52701200
H	3.98024700	3.24338200	-0.32456000
H	4.84275200	7.35138500	-0.98692200
H	0.74111700	6.09934000	-0.48325300
N	2.28855800	8.22777300	-0.94434000
H	1.45907600	8.45500800	-0.41367300
H	3.01631800	8.90593100	-0.76555000
C	6.05883800	4.96194700	-0.73411900
O	6.34868300	3.76389600	-0.57524000
O	6.78612100	5.95116600	-0.93740300
Br	0.97261300	3.19916500	-0.08139000

$^{-}$OOC-phBr-NH_2 TCM

C	2.27350300	4.58518000	-0.36854100
C	3.61536000	4.25242700	-0.44142600
C	4.53602200	5.27952600	-0.66145100
C	4.09808800	6.58864100	-0.80831500
C	2.73834500	6.90833000	-0.73448700
C	1.81029600	5.88596600	-0.50935800
H	3.96610800	3.23518500	-0.33464000
H	4.83910900	7.36086600	-0.98169700
H	0.75120200	6.10692400	-0.45159900
N	2.30138400	8.22031400	-0.94227500
H	1.41945900	8.44666300	-0.50474600
H	2.99929800	8.92423800	-0.74670200
C	6.04440600	4.95999800	-0.73779400
O	6.35393400	3.75527600	-0.63151500
O	6.80183900	5.94054900	-0.89558600

Br	0.98658300	3.20066000	-0.07007500

$^{-}$OOC-phBr-NH$_2$ DCE

C	2.27365400	4.58574800	-0.36734900
C	3.61604300	4.25287300	-0.44067400
C	4.53679400	5.27994400	-0.66034900
C	4.09998500	6.58991900	-0.80566300
C	2.73948700	6.91027200	-0.73190600
C	1.81152800	5.88662400	-0.50729500
H	3.96402100	3.23492200	-0.33328800
H	4.83825600	7.36474200	-0.97810600
H	0.75276600	6.10868800	-0.44811800
N	2.30324800	8.21938000	-0.94063000
H	1.41377600	8.44513700	-0.51805500
H	2.99606500	8.92807400	-0.74385900
C	6.04125900	4.95778200	-0.73995000
O	6.35311800	3.75214900	-0.63562800
O	6.80577400	5.93363800	-0.89996600
Br	0.98916200	3.20085000	-0.06937200

$^{-}$OOC-phBr-NH$_2$ Acetone

C	2.27294000	4.58632000	-0.36957200
C	3.61559300	4.25292300	-0.44162200
C	4.53706700	5.27985200	-0.65887400
C	4.10155200	6.59065000	-0.80240800
C	2.74066000	6.91170900	-0.73043600
C	1.81198900	5.88747000	-0.50857300
H	3.96173100	3.23441700	-0.33432900
H	4.83892700	7.36682700	-0.97222300
H	0.75338800	6.11045500	-0.45018000
N	2.30539300	8.21966100	-0.93876700
H	1.41174400	8.44493100	-0.52471900
H	2.99563200	8.93039000	-0.74022100
C	6.03961100	4.95562200	-0.73893700
O	6.35166200	3.74916500	-0.63714700
O	6.80830000	5.92893100	-0.89777700
Br	0.98874700	3.20141800	-0.07442300

$^{-}$OOC-phBr-NH$_2$ DMSO

C	2.27387100	4.58581700	-0.36864000
C	3.61690500	4.25328900	-0.44109700
C	4.53771400	5.28072300	-0.65871800
C	4.10165600	6.59154800	-0.80160500
C	2.74035000	6.91188300	-0.72929500
C	1.81235200	5.88663600	-0.50743600
H	3.96292900	3.23481400	-0.33336800
H	4.83765100	7.36904100	-0.97134100
H	0.75373500	6.10935400	-0.44830300
N	2.30435100	8.21862100	-0.93760900
H	1.40833300	8.44290200	-0.52814100
H	2.99256500	8.93120900	-0.73877500
C	6.03931600	4.95642000	-0.74098500
O	6.35275000	3.75010400	-0.63748000
O	6.80912400	5.92844000	-0.90395200

Br	0.99133500	3.19993800	-0.07346500

$^{-}$OOC-phBr-NH$_2$ Water

C	2.27401800	4.58605300	-0.36724900
C	3.61707900	4.25351900	-0.43939600
C	4.53781300	5.28084100	-0.65814800
C	4.10185600	6.59157800	-0.80206900
C	2.74035200	6.91192500	-0.72999200
C	1.81248000	5.88675800	-0.50731100
H	3.96311400	3.23520500	-0.33065300
H	4.83744400	7.36928500	-0.97231400
H	0.75382400	6.10937400	-0.44877100
N	2.30437000	8.21826500	-0.93949900
H	1.40776700	8.44283300	-0.53147300
H	2.99215400	8.93141000	-0.74110000
C	6.03898900	4.95606700	-0.74062900
O	6.35248700	3.74968700	-0.63652300
O	6.80961900	5.92746900	-0.90440300
Br	0.99157100	3.20047300	-0.07067900

$^{-}$OOC-phI-NH$_2$ Vacuum

C	2.27365000	4.58473700	-0.38178800
C	3.61351600	4.25350400	-0.44385000
C	4.53414200	5.28248000	-0.66559600
C	4.09130000	6.58870200	-0.81603400
C	2.73368700	6.90270200	-0.74556500
C	1.80305100	5.88361700	-0.52970900
H	3.98960200	3.24547600	-0.32810700
H	4.84389400	7.35297900	-0.98525700
H	0.74358300	6.10567200	-0.48771400
N	2.28949700	8.22854100	-0.94361800
H	1.45694100	8.45418800	-0.41713600
H	3.01562900	8.90737700	-0.76088900
C	6.06110400	4.96373900	-0.73308900
O	6.35060600	3.76602700	-0.57363500
O	6.78692000	5.95376900	-0.93590800
I	0.82261900	3.03537300	-0.05492500

$^{-}$OOC-phI-NH$_2$ TCM

C	2.27307900	4.58450600	-0.37437700
C	3.61547300	4.25270400	-0.44538200
C	4.53705800	5.28081300	-0.66215000
C	4.09970100	6.59003800	-0.80741500
C	2.74026200	6.90948400	-0.73528900
C	1.81134300	5.88613700	-0.51372600
H	3.97274100	3.23769900	-0.33979400
H	4.84127700	7.36241900	-0.97816400
H	0.75397800	6.11507900	-0.45761300
N	2.30334300	8.22233700	-0.94093500
H	1.42031100	8.44676800	-0.50443000
H	3.00043700	8.92548600	-0.73934800
C	6.04589900	4.96102000	-0.73633900
O	6.35525100	3.75603100	-0.63316700
O	6.80347300	5.94209600	-0.88994900

I	0.83611600	3.03626600	-0.04474000

$^{-}$OOC-phI-NH$_2$ DCE

C	2.27281600	4.58459500	-0.37419100
C	3.61603200	4.25309800	-0.44553100
C	4.53783900	5.28119100	-0.66075800
C	4.10181400	6.59142600	-0.80387400
C	2.74156900	6.91143200	-0.73256000
C	1.81272300	5.88656200	-0.51240500
H	3.97066600	3.23729800	-0.34031400
H	4.84059800	7.36665900	-0.97259500
H	0.75565300	6.11667200	-0.45577500
N	2.30535500	8.22127800	-0.93868800
H	1.41461300	8.44508600	-0.51767400
H	2.99714100	8.92944100	-0.73632400
C	6.04279400	4.95909300	-0.73743800
O	6.35466600	3.75312100	-0.63750000
O	6.80751100	5.93581000	-0.89104400
I	0.83795000	3.03612100	-0.04614700

$^{-}$OOC-phI-NH$_2$ Acetone

C	2.27255300	4.58471700	-0.37503600
C	3.61620400	4.25334600	-0.44578800
C	4.53832900	5.28145800	-0.65954800
C	4.10308300	6.59231500	-0.80131300
C	2.74237800	6.91253200	-0.73122600
C	1.81335400	5.88686100	-0.51273500
H	3.96953200	3.23713900	-0.34057500
H	4.84058800	7.36908300	-0.96821200
H	0.75641600	6.11762300	-0.45636300
N	2.30650400	8.22097400	-0.93758500
H	1.41163000	8.44404200	-0.52487600
H	2.99541000	8.93151800	-0.73365900
C	6.04139300	4.95781100	-0.73731500
O	6.35397500	3.75116100	-0.63977000
O	6.80992800	5.93219100	-0.89028700
I	0.83846400	3.03611200	-0.04853100

$^{-}$OOC-phI-NH$_2$ DMSO

C	2.27313500	4.58468700	-0.37262300
C	3.61707700	4.25378900	-0.44427000
C	4.53878900	5.28197300	-0.65941700
C	4.10339200	6.59292000	-0.80122500
C	2.74239200	6.91286700	-0.73045900
C	1.81384300	5.88662300	-0.51086200
H	3.97009300	3.23757200	-0.33842300
H	4.83966600	7.37069500	-0.96871600
H	0.75697100	6.11746600	-0.45369100
N	2.30595000	8.22008500	-0.93783300
H	1.40907300	8.44278500	-0.52920600
H	2.99315800	8.93249700	-0.73461100
C	6.04074300	4.95769500	-0.73971400
O	6.35416200	3.75092200	-0.64151200
O	6.81090300	5.93062300	-0.89581200

I	0.84039500	3.03568500	-0.04444300

$^{-}$OOC-phI-NH$_2$ Water

C	2.27295800	4.58472900	-0.37341000
C	3.61684500	4.25374500	-0.44557200
C	4.53878700	5.28197000	-0.65989300
C	4.10372400	6.59312900	-0.80049100
C	2.74256700	6.91319600	-0.72966500
C	1.81396900	5.88691800	-0.51071300
H	3.96954300	3.23729800	-0.34056800
H	4.83967400	7.37136000	-0.96721700
H	0.75718300	6.11798700	-0.45272100
N	2.30647100	8.22058100	-0.93611500
H	1.40911000	8.44298500	-0.52829700
H	2.99349100	8.93282700	-0.73174400
C	6.04029900	4.95705000	-0.74065400
O	6.35338200	3.74993300	-0.64423800
O	6.81160300	5.92937900	-0.89546100
I	0.84013500	3.03579600	-0.04605900

HOOC-CH$_2$-NH$_3^+$ Vacuum

N	-2.56041600	-1.27111200	0.03463200
H	-1.57335100	-1.01328300	-0.19131800
C	-3.31527900	0.02375200	0.02432000
C	-2.24000100	1.12178000	-0.08550100
H	-3.97828900	0.04795100	-0.84105500
H	-3.90492000	0.11523300	0.93627600
O	-1.09654100	0.79867800	-0.21877200
H	-2.90539200	-1.94570600	-0.65219000
O	-2.63845300	2.37121900	-0.04037600
H	-3.58917800	2.49017700	0.08056600
H	-2.56451800	-1.72193100	0.95341900

HOOC-CH$_2$-NH$_3^+$ TCM

N	-2.56455700	-1.27105100	0.01738800
H	-1.67258300	-1.18894700	-0.48844200
C	-3.28360100	0.03183300	-0.04110400
C	-2.22858200	1.13324600	-0.01194000
H	-3.84763900	0.08059400	-0.97249900
H	-3.96992300	0.09747300	0.80184300
O	-1.06303500	0.86782700	-0.07885000
H	-3.11247800	-2.03507300	-0.38568400
O	-2.66650000	2.37755900	0.06536300
H	-3.62886800	2.44961000	0.11355200
H	-2.32857200	-1.52631100	0.98037500

HOOC-CH$_2$-NH$_3^+$ DCE

N	-2.55932200	-1.26973700	-0.02873300
H	-1.89716100	-1.35299700	-0.80597000
C	-3.27060900	0.03522800	-0.06564200
C	-2.23400500	1.13419300	0.10972400
H	-3.78456800	0.12520900	-1.02218700
H	-4.00183600	0.05611500	0.74215000
O	-1.07411700	0.87594500	0.25736200

H	-3.21590000	-2.05250400	-0.08288200
O	-2.68025300	2.38089200	0.09412100
H	-3.63641000	2.44867400	-0.03083800
H	-2.01215600	-1.36425900	0.83289600

$HOOC-CH_2-NH_3^+$ Acetone

N	-2.55918900	-1.27008400	-0.02919900
H	-1.90105000	-1.35765100	-0.80907800
C	-3.26778300	0.03547500	-0.06591500
C	-2.23384000	1.13475300	0.11291600
H	-3.78006400	0.12665400	-1.02310600
H	-4.00087400	0.05641700	0.74005000
O	-1.07298700	0.88184800	0.26664900
H	-3.21879500	-2.05054400	-0.07978200
O	-2.68266100	2.38105000	0.09420900
H	-3.63824800	2.44531600	-0.03792500
H	-2.01084500	-1.36647500	0.83118100

$HOOC-CH_2-NH_3^+$ DMSO

N	-2.55875800	-1.27033600	-0.02902900
H	-1.90676000	-1.36255900	-0.81327800
C	-3.26585000	0.03551400	-0.06544900
C	-2.23371600	1.13553200	0.11424600
H	-3.77775100	0.12682600	-1.02274600
H	-3.99925600	0.05695500	0.74019200
O	-1.07222900	0.88657200	0.27170200
H	-3.22062600	-2.04920400	-0.07340300
O	-2.68509900	2.38131000	0.09307100
H	-3.64032300	2.44252300	-0.04374000
H	-2.00597100	-1.36637300	0.82843400

$HOOC-CH_2-NH_3^+$ Water

N	-2.55888500	-1.27054100	-0.02942200
H	-1.90832700	-1.36371400	-0.81483500
C	-3.26520400	0.03557600	-0.06527900
C	-2.23350900	1.13560200	0.11508900
H	-3.77640300	0.12776400	-1.02298000
H	-3.99903000	0.05726300	0.73975200
O	-1.07189900	0.88762500	0.27410000
H	-3.22192200	-2.04837800	-0.07231000
O	-2.68539400	2.38114700	0.09262100
H	-3.64073200	2.44126600	-0.04422500
H	-2.00503300	-1.36685200	0.82748700

$HOOC-CH_2-NH_2$ Vacuum

N	-2.72178600	-1.30433700	-0.20581000
C	-3.32481100	-0.00074300	-0.02810700
C	-2.24652200	1.05389700	0.15717100
H	-3.93194000	0.26316900	-0.90186700
H	-3.97590500	0.08550800	0.85573800
O	-1.12102900	0.80316900	0.46180300
H	-3.31474600	-2.04442200	0.14414000
O	-2.65108600	2.33127300	0.00502900
H	-3.56458200	2.36754800	-0.29613800

H	-1.83110900	-1.33766600	0.27944500

HOOC-CH_2-NH_2 TCM

N	-2.67369600	-1.29967800	-0.19331200
C	-3.29824900	-0.00082800	-0.02532000
C	-2.23939500	1.07151500	0.12486300
H	-3.91724200	0.23293400	-0.89641300
H	-3.94241500	0.08937100	0.86275100
O	-1.09152500	0.84686500	0.38356100
H	-3.34242000	-2.03872600	-0.01273100
O	-2.66657500	2.34026200	-0.00017300
H	-3.59967800	2.37568400	-0.24206100
H	-1.91232000	-1.40000300	0.47024200

HOOC-CH_2-NH_2 DCE

N	-2.65589400	-1.29869400	-0.18272600
C	-3.28673400	-0.00093600	-0.02411800
C	-2.23524000	1.07916500	0.11235100
H	-3.90700500	0.22022600	-0.89703900
H	-3.93237900	0.09273800	0.86218100
O	-1.07879100	0.86565800	0.34718600
H	-3.34476600	-2.03392100	-0.07297700
O	-2.67386300	2.34448000	0.00124000
H	-3.61388400	2.37642000	-0.21473300
H	-1.95496100	-1.42773900	0.54004100

HOOC-CH_2-NH_2 Acetone

N	-2.64524100	-1.29851700	-0.17451800
C	-3.27891700	-0.00094100	-0.02350100
C	-2.23216000	1.08417300	0.10459500
H	-3.89934100	0.21229500	-0.89807400
H	-3.92626900	0.09586600	0.86102000
O	-1.07052200	0.87830500	0.32332000
H	-3.34407200	-2.03002700	-0.11022400
O	-2.67907700	2.34707000	0.00334700
H	-3.62301400	2.37532500	-0.19661400
H	-1.98490400	-1.44615400	0.58205500

HOOC-CH_2-NH_2 DMSO

N	-2.64026200	-1.29887800	-0.17011200
C	-3.27505100	-0.00100200	-0.02402700
C	-2.23064600	1.08645300	0.10039500
H	-3.89461000	0.20839200	-0.90004700
H	-3.92410900	0.09762400	0.85884800
O	-1.06626100	0.88435200	0.31003100
H	-3.34326900	-2.02800700	-0.12570000
O	-2.68165300	2.34810000	0.00540100
H	-3.62769900	2.37473000	-0.18536900
H	-1.99995600	-1.45436800	0.60198700

HOOC-CH_2-NH_2 Water

N	-2.63882000	-1.29906500	-0.16859100
C	-3.27388300	-0.00104100	-0.02441600
C	-2.23018000	1.08709700	0.09893900

H	-3.89289800	0.20716100	-0.90108600
H	-3.92371600	0.09832400	0.85773500
O	-1.06487600	0.88611600	0.30528900
H	-3.34296800	-2.02745000	-0.12978400
O	-2.68247300	2.34836300	0.00638800
H	-3.62924700	2.37449600	-0.18106700
H	-2.00445500	-1.45660600	0.60799800

$^{-}$OOC-CH$_2$-NH$_2$ Vacuum

N	-2.91576000	-1.41921400	-0.06787000
C	-3.33829000	-0.01624400	-0.18928400
C	-2.27126200	1.04491200	0.22649300
H	-3.59757800	0.18890100	-1.23401400
H	-4.24686700	0.15458000	0.39324000
O	-1.10704000	0.61222900	0.37503500
H	-2.92352700	-1.64995600	0.92188200
O	-2.70333900	2.20963400	0.33184600
H	-1.91928500	-1.40036100	-0.28592400

$^{-}$OOC-CH$_2$-NH$_2$ TCM

N	-2.93676400	-1.41597700	-0.04603100
C	-3.33308900	-0.01388000	-0.17760300
C	-2.28735200	1.04688700	0.24907100
H	-3.58741500	0.18864500	-1.22251600
H	-4.24612600	0.16052300	0.39735600
O	-1.15135400	0.63301800	0.57077900
H	-2.78508400	-1.60673200	0.94025900
O	-2.68739200	2.23358700	0.21179900
H	-2.00837000	-1.50159100	-0.45171100

$^{-}$OOC-CH$_2$-NH$_2$ DCE

N	-2.72006700	-1.34623200	-0.18776400
C	-3.30725100	-0.00792900	-0.10890300
C	-2.24422500	1.09372300	0.10193900
H	-3.85577600	0.23051700	-1.02355700
H	-4.01670800	0.09694400	0.72205600
O	-1.10089500	0.72476000	0.45398500
H	-3.30393300	-2.02740900	0.28231800
O	-2.64228300	2.26788700	-0.07412400
H	-1.83180800	-1.30778000	0.30545700

$^{-}$OOC-CH$_2$-NH$_2$ Acetone

N	-2.70440200	-1.33874200	-0.19176200
C	-3.30208500	-0.00663700	-0.09708800
C	-2.24310200	1.10012500	0.09178300
H	-3.87270400	0.22487200	-0.99953200
H	-3.99340400	0.09323000	0.75060700
O	-1.09925100	0.74296500	0.45499200
H	-3.31638200	-2.03913900	0.21039400
O	-2.64168900	2.27146600	-0.10606900
H	-1.84992900	-1.32365800	0.35808000

$^{-}$OOC-CH$_2$-NH$_2$ DMSO

N	-2.69842000	-1.33629100	-0.19012500

C	-3.29941900	-0.00605000	-0.09311500
C	-2.24192700	1.10243300	0.08628600
H	-3.87708500	0.22089300	-0.99204300
H	-3.98493800	0.09411000	0.75961300
O	-1.09925000	0.75087100	0.45905900
H	-3.32276100	-2.04195500	0.18316700
O	-2.63859700	2.27230000	-0.12606400
H	-1.86054900	-1.33183100	0.38462700

$^{-}$OOC-CH$_2$-NH$_2$ Water

N	-2.69608200	-1.33526700	-0.19107700
C	-3.29858700	-0.00589200	-0.09166800
C	-2.24198800	1.10336200	0.08564100
H	-3.87882900	0.22027400	-0.98906200
H	-3.98207400	0.09309500	0.76293400
O	-1.09952800	0.75369300	0.46104700
H	-3.32386200	-2.04301100	0.17255300
O	-2.63846800	2.27277700	-0.13027200
H	-1.86352800	-1.33455000	0.39130800

Six-membered Oxocarbenium Vacuum

C	-4.62202300	-3.17722600	-0.07110900
C	-3.10112800	-3.32721500	-0.07519200
C	-2.45978900	-1.95961200	0.15566100
C	-3.20462700	-1.09679600	1.08208100
C	-5.07788600	-2.59811800	1.24524800
H	-1.42669400	-2.00342000	0.52339400
H	-2.79059500	-4.01754100	0.71304000
H	-2.75077900	-3.73887600	-1.02046300
H	-4.95260700	-2.53745900	-0.89503000
H	-5.11350500	-4.14371500	-0.19605900
H	-2.80195300	-0.13316500	1.40177400
H	-4.88280300	-3.24536200	2.10112100
H	-6.11171100	-2.26290900	1.26163600
H	-2.38399200	-1.36264200	-0.76939900
O	-4.32415900	-1.34865800	1.56734400

Dimethyloxidanium Vacuum

O	-0.24745500	0.34395600	0.03999200
C	1.22818100	0.24706300	-0.00594900
H	1.46265800	-0.80997100	0.08489900
H	1.57604000	0.67590900	-0.94387700
H	1.57834300	0.80225800	0.85973900
C	-0.83182400	1.70294100	0.00076400
H	-0.53423700	2.18204300	-0.93014500
H	-1.90726600	1.57014300	0.07998200
H	-0.43417900	2.21076200	0.87501700
H	-0.68330000	-0.26988200	-0.57452900

Methylguanidinium Vacuum

C	0.03687000	-0.02178900	-0.00611700
N	0.04980700	-0.12230200	1.32274400
N	1.19121300	0.04835300	-0.67465000
N	-1.11882300	0.01639300	-0.65698800

C	-2.42428100	0.06103600	0.00150600
H	-0.79643300	-0.29540300	1.84211400
H	0.90594400	-0.02646400	1.84639300
H	2.07361200	-0.11897800	-0.21704100
H	1.21428800	0.26993900	-1.65780900
H	-1.09396800	-0.04557600	-1.66410700
H	-2.46768900	0.90018300	0.69754000
H	-3.18101800	0.21339400	-0.76341500
H	-2.63897100	-0.87878600	0.51492800

Cation-Anion-Cl Vacuum ModRedundant

N	-2.52420300	-0.96130500	0.04428900
H	-1.66280800	-1.15976500	-0.46018800
C	-2.81481300	0.45241500	-0.19502500
C	-1.59767400	1.40694800	-0.20429300
H	-3.30249100	0.55872900	-1.17001900
H	-3.53122100	0.81757700	0.54412200
O	-0.46125600	0.86181800	-0.24043600
H	-2.25592300	-1.06422700	1.01839300
O	-1.85729800	2.62785900	-0.20594600
C	2.15138600	4.17843200	-0.47938300
C	3.54789600	4.03190500	-0.48980300
C	4.38677300	5.13541100	-0.55887800
C	3.87304100	6.43458000	-0.61950000
C	2.49986000	6.54364100	-0.60779700
C	1.63274200	5.47180500	-0.54074400
H	3.98333100	3.04020100	-0.44356100
H	4.53712300	7.28921400	-0.67127400
H	0.55236800	5.59643700	-0.53187400
Cl	1.12250900	2.82457700	-0.38930000
N	1.88314700	7.89990700	-0.65514400
H	2.58620400	8.61447100	-0.86035700
H	1.16231200	7.94438400	-1.38276000
C	5.86321200	4.89930700	-0.56857000
O	6.37725200	3.82130700	-0.52262600
O	6.56123500	6.05046600	-0.63539800
H	7.50054400	5.82018300	-0.63833500
H	1.43988200	8.13532900	0.23897900

A 7 10 15 120.0 F

D 4 7 10 15 -2.0 F

Cation-Anion-Cl TCM ModRedundant

N	-2.44073500	-1.01578300	0.60045100
H	-1.43950900	-0.96182400	0.42716100
C	-3.02791600	0.18506400	0.00316300
C	-1.98220000	1.29904100	-0.24094700
H	-3.49146900	-0.01029400	-0.97188500
H	-3.80795300	0.60110900	0.64596800
O	-0.77545200	0.96777300	-0.17118700
H	-2.78455700	-1.85363800	0.14760900
O	-2.44724800	2.42794700	-0.51125000
C	2.13087100	4.40023100	-0.48177100
C	3.49438800	4.14477200	-0.56783500

C	4.39155900	5.20346400	-0.66857400
C	3.94665200	6.52293600	-0.68295200
C	2.58376700	6.73641700	-0.59474300
C	1.66124500	5.71134500	-0.49468400
H	3.86536100	3.12734600	-0.56061500
H	4.65093800	7.34150600	-0.76161700
H	0.59680900	5.90408800	-0.42978600
Cl	1.00041200	3.10252100	-0.36559300
N	2.08661800	8.12923900	-0.59043300
H	2.27045900	8.59216600	0.30640000
H	2.52856200	8.68964600	-1.32585000
C	5.84796100	4.87897000	-0.76499100
O	6.28753400	3.76206700	-0.75536800
O	6.61064100	5.97429000	-0.86442900
H	7.53613300	5.69707400	-0.92710300
H	1.07526100	8.16413200	-0.74956600

A 15 10 7 120.0 F

D 15 10 7 4 7.0 F

Cation-Anion-Cl DCE

N	-2.23452500	-1.20042000	0.31494600
H	-1.28580500	-0.97173700	0.02981200
C	-3.05777800	-0.02355800	0.03459300
C	-2.23568600	1.28401100	0.04584900
H	-3.54063000	-0.06537000	-0.95081400
H	-3.85579600	0.07844900	0.77411300
O	-0.98936300	1.17511700	-0.02095600
H	-2.53882000	-1.99616900	-0.23309600
O	-2.90194500	2.34307600	0.09049700
C	2.07332400	4.54342600	-0.45695200
C	3.41898000	4.20585100	-0.49905100
C	4.37595400	5.20888100	-0.62440000
C	4.00501300	6.54764200	-0.70812700
C	2.65469200	6.84304200	-0.66118000
C	1.67485300	5.87460300	-0.53910300
H	3.73175000	3.17112600	-0.43554200
H	4.75306400	7.32430800	-0.80690000
H	0.62265500	6.13148300	-0.50665800
Cl	0.87227600	3.30883700	-0.29934100
N	2.24031400	8.25758800	-0.73961900
H	2.57830000	8.79487100	0.06600300
H	2.59844600	8.71019600	-1.58711200
C	5.81373100	4.80134300	-0.66712600
O	6.18885100	3.66208100	-0.59219900
O	6.63730600	5.84503400	-0.79831800
H	7.54872900	5.51885000	-0.82239400
H	1.22023900	8.34904600	-0.75735400

Cation-Anion-Cl Acetone

N	-2.23006300	-1.21171400	0.34385400
H	-1.28982500	-0.99799100	0.02270000
C	-3.06701400	-0.05488700	0.02450200
C	-2.26616700	1.26430900	0.02847000

H	-3.52960500	-0.12216600	-0.96947200
H	-3.88072100	0.04476300	0.74675600
O	-1.01758400	1.17651600	-0.02308900
H	-2.54649900	-2.03617000	-0.15286000
O	-2.94839200	2.31474200	0.05068600
C	2.07215200	4.56873900	-0.45069500
C	3.41391900	4.21961100	-0.49860200
C	4.37765900	5.21592700	-0.62721700
C	4.01562800	6.55709200	-0.70809900
C	2.66795400	6.86381100	-0.65516300
C	1.68163000	5.90212200	-0.52978800
H	3.71883300	3.18245500	-0.43804900
H	4.76796000	7.32898900	-0.81003700
H	0.63182600	6.16761500	-0.49345400
Cl	0.86265600	3.33931700	-0.29169200
N	2.26580100	8.28062000	-0.73133500
H	2.60329900	8.81288700	0.07787200
H	2.63331700	8.73319900	-1.57488500
C	5.81199100	4.79779300	-0.67753700
O	6.17834400	3.65470500	-0.60596400
O	6.64234600	5.83438400	-0.81136100
H	7.55180100	5.50293100	-0.84091500
H	1.24688500	8.38200700	-0.75505300

Cation-Anion-Cl DMSO

N	-2.20285300	-1.20929200	0.37663600
H	-1.28172000	-1.00154500	0.00104600
C	-3.07150300	-0.08172900	0.03818700
C	-2.29991400	1.25283700	-0.01162000
H	-3.54965500	-0.18837200	-0.94512800
H	-3.87432100	0.02008300	0.77197000
O	-1.05188200	1.19034600	-0.09969600
H	-2.52968900	-2.06153700	-0.06356600
O	-3.00233600	2.29047800	0.00654300
C	2.06735100	4.58715400	-0.46696400
C	3.40620400	4.22823800	-0.51242200
C	4.37714900	5.21911200	-0.62870000
C	4.02416300	6.56316800	-0.69993100
C	2.67857000	6.87943900	-0.64951000
C	1.68528300	5.92335100	-0.53554100
H	3.70337000	3.18841600	-0.46031400
H	4.78152500	7.33107500	-0.79365800
H	0.63736500	6.19620900	-0.50109100
Cl	0.84831700	3.36248700	-0.32735700
N	2.28790400	8.29907800	-0.71788600
H	2.62417800	8.82326000	0.09711300
H	2.66506900	8.75466000	-1.55558200
C	5.80864500	4.79155300	-0.67807700
O	6.16653800	3.64483400	-0.61461800
O	6.64631200	5.82271000	-0.80118800
H	7.55388600	5.48602900	-0.83105500
H	1.27017500	8.40956500	-0.74801700

Cation-Anion-Cl Water

N	-2.20699100	-1.21372200	0.37467400
H	-1.28761700	-1.01054400	-0.00753600
C	-3.07502100	-0.08553300	0.03684300
C	-2.30328400	1.24880200	-0.00948600
H	-3.55199100	-0.19039700	-0.94728100
H	-3.87875100	0.01461400	0.76983100
O	-1.05516500	1.18680800	-0.09674200
H	-2.53898200	-2.06687600	-0.06002300
O	-3.00547400	2.28675200	0.01016800
C	2.06905800	4.59041000	-0.46595800
C	3.40768300	4.23073100	-0.50795100
C	4.37900800	5.22113700	-0.62517700
C	4.02631600	6.56497600	-0.70075500
C	2.68076300	6.88201700	-0.65348500
C	1.68707700	5.92635200	-0.53876500
H	3.70444300	3.19100100	-0.45234600
H	4.78394500	7.33248100	-0.79510900
H	0.63920800	6.19963900	-0.50688000
Cl	0.84958400	3.36567800	-0.32518900
N	2.29107500	8.30147200	-0.72611600
H	2.62849800	8.82804600	0.08688200
H	2.66806400	8.75411900	-1.56548200
C	5.81051400	4.79326700	-0.67025900
O	6.16797800	3.64651700	-0.60251500
O	6.64850900	5.82372900	-0.79458400
H	7.55622300	5.48713300	-0.82141800
H	1.27346100	8.41299600	-0.75576900

Cation-Anion-Br Vacuum ModRedundant

N	-2.45363900	-0.99222700	-0.03795400
H	-1.59167600	-1.05749300	0.49779900
C	-2.89676900	0.39752100	0.05198600
C	-1.80832700	1.48109700	-0.10767300
H	-3.67442500	0.58792700	-0.69089000
H	-3.36227200	0.56322200	1.02901700
O	-0.60948000	1.06520100	-0.08075800
H	-2.15387800	-1.16467000	-0.99280800
O	-2.19170700	2.65458100	-0.22094600
C	2.17045400	4.35974700	-0.44692600
C	3.56092500	4.17130900	-0.44533800
C	4.43661100	5.24351700	-0.56343100
C	3.96344400	6.55342100	-0.68655400
C	2.59380200	6.70595000	-0.68527600
C	1.69305900	5.66462900	-0.57228800
H	3.97039900	3.17162300	-0.35213800
H	4.65358500	7.38397900	-0.77624400
H	0.61867800	5.83318100	-0.57675600
N	2.02482200	8.08062800	-0.79715400
H	2.75046400	8.75738700	-1.04693200
H	1.29772100	8.11292000	-1.51881600
C	5.90462500	4.96379500	-0.55816300
O	6.38832200	3.87485300	-0.45905800
O	6.63868800	6.08900800	-0.67889700
H	7.56986300	5.82837300	-0.66765600

H	1.60133400	8.37858600	0.08757600
Br	0.95418300	2.91703600	-0.28769000

A 15 10 7 120.0 F

D 15 10 7 4 0.0 F

Cation-Anion-Br TCM

N	-2.39157800	-1.07225200	0.38093000
H	-1.42914300	-0.99378900	0.06025600
C	-3.02644400	0.21809000	0.10664000
C	-2.00124600	1.34601400	-0.15066900
H	-3.67160000	0.19126100	-0.77999400
H	-3.65470100	0.53250400	0.94420300
O	-0.81208000	0.99396700	-0.35136200
H	-2.83016900	-1.81397800	-0.15080200
O	-2.45873500	2.50751600	-0.15837700
C	2.25436300	4.46972100	-0.54524600
C	3.62592100	4.24239400	-0.55907600
C	4.50924400	5.31742200	-0.62115100
C	4.04227700	6.62805900	-0.66934900
C	2.67254600	6.81575300	-0.65500900
C	1.76555900	5.77401600	-0.59489900
H	4.02012800	3.23434100	-0.52221600
H	4.73296500	7.46080700	-0.71819100
H	0.69656000	5.95467300	-0.58726400
N	2.15117900	8.19824600	-0.71391800
H	2.50696500	8.76994900	0.05913100
H	2.41129900	8.66220900	-1.59084100
C	5.97446900	5.02086500	-0.63798100
O	6.43545500	3.91304200	-0.60088400
O	6.72020700	6.13085700	-0.70070600
H	7.65299800	5.87157300	-0.70986600
H	1.12874900	8.21159600	-0.65546600
Br	1.02361600	3.04024400	-0.46186100

Cation-Anion-Br DCE

N	-2.24272700	-1.18790800	0.28684400
H	-1.29374700	-0.98702500	-0.01713500
C	-3.03703800	0.01332700	0.02842500
C	-2.18297600	1.29876400	0.05882600
H	-3.52283600	0.00162300	-0.95666300
H	-3.83036200	0.12208500	0.77184200
O	-0.93958800	1.15581900	-0.03348200
H	-2.58241100	-1.97170300	-0.25764600
O	-2.81550600	2.37404700	0.14046400
C	2.16777500	4.63407800	-0.45522600
C	3.51729900	4.30800100	-0.49537100
C	4.46923300	5.31559200	-0.62972800
C	4.09046600	6.65131600	-0.72459700
C	2.73819500	6.93820400	-0.68004600
C	1.76459000	5.96387500	-0.54902700
H	3.84234800	3.27761400	-0.42296000
H	4.83403600	7.43153800	-0.82920100
H	0.71212600	6.22091600	-0.51843300

N	2.31467100	8.34972900	-0.77072200
H	2.66521400	8.90030200	0.02029300
H	2.65350800	8.79219000	-1.63135800
C	5.90947000	4.91733100	-0.66779000
O	6.29302500	3.78135300	-0.58432700
O	6.72686100	5.96559700	-0.80521100
H	7.64022200	5.64467700	-0.82525200
H	1.29399600	8.43543400	-0.76978100
Br	0.86296200	3.27832400	-0.26670400

Cation-Anion-Br Acetone

N	-2.25822200	-1.12108700	0.53734500
H	-1.27296700	-0.88558500	0.45596200
C	-3.01090500	-0.06302700	-0.13659400
C	-2.28791300	1.29810600	-0.07642100
H	-3.17573100	-0.26630300	-1.20342200
H	-3.99660300	0.06019300	0.31829800
O	-1.06849100	1.28261700	0.21753200
H	-2.40069500	-2.01395000	0.07989700
O	-2.98157200	2.29956500	-0.36189600
C	2.14299300	4.68442400	-0.38623900
C	3.47785200	4.32067700	-0.49893200
C	4.44893000	5.30454000	-0.66974900
C	4.10195000	6.65084000	-0.72864500
C	2.76224800	6.97441200	-0.61333100
C	1.77016400	6.02475700	-0.44412900
H	3.77696500	3.28079500	-0.45708100
H	4.85943100	7.41287800	-0.86240300
H	0.72848200	6.31028600	-0.35838500
N	2.37481800	8.39653000	-0.66956600
H	2.77898400	8.92835500	0.10850700
H	2.68400600	8.83949000	-1.54133700
C	5.87343100	4.86800900	-0.79070600
O	6.22830900	3.71989800	-0.74290900
O	6.71037100	5.89458800	-0.95884400
H	7.61320900	5.55183700	-1.03149400
H	1.35832700	8.51115600	-0.61797600
Br	0.81143200	3.36109700	-0.15145100

Cation-Anion-Br DMSO

N	-2.20811200	-1.18621700	0.38635600
H	-1.25139900	-0.96759900	0.12299300
C	-3.04568200	-0.07104400	-0.05510600
C	-2.30469000	1.27880800	0.01661300
H	-3.38290500	-0.17157200	-1.09601500
H	-3.94335000	0.00288500	0.56300800
O	-1.05335800	1.23995400	0.09514100
H	-2.47004200	-2.04277000	-0.08775800
O	-3.02302500	2.30213200	-0.04567400
C	2.15410900	4.69606800	-0.40744300
C	3.49168800	4.33376700	-0.48142400
C	4.46386200	5.31815700	-0.64270100
C	4.11442400	6.66209100	-0.73060200
C	2.77159900	6.98416100	-0.65163700

C	1.77820200	6.03373200	-0.49334100
H	3.79230600	3.29562600	-0.41643600
H	4.87224900	7.42484800	-0.85747700
H	0.73407700	6.31770600	-0.43756200
N	2.38317700	8.40372900	-0.73613800
H	2.76895200	8.94761500	0.04304300
H	2.71154800	8.83473600	-1.60671800
C	5.89213400	4.88423400	-0.71905200
O	6.24817600	3.73754700	-0.64406900
O	6.73046800	5.90998300	-0.87978900
H	7.63598600	5.56935500	-0.92395200
H	1.36580600	8.51836700	-0.70891800
Br	0.82260200	3.36880200	-0.18930800

Cation-Anion-Br Water

N	-2.15734100	-1.19530300	0.28945200
H	-1.19951600	-0.91706200	0.09597500
C	-3.01945400	-0.07513900	-0.08688700
C	-2.33921500	1.28808500	0.14700300
H	-3.30420600	-0.08852100	-1.14806200
H	-3.94662600	-0.09317500	0.49037600
O	-1.09229200	1.28864900	0.28314900
H	-2.36052400	-2.01122200	-0.27645300
O	-3.09559800	2.28581700	0.14526200
C	2.13420800	4.71427100	-0.34743400
C	3.46647800	4.33466300	-0.43102300
C	4.44596600	5.30304700	-0.63615500
C	4.10815400	6.64716600	-0.76063300
C	2.77063800	6.98663000	-0.67117800
C	1.76990400	6.05245800	-0.46619900
H	3.75657400	3.29542800	-0.34128200
H	4.87174200	7.39737900	-0.92251200
H	0.72981900	6.34815300	-0.40002100
N	2.39812700	8.40783300	-0.78728500
H	2.64745200	8.93413600	0.05728100
H	2.86748300	8.85830700	-1.57957000
C	5.86844400	4.85203200	-0.72097000
O	6.21364500	3.70391900	-0.62028300
O	6.71461400	5.86420300	-0.92019800
H	7.61626500	5.51369600	-0.96654000
H	1.39074500	8.52414100	-0.93046800
Br	0.79332000	3.40551000	-0.07931100

Cation-Anion-I Vacuum

N	-2.38568300	-0.88249100	0.47628200
H	-1.37976800	-0.83446900	0.34143700
C	-2.95802000	0.34214700	-0.07727000
C	-1.93055900	1.47737500	-0.21654600
H	-3.37745000	0.20774000	-1.08306200
H	-3.76446100	0.72199300	0.55469800
O	-0.70533400	1.11116900	-0.15652200
H	-2.73031900	-1.70097300	-0.00800900
O	-2.34774200	2.61957600	-0.39766600
C	2.36875400	4.50040400	-0.49238400

C	3.75756900	4.33537200	-0.56009600
C	4.62323300	5.42237800	-0.64923000
C	4.13214900	6.72985300	-0.67630900
C	2.76116800	6.86563000	-0.61093300
C	1.87743000	5.80629600	-0.52173400
H	4.18803800	3.33978100	-0.53973100
H	4.80899400	7.57358800	-0.74413900
H	0.80316800	5.97395600	-0.47201300
N	2.17920100	8.24014500	-0.66397800
H	2.85350300	8.93792300	-0.33944400
H	1.89359300	8.48915200	-1.61605800
C	6.09218900	5.16184900	-0.71230500
O	6.59275500	4.07557300	-0.70172600
O	6.81268800	6.30124100	-0.78512800
H	7.74506300	6.04841500	-0.82444800
H	1.35066000	8.29625500	-0.06395700
I	0.91690700	2.87625600	-0.33953300

Cation-Anion-I TCM

N	-2.33045100	-1.07640000	0.48056700
H	-1.33550700	-0.95697900	0.31126200
C	-3.00359100	0.10068900	-0.06684300
C	-2.08989700	1.34113800	-0.09704400
H	-3.34116300	-0.04021500	-1.10248400
H	-3.88711500	0.35538400	0.52311600
O	-0.85084000	1.12542300	0.01560000
H	-2.62767500	-1.91931900	0.00429900
O	-2.64339700	2.44169800	-0.26486800
C	2.29230300	4.71070700	-0.45629800
C	3.65133700	4.42149900	-0.53857100
C	4.58966200	5.44321600	-0.67095700
C	4.19162700	6.77613900	-0.72360200
C	2.83671600	7.03609800	-0.64119900
C	1.88218200	6.04242800	-0.50942200
H	4.00308000	3.39726700	-0.50190000
H	4.92263900	7.56847800	-0.82705100
H	0.82828800	6.29270300	-0.44906500
N	2.38738500	8.44578100	-0.69272500
H	2.73670500	8.98284100	0.10778400
H	2.70787100	8.91384400	-1.54675500
C	6.03319400	5.06865400	-0.75823600
O	6.43973700	3.93922100	-0.71886900
O	6.83365900	6.13520100	-0.88753500
H	7.74860600	5.82391300	-0.94213400
H	1.36519300	8.50910500	-0.67890400
I	0.83717700	3.15762200	-0.24797100

Cation-Anion-I DCE

N	-2.26574900	-1.17663100	0.26472500
H	-1.33402400	-1.02859000	-0.11269500
C	-3.02230200	0.05584900	0.04732300
C	-2.12205000	1.30571800	0.06344100
H	-3.54003500	0.07818900	-0.92158500
H	-3.78566100	0.18283700	0.81816400

O	-0.88774000	1.11089500	-0.09982500
H	-2.68342600	-1.95032600	-0.23874800
O	-2.69282400	2.40498100	0.19863400
C	2.29091900	4.74720000	-0.49616100
C	3.64783300	4.44399300	-0.52388000
C	4.59624600	5.45829000	-0.64102900
C	4.20813600	6.79154200	-0.73299500
C	2.85312800	7.06446200	-0.70269000
C	1.88804200	6.07831100	-0.58765500
H	3.99031100	3.41859000	-0.45417100
H	4.94589700	7.57894600	-0.82439000
H	0.83514300	6.33739900	-0.56791400
N	2.41836500	8.47375200	-0.79214200
H	2.75745800	9.02468900	0.00335400
H	2.76025800	8.92222700	-1.64825500
C	6.03953900	5.07376600	-0.66397200
O	6.43527700	3.94127700	-0.58320300
O	6.85043100	6.13034400	-0.78479000
H	7.76618400	5.81611600	-0.79480800
H	1.39713500	8.55026000	-0.79957200
I	0.83123300	3.20204700	-0.30496800

Cation-Anion-I Acetone

N	-2.33038500	-1.10543000	0.56802400
H	-1.33699600	-0.98404200	0.39337200
C	-3.02643900	-0.00022000	-0.08999500
C	-2.18753500	1.29115100	-0.10904100
H	-3.27158200	-0.20971200	-1.14032200
H	-3.96815100	0.21895100	0.41827200
O	-0.95285100	1.16733100	0.10385300
H	-2.60722300	-1.99408500	0.16737500
O	-2.79880000	2.34665300	-0.37051100
C	2.27965100	4.79103000	-0.44135500
C	3.62345300	4.45593200	-0.55733200
C	4.58690200	5.45201800	-0.70532200
C	4.22530600	6.79530900	-0.73865000
C	2.88153500	7.09893000	-0.62220300
C	1.90146400	6.13181700	-0.47488400
H	3.94389100	3.42139900	-0.53644100
H	4.97394100	7.56886800	-0.85395600
H	0.85840900	6.41413100	-0.38778500
N	2.47660800	8.51829200	-0.65025000
H	2.82587500	9.02727900	0.16856700
H	2.82780000	8.99801900	-1.48571500
C	6.01598200	5.03533500	-0.83118900
O	6.38699300	3.89117100	-0.80495500
O	6.84246300	6.07472800	-0.97814000
H	7.74861200	5.74235300	-1.05618900
H	1.45728100	8.61648800	-0.65404700
I	0.80152000	3.27244100	-0.21098400

Cation-Anion-I DMSO

N	-2.27466400	-1.16797700	0.43165700
H	-1.30741400	-1.03896700	0.14991800

C	-3.03146300	-0.01417600	-0.05272000
C	-2.20629200	1.28504500	-0.01464600
H	-3.36522100	-0.12299500	-1.09405100
H	-3.92742700	0.13802700	0.55301700
O	-0.95712800	1.16100300	0.07202500
H	-2.60857400	-2.02204800	-0.00003100
O	-2.84604200	2.35278800	-0.11042500
C	2.27971900	4.80266300	-0.44591500
C	3.62556900	4.46655200	-0.52476900
C	4.59044600	5.46149400	-0.67124700
C	4.22740500	6.80278400	-0.74059700
C	2.88109300	7.10726400	-0.65985600
C	1.89931700	6.14127400	-0.51525100
H	3.94675600	3.43334400	-0.47499700
H	4.97688700	7.57555600	-0.85543800
H	0.85427200	6.42358800	-0.45752200
N	2.47689900	8.52460100	-0.72628300
H	2.83304500	9.05711700	0.07446000
H	2.82311400	8.97861500	-1.57803000
C	6.02270600	5.04528800	-0.75383300
O	6.39409300	3.90191700	-0.69769800
O	6.85100600	6.08275700	-0.89796200
H	7.75950900	5.75127200	-0.94811300
H	1.45782600	8.62512700	-0.72539600
I	0.80228800	3.28422200	-0.21610000

Cation-Anion-I Water

N	-2.27474800	-1.17093300	0.43103700
H	-1.30869700	-1.04355400	0.14454600
C	-3.03324200	-0.01813100	-0.05316500
C	-2.21142500	1.28291600	-0.01009400
H	-3.36391600	-0.12573200	-1.09565400
H	-3.93126600	0.13001500	0.55048400
O	-0.96209800	1.16215400	0.07687000
H	-2.61108900	-2.02584100	0.00276500
O	-2.85391600	2.34956000	-0.10279800
C	2.28052900	4.80573300	-0.44427200
C	3.62577300	4.46811000	-0.52480000
C	4.59116100	5.46236300	-0.67261900
C	4.22895900	6.80385000	-0.74167700
C	2.88304200	7.10972600	-0.65924700
C	1.90068300	6.14448900	-0.51316100
H	3.94608500	3.43463600	-0.47542000
H	4.97880200	7.57605800	-0.85761500
H	0.85598800	6.42765300	-0.45402500
N	2.48034300	8.52723400	-0.72579300
H	2.84047500	9.06032000	0.07279700
H	2.82384600	8.97979900	-1.57943800
C	6.02298800	5.04510500	-0.75708400
O	6.39345800	3.90127700	-0.70131200
O	6.85175300	6.08175200	-0.90240900
H	7.76009100	5.74994400	-0.95372400
H	1.46146000	8.62940300	-0.72102000
I	0.80268500	3.28823000	-0.21297800

H	7.55237600	5.63747800	-0.78660800

Neutral-Anion-Cl Vacuum ModRedundant

N	-2.52604100	-1.11555300	-0.01728100
H	-1.62038000	-1.08421200	0.45019400
C	-3.02131200	0.26584200	0.04437000
C	-1.93670400	1.37515900	-0.08196400
H	-3.77789300	0.42772900	-0.72707600
H	-3.52220100	0.42239100	1.00614700
O	-0.74884700	0.98886500	0.03944600
H	-2.27256800	-1.30102300	-0.98384500
O	-2.36869900	2.52965700	-0.25868500
C	2.16271400	4.36686400	-0.34778400
C	3.52978600	4.10342600	-0.39631300
C	4.41341800	5.16797800	-0.54872600
C	3.96125400	6.48258200	-0.65151000
C	2.59135500	6.73941300	-0.60271700
C	1.70091900	5.67492800	-0.44786100
H	3.90361600	3.09092500	-0.32155500
H	4.66964500	7.29399500	-0.76280100
H	0.63158500	5.85362600	-0.40732000
Cl	1.02747300	3.07664400	-0.18092300
N	2.11257000	8.05564200	-0.65449400
H	2.70451500	8.69196800	-1.16770400
H	1.14897800	8.13158700	-0.94658200
C	5.86445200	4.85729800	-0.60105900
O	6.35101100	3.76118400	-0.51044900
O	6.64157900	5.95616400	-0.76797500

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Neutral-Anion-Cl TCM

N	-2.32213900	-1.26736000	0.10802000
H	-1.61382700	-1.06056600	0.80838700
C	-3.12611500	-0.05422600	-0.04942300
C	-2.35389900	1.28934000	-0.07309800
H	-3.71933100	-0.12492700	-0.96337500
H	-3.84246900	0.00899600	0.77649600
O	-1.14795000	1.25848000	0.25823000
H	-1.78775100	-1.40662400	-0.74462700
O	-3.03151100	2.29096600	-0.39990000
C	2.15177100	4.57612200	-0.33114300
C	3.48262000	4.19569300	-0.42944500
C	4.43761600	5.19574000	-0.60466300
C	4.08034600	6.53804500	-0.68034400
C	2.73487600	6.90687800	-0.57965700
C	1.77006100	5.90855400	-0.40233200
H	3.77792900	3.15662900	-0.37496100
H	4.84163100	7.29625700	-0.81453100
H	0.72186500	6.17124200	-0.31965900
Cl	0.92266700	3.36371500	-0.11710800
N	2.36444600	8.24646300	-0.59547300
H	3.00841300	8.86733600	-1.06354400
H	1.40563300	8.42771800	-0.85551200

C	5.86268900	4.77541000	-0.70975200
O	6.24733300	3.63542100	-0.64673700
O	6.70550700	5.80680400	-0.88572000
H	7.60218600	5.44845500	-0.94120500

Neutral-Anion-Cl DCE

N	-2.28465200	-1.15140400	0.52952500
H	-1.34624900	-0.96254700	0.18533000
C	-3.12650100	-0.04109000	0.07980900
C	-2.30667500	1.23005000	-0.24123600
H	-3.68536300	-0.27707200	-0.83472700
H	-3.86485200	0.22295100	0.84149200
O	-1.06769100	1.09504200	-0.35730200
H	-2.58991800	-2.02703800	0.12208700
O	-2.97224900	2.28161700	-0.38258400
C	2.16104000	4.59436600	-0.56297900
C	3.49514400	4.21912000	-0.61201400
C	4.45545100	5.22945100	-0.62739700
C	4.09834300	6.57299100	-0.59398100
C	2.74699800	6.93523100	-0.54494300
C	1.77589200	5.92665700	-0.52898800
H	3.78924700	3.17864300	-0.63787000
H	4.86295400	7.33954000	-0.60495700
H	0.72385300	6.18379700	-0.48873100
Cl	0.92684700	3.36083600	-0.54097200
N	2.37498500	8.26878600	-0.45247500
H	3.04872800	8.93456000	-0.80255900
H	1.43470700	8.48232500	-0.75244200
C	5.88657100	4.81726100	-0.68366100
O	6.26625600	3.67364000	-0.71940200
O	6.73407800	5.85609100	-0.69138800
H	7.63565600	5.50675600	-0.72871000

Neutral-Anion-Cl Acetone

N	-2.28719200	-1.15062600	0.54468500
H	-1.37834000	-1.03239700	0.10496500
C	-3.13151000	-0.04671900	0.08651200
C	-2.31005500	1.21439000	-0.25877300
H	-3.69972500	-0.29149400	-0.82093600
H	-3.86119000	0.22601100	0.85278300
O	-1.07746500	1.06735400	-0.42066000
H	-2.66183300	-2.04246700	0.24320900
O	-2.96696900	2.27514400	-0.37776200
C	2.17054800	4.60250900	-0.57744900
C	3.50441000	4.22751600	-0.62246800
C	4.46365000	5.23923100	-0.62816100
C	4.10487100	6.58185000	-0.58892700
C	2.75259400	6.94328100	-0.54372900
C	1.78211900	5.93339800	-0.53800500
H	3.79947200	3.18749700	-0.65297200
H	4.86843500	7.34949900	-0.59281500
H	0.72977600	6.18987200	-0.50175700
Cl	0.93786700	3.36496000	-0.56804100
N	2.37951900	8.27473900	-0.44495800

H	3.05612200	8.94489400	-0.78099700
H	1.44106000	8.49173900	-0.74814500
C	5.89572800	4.82828000	-0.68065400
O	6.27450200	3.68415200	-0.72052100
O	6.74151300	5.86691600	-0.67963100
H	7.64469400	5.52103000	-0.71587000

Neutral-Anion-Cl DMSO

N	-2.27645000	-1.27870800	0.08228700
H	-1.40747300	-1.01166300	-0.37188700
C	-3.14132300	-0.09847400	0.08477600
C	-2.33499300	1.21433200	0.16761500
H	-3.75663100	-0.01607600	-0.82164600
H	-3.82867600	-0.12647100	0.93333300
O	-1.11536900	1.15705100	-0.10918700
H	-2.68954000	-2.02798700	-0.46070100
O	-2.99020600	2.23763300	0.47590900
C	2.17420500	4.62963400	-0.47232800
C	3.50634300	4.24707600	-0.45477800
C	4.47053700	5.24968900	-0.55324400
C	4.11773000	6.58956600	-0.66505300
C	2.76652100	6.95892900	-0.67949700
C	1.79108700	5.95813600	-0.58116800
H	3.79679700	3.20905200	-0.36874000
H	4.88541000	7.34932900	-0.74181300
H	0.73952000	6.22010900	-0.58988300
Cl	0.93527800	3.40399600	-0.35670300
N	2.39932200	8.29422300	-0.72937300
H	3.08344400	8.92179400	-1.12696200
H	1.46589000	8.48184400	-1.06611700
C	5.90137600	4.83061300	-0.53384300
O	6.27347400	3.68786400	-0.43366800
O	6.75187300	5.85904400	-0.63949600
H	7.65445200	5.51002200	-0.61891200

Neutral-Anion-Cl Water

N	-2.29032300	-1.15092200	0.55848400
H	-1.40407000	-1.07544000	0.06712500
C	-3.13770300	-0.05225000	0.09440100
C	-2.31706200	1.19852000	-0.28270800
H	-3.72072300	-0.30885700	-0.80063800
H	-3.85440200	0.23358100	0.86777000
O	-1.08954800	1.04309900	-0.47392800
H	-2.69856100	-2.04719000	0.31985200
O	-2.96872300	2.26372900	-0.39778700
C	2.17825200	4.60905200	-0.58726700
C	3.51172600	4.23392800	-0.63040800
C	4.47029400	5.24656200	-0.62890800
C	4.11047300	6.58846800	-0.58428500
C	2.75762000	6.94952200	-0.54081100
C	1.78748800	5.93890600	-0.54268800
H	3.80740300	3.19427500	-0.66521200
H	4.87332800	7.35682500	-0.58308200
H	0.73497300	6.19495400	-0.50873900

Cl	0.94616000	3.36901800	-0.58748200
N	2.38401500	8.27952600	-0.43599200
H	3.06206500	8.95252700	-0.76356800
H	1.44660200	8.49899200	-0.74082400
C	5.90301200	4.83632400	-0.67975800
O	6.28075600	3.69170800	-0.72323400
O	6.74761700	5.87453800	-0.67262700
H	7.65193100	5.53116300	-0.70876500

Neutral-Anion-Br Vacuum

N	-2.45601300	-1.11453800	-0.05040300
H	-1.56639400	-1.05505600	0.44347000
C	-3.02617200	0.23514000	0.03682400
C	-2.00873800	1.40653400	-0.05542900
H	-3.78456400	0.37240400	-0.73736300
H	-3.54203000	0.34256200	0.99734900
O	-0.79990600	1.08554000	0.08445300
H	-2.16991600	-1.25973500	-1.01462700
O	-2.49592900	2.53673400	-0.22516200
C	2.25367900	4.48856300	-0.34706500
C	3.61872400	4.21484700	-0.39343900
C	4.51245200	5.27038400	-0.55739200
C	4.07096300	6.58750600	-0.67490100
C	2.70347100	6.85642400	-0.62933400
C	1.80414200	5.80025000	-0.46212400
H	3.98924600	3.20190100	-0.30758700
H	4.78599400	7.39200400	-0.79476700
H	0.73759300	5.99620700	-0.42364900
N	2.23611700	8.17690900	-0.69550600
H	2.83307700	8.80128400	-1.21770800
H	1.27355100	8.25691600	-0.99006500
C	5.96087800	4.94843200	-0.60589100
O	6.44018100	3.84986800	-0.50440700
O	6.74685800	6.03991400	-0.78290800
H	7.65498500	5.71360300	-0.79696100
Br	0.98216300	3.09748300	-0.14629000

Neutral-Anion-Br TCM

N	-2.33023900	-1.24463000	0.08496600
H	-1.51234700	-1.09942600	0.67115000
C	-3.08303700	0.00976200	0.07831200
C	-2.27148000	1.30853200	-0.15459500
H	-3.86575900	-0.04276500	-0.68240600
H	-3.59683400	0.12342700	1.03809800
O	-1.02397900	1.20025600	-0.19795900
H	-1.93894500	-1.38127900	-0.84269600
O	-2.95137300	2.35415800	-0.25827600
C	2.22681200	4.65200600	-0.42544800
C	3.56593500	4.28710000	-0.47388100
C	4.51978600	5.29671700	-0.59411600
C	4.15467800	6.63740400	-0.66469600
C	2.80331400	6.99335300	-0.61402400
C	1.84034500	5.98415700	-0.49159600
H	3.87301200	3.25110300	-0.42336200

H	4.91431100	7.40341000	-0.75820800
H	0.78873400	6.24434700	-0.45016300
N	2.42197000	8.33091900	-0.62564400
H	3.07740600	8.96176700	-1.06388900
H	1.47287600	8.50616000	-0.92301900
C	5.95133000	4.89004100	-0.64778600
O	6.34403900	3.75218100	-0.59412000
O	6.79230400	5.93178500	-0.76475800
H	7.69307900	5.58069600	-0.79133300
Br	0.88847400	3.31090000	-0.28143000

Neutral-Anion-Br DCE

N	-2.28314000	-1.16923700	0.34581900
H	-1.31007400	-0.93815800	0.16190700
C	-3.07679100	-0.00823000	-0.06067800
C	-2.26161900	1.30416800	-0.03083200
H	-3.46663800	-0.09597200	-1.08301600
H	-3.93975600	0.12281700	0.59704600
O	-1.01489500	1.19877000	0.04272700
H	-2.51675400	-1.98177000	-0.21233300
O	-2.93017600	2.35863600	-0.11230500
C	2.23955200	4.69222800	-0.36705600
C	3.57282600	4.31496900	-0.44733000
C	4.52935700	5.31744600	-0.60513200
C	4.17069200	6.65898800	-0.68104700
C	2.82299100	7.02625900	-0.59798300
C	1.85646800	6.02455600	-0.43851500
H	3.87413900	3.27760800	-0.39295200
H	4.93179500	7.41940900	-0.80365600
H	0.80845300	6.29298200	-0.37174200
N	2.45175000	8.36407700	-0.61278200
H	3.10347900	8.99034700	-1.06315900
H	1.49712800	8.54797400	-0.88649100
C	5.95704000	4.89928600	-0.69259200
O	6.33898700	3.75735500	-0.63310600
O	6.79967600	5.93113600	-0.84715300
H	7.69957100	5.57865000	-0.89444600
Br	0.90035400	3.35778600	-0.16407300

Neutral-Anion-Br Acetone

N	-2.22014800	-1.18720800	0.30163000
H	-1.27533700	-0.93053500	0.02833100
C	-3.08410900	-0.05316900	-0.02808600
C	-2.32664400	1.29120800	0.00770500
H	-3.51879900	-0.12545600	-1.03396200
H	-3.91895100	0.01496500	0.67363100
O	-1.07429200	1.24208900	-0.00562600
H	-2.48232900	-2.00881000	-0.23024100
O	-3.04210500	2.31842000	0.01534800
C	2.23199600	4.72432800	-0.39128000
C	3.56083300	4.33021500	-0.45390100
C	4.53059000	5.32202300	-0.60037400
C	4.18809400	6.66718600	-0.68186200
C	2.84335500	7.05074200	-0.61644100

C	1.86318200	6.06003300	-0.46881800
H	3.84917800	3.28955400	-0.39418700
H	4.95904800	7.41897800	-0.79611300
H	0.81768900	6.34079300	-0.41585600
N	2.48856600	8.39160600	-0.63623900
H	3.15510900	9.01217500	-1.07277300
H	1.54011100	8.58912300	-0.92165200
C	5.95470200	4.88663600	-0.66865900
O	6.32001600	3.73914500	-0.60478500
O	6.81074700	5.90739400	-0.81029400
H	7.70806200	5.54657100	-0.84662300
Br	0.87585200	3.40407200	-0.19975200

Neutral-Anion-Br DMSO

N	-2.17723000	-1.14502600	0.25240100
H	-1.20591600	-0.84719400	0.23833000
C	-2.98427400	-0.01298500	-0.20315800
C	-2.37942600	1.34068600	0.21983800
H	-3.08348800	0.03260700	-1.29662500
H	-3.99554900	-0.07445600	0.20474900
O	-1.17224100	1.34841500	0.55625700
H	-2.26753700	-1.92998100	-0.38227700
O	-3.14849800	2.32750200	0.15405400
C	2.19632000	4.72380000	-0.30725400
C	3.51645200	4.30939900	-0.40407700
C	4.49220600	5.28425500	-0.61296500
C	4.16314600	6.63065300	-0.72212900
C	2.82595100	7.03383900	-0.62325900
C	1.83946900	6.06060400	-0.41302400
H	3.79409600	3.26747900	-0.32203200
H	4.93885900	7.36913100	-0.88210200
H	0.80018200	6.35653600	-0.33168100
N	2.48713600	8.37735300	-0.66984800
H	3.14786900	8.97832000	-1.14119300
H	1.53253100	8.58067200	-0.92979900
C	5.90818700	4.82814000	-0.71518100
O	6.25951000	3.67727000	-0.63323500
O	6.77127700	5.83307400	-0.90924500
H	7.66342800	5.46144800	-0.96390400
Br	0.83195400	3.43053900	-0.01352000

Neutral-Anion-Br Water

N	-2.22235900	-1.18651200	0.31715900
H	-1.28696000	-0.96021300	-0.00863400
C	-3.08931800	-0.06260300	-0.03683000
C	-2.34229100	1.28565600	0.00428000
H	-3.50590000	-0.14361900	-1.05022400
H	-3.93658400	0.00003300	0.64990900
O	-1.08957100	1.24714900	-0.00961200
H	-2.51737400	-2.03228900	-0.15683500
O	-3.06394200	2.30953800	0.01341500
C	2.23947500	4.73126800	-0.38955200
C	3.56749900	4.33591900	-0.45393700
C	4.53709700	5.32802200	-0.60138200

C	4.19457900	6.67301900	-0.68156800
C	2.84976600	7.05737100	-0.61389500
C	1.86942100	6.06653200	-0.46584800
H	3.85567900	3.29520600	-0.39537500
H	4.96520900	7.42493700	-0.79711800
H	0.82412200	6.34761700	-0.41202600
N	2.49564800	8.39756300	-0.63166800
H	3.16276300	9.01966300	-1.06534300
H	1.54713000	8.59697700	-0.91576100
C	5.96130200	4.89213100	-0.67249100
O	6.32488200	3.74379400	-0.60879300
O	6.81651700	5.91190300	-0.81614300
H	7.71457500	5.55278700	-0.85517000
Br	0.88305000	3.41022900	-0.19743600

Neutral-Anion-I Vacuum

N	-2.34305600	-1.15347100	0.04714600
H	-1.44190700	-1.03385200	0.50646800
C	-3.01245000	0.14571700	0.15722700
C	-2.11253300	1.39555400	-0.02135100
H	-3.82961100	0.20812600	-0.56482200
H	-3.47014300	0.22965200	1.14870900
O	-0.86788100	1.17306500	0.01975400
H	-2.08742000	-1.28277000	-0.92765800
O	-2.69118300	2.48086600	-0.15574700
C	2.32495800	4.68612800	-0.51802600
C	3.68502700	4.37993700	-0.53242700
C	4.61959700	5.40395000	-0.67407700
C	4.22348100	6.73489600	-0.80292100
C	2.86545600	7.04511200	-0.78790600
C	1.93067200	6.01395000	-0.64888000
H	4.03100500	3.35884200	-0.43301500
H	4.96532400	7.51551100	-0.91994900
H	0.87230000	6.25764600	-0.64215500
N	2.43613300	8.37038500	-0.96554200
H	1.50916800	8.54907300	-0.60666400
H	3.09332200	9.06284400	-0.63685400
C	6.05715300	5.03732100	-0.68147900
O	6.50133400	3.92351300	-0.58169400
O	6.88311800	6.10643400	-0.81539000
H	7.77980400	5.74995200	-0.80993300
I	0.83643600	3.15290300	-0.28213200

Neutral-Anion-I TCM

N	-2.34104300	-1.23529800	-0.02912200
H	-1.58221700	-1.15071100	0.64239700
C	-3.07684300	0.02839700	-0.01044900
C	-2.23323100	1.32523500	-0.02968000
H	-3.76634800	0.05962400	-0.85700400
H	-3.69670600	0.06782300	0.89114100
O	-0.99352500	1.19417300	0.13242800
H	-1.86699900	-1.31236000	-0.92432500
O	-2.87016600	2.38778300	-0.18234800
C	2.34246000	4.78539500	-0.38434300

C	3.68525000	4.42946400	-0.44127400
C	4.63942900	5.43405600	-0.60106900
C	4.27309700	6.77268900	-0.70424100
C	2.92273100	7.12699000	-0.64704900
C	1.96361200	6.11861200	-0.48375200
H	4.00378900	3.39806800	-0.36625700
H	5.03093600	7.53660100	-0.82672600
H	0.91475400	6.39122300	-0.43600700
N	2.53786500	8.46475800	-0.69125300
H	3.18595900	9.08169700	-1.15939800
H	1.58590500	8.62705400	-0.98721800
C	6.07001000	5.02706100	-0.65826700
O	6.46629900	3.89157100	-0.57834400
O	6.91016900	6.06585500	-0.81097100
H	7.81034100	5.71331600	-0.83645800
I	0.84257600	3.28221300	-0.14972800

Neutral-Anion-I DCE

N	-2.35847100	-1.09303200	0.53030400
H	-1.36793800	-0.86445100	0.51184900
C	-3.05568700	-0.01923700	-0.17878500
C	-2.25910300	1.30320700	-0.18225600
H	-3.24422100	-0.25700200	-1.23356800
H	-4.02790800	0.18176600	0.27853000
O	-1.05119500	1.23727100	0.15782100
H	-2.47881900	-1.97940700	0.05512100
O	-2.88481100	2.31836500	-0.55156100
C	2.35409200	4.83067600	-0.36320100
C	3.68675200	4.45579900	-0.48135800
C	4.64890900	5.45389500	-0.63747200
C	4.29856800	6.79974600	-0.67480100
C	2.95611400	7.17136900	-0.55423200
C	1.98760500	6.17016500	-0.39690900
H	3.99144100	3.41785800	-0.45798300
H	5.06177200	7.55844900	-0.79621600
H	0.94552500	6.45478100	-0.30218700
N	2.59155800	8.51268000	-0.52967900
H	3.23592700	9.14329700	-0.98483900
H	1.63299700	8.70494100	-0.78375400
C	6.07085900	5.02880000	-0.76616900
O	6.44827600	3.88373000	-0.73854800
O	6.91764600	6.05822500	-0.91974700
H	7.81346500	5.70006900	-0.99399500
I	0.84474800	3.33932700	-0.13567900

Neutral-Anion-I Acetone

N	-2.32364100	-1.10710800	0.51771400
H	-1.33412400	-0.88478600	0.45352300
C	-3.05010700	-0.05143700	-0.18782800
C	-2.31550800	1.30315400	-0.13166700
H	-3.19354500	-0.26799200	-1.25512800
H	-4.04392400	0.08809700	0.24390100
O	-1.10117000	1.27668600	0.18851900
H	-2.46766200	-2.00537300	0.07144300

O	-2.98976600	2.30761600	-0.44423000
C	2.35033900	4.85594000	-0.36127100
C	3.67786800	4.46679600	-0.48540100
C	4.64841000	5.45637200	-0.64581900
C	4.31034200	6.80513400	-0.68108000
C	2.97165900	7.19014100	-0.55459100
C	1.99405400	6.19798400	-0.39327700
H	3.97234400	3.42597300	-0.46331100
H	5.07973900	7.55700500	-0.80596800
H	0.95525600	6.49238900	-0.29406200
N	2.62076600	8.53374900	-0.52745800
H	3.27137100	9.16020600	-0.97965600
H	1.66350800	8.73783700	-0.77739800
C	6.06599000	5.01713900	-0.78166200
O	6.42986400	3.86724800	-0.75746100
O	6.92129500	6.03730400	-0.93710000
H	7.81434200	5.67288300	-1.01718800
I	0.83040200	3.37832900	-0.12286200

Neutral-Anion-I DMSO

N	-2.32091400	-1.16257600	0.38878300
H	-1.34839500	-1.01397800	0.13557300
C	-3.07941700	-0.00999900	-0.09694000
C	-2.26335000	1.29577600	-0.03478900
H	-3.39614300	-0.11300300	-1.14411300
H	-3.98593800	0.13018700	0.49601700
O	-1.01708700	1.18252100	0.07420400
H	-2.63033400	-2.01358100	-0.06645000
O	-2.91490100	2.35804700	-0.13537900
C	2.37397900	4.83060000	-0.40483400
C	3.71133100	4.46488600	-0.48609600
C	4.66751300	5.47122000	-0.62777000
C	4.30568200	6.81269100	-0.68699000
C	2.95670200	7.17418100	-0.60343200
C	1.99331200	6.16509900	-0.46086400
H	4.02448400	3.43021600	-0.44398900
H	5.06428900	7.57751700	-0.79787000
H	0.94670400	6.44076000	-0.39489900
N	2.58059700	8.51061500	-0.59913100
H	3.23228900	9.14619400	-1.03702200
H	1.62720500	8.69518800	-0.87737900
C	6.09686200	5.05826900	-0.71531600
O	6.48049500	3.91522400	-0.67177800
O	6.93682800	6.09323000	-0.84931700
H	7.83917200	5.74672700	-0.89966300
I	0.87713900	3.32527400	-0.18987300

Neutral-Anion-I Water

N	-2.32435900	-1.11584100	0.50468100
H	-1.33252300	-0.91452700	0.41544200
C	-3.04866300	-0.05755000	-0.19877200
C	-2.32458400	1.30000100	-0.11519300
H	-3.17631500	-0.26174500	-1.27076800
H	-4.04909400	0.06774600	0.22153600

O	-1.11282000	1.27900300	0.21422600
H	-2.49555600	-2.01678900	0.07319200
O	-3.00275400	2.30564000	-0.41875100
C	2.35340900	4.86133900	-0.36058200
C	3.68123200	4.47132100	-0.47492700
C	4.65160900	5.46106800	-0.63684700
C	4.31247900	6.80897900	-0.68295100
C	2.97257900	7.19432500	-0.56609400
C	1.99469900	6.20228700	-0.40348500
H	3.97625200	3.43096200	-0.44398000
H	5.08164300	7.56082600	-0.80924800
H	0.95519700	6.49645200	-0.31194200
N	2.62099400	8.53701400	-0.54910600
H	3.27490800	9.16245900	-0.99809500
H	1.66529700	8.74039700	-0.80564400
C	6.07061800	5.02197900	-0.76170500
O	6.43339000	3.87164100	-0.73054900
O	6.92564700	6.04135300	-0.91486600
H	7.82029700	5.67909000	-0.98835700
I	0.83452300	3.38385700	-0.11652800
H	-3.91923700	-0.33694700	0.73458800
O	-1.43071900	1.38401300	0.49414400
H	-1.67921400	-1.07888400	-0.99036800
O	-3.48239900	2.22244100	0.11867100
C	2.22808000	4.54367100	-0.31955100
C	3.56438600	4.18198200	-0.40649300
C	4.51493700	5.18517800	-0.60471100
C	4.11524900	6.51122500	-0.71536000
C	2.76549200	6.86466400	-0.63281400
C	1.81135200	5.86404700	-0.42867900
H	3.88089200	3.15083200	-0.32418500
H	4.87919700	7.26562000	-0.86683300
H	0.75853200	6.10964900	-0.35315900
Cl	1.00498300	3.31670600	-0.05742900
N	2.37472200	8.20926600	-0.69234400
H	3.02157400	8.80037600	-1.19552700
H	1.42722100	8.35406500	-1.01246200
C	6.01258000	4.83144100	-0.70149100
O	6.30015100	3.61930400	-0.61330000
O	6.79400700	5.79544300	-0.85773900

Anion-Anion-Cl Vacuum SP

N	-2.23769900	-1.21586300	-0.15293600
H	-1.57383700	-1.08203100	0.60593800
C	-3.20774900	-0.12318700	-0.06991900
C	-2.64194900	1.29522300	0.19998600
H	-3.79278600	-0.08742100	-0.99196200

Anion-Anion-Cl TCM

N	-2.23769900	-1.21586300	-0.15293600
H	-1.57383700	-1.08203100	0.60593800
C	-3.20774900	-0.12318700	-0.06991900
C	-2.64194900	1.29522300	0.19998600
H	-3.79278600	-0.08742100	-0.99196200

H	-3.91923700	-0.33694700	0.73458800
O	-1.43071900	1.38401300	0.49414400
H	-1.67921400	-1.07888400	-0.99036800
O	-3.48239900	2.22244100	0.11867100
C	2.22808000	4.54367100	-0.31955100
C	3.56438600	4.18198200	-0.40649300
C	4.51493700	5.18517800	-0.60471100
C	4.11524900	6.51122500	-0.71536000
C	2.76549200	6.86466400	-0.63281400
C	1.81135200	5.86404700	-0.42867900
H	3.88089200	3.15083200	-0.32418500
H	4.87919700	7.26562000	-0.86683300
H	0.75853200	6.10964900	-0.35315900
Cl	1.00498300	3.31670600	-0.05742900
N	2.37472200	8.20926600	-0.69234400
H	3.02157400	8.80037600	-1.19552700
H	1.42722100	8.35406500	-1.01246200
C	6.01258000	4.83144100	-0.70149100
O	6.30015100	3.61930400	-0.61330000
O	6.79400700	5.79544300	-0.85773900

H	-4.01605000	0.04286300	0.68137000
O	-1.10192900	1.09938600	0.09003000
H	-2.62195600	-2.01240600	-0.38074400
O	-2.99871300	2.29655900	0.02282200
C	2.19968200	4.59274300	-0.38330400
C	3.53496400	4.22367500	-0.45299900
C	4.49630200	5.22595300	-0.59533700
C	4.10877000	6.55851600	-0.66559100
C	2.75922800	6.92005500	-0.59723600
C	1.79367700	5.91849300	-0.45155100
H	3.83932900	3.18697300	-0.40038300
H	4.87711200	7.31512200	-0.77687400
H	0.74145100	6.17091800	-0.39187200
Cl	0.97073200	3.35506600	-0.20739100
N	2.38026000	8.26559800	-0.61243400
H	3.04029600	8.87682400	-1.07273400
H	1.43824500	8.43466600	-0.93695700
C	5.98926600	4.86001100	-0.67792700
O	6.26538700	3.64170200	-0.63606800
O	6.78784900	5.81766200	-0.77918700

Anion-Anion-Cl DCE

N	-2.40407400	-1.26740600	0.26976500
H	-1.42785800	-1.01636100	0.13187600
C	-3.18878900	-0.06674900	-0.02516100
C	-2.34530700	1.22818300	0.04325100
H	-3.63010500	-0.08723500	-1.02930000

Anion-Anion-Cl Acetone

N	-2.41425200	-1.25333400	0.36118200
H	-1.44805800	-1.06908400	0.10455400
C	-3.19242200	-0.07772900	-0.03193800
C	-2.35017700	1.21650800	-0.00940600
H	-3.59802600	-0.15416600	-1.04967900

H	-4.04330300	0.06384300	0.63867400
O	-1.10553500	1.08919700	0.01573100
H	-2.71694900	-2.07498800	-0.14863000
O	-3.00017700	2.28747500	-0.05062200
C	2.20655000	4.60288400	-0.42045900
C	3.54129800	4.23275400	-0.48815400
C	4.50421000	5.23694100	-0.60412600
C	4.11871900	6.57111800	-0.64910200
C	2.76865100	6.93347900	-0.58093000
C	1.80097800	5.92944200	-0.46361800
H	3.84341900	3.19469200	-0.45421600
H	4.88661500	7.33066600	-0.74064700
H	0.74866400	6.18212800	-0.40693200
Cl	0.97673900	3.36023700	-0.27978400
N	2.39219500	8.27751300	-0.56778400
H	3.05481700	8.90183400	-1.00630200
H	1.45035000	8.45838400	-0.88620700
C	5.99546000	4.86853400	-0.68556100
O	6.26932700	3.64874900	-0.65763600
O	6.79867400	5.82373500	-0.77234400

H	-4.11983900	0.16248700	0.47763800
O	-1.08367000	0.97764300	0.02784600
H	-2.87411200	-2.10974600	0.08923300
O	-2.89608500	2.24555200	-0.34092800
C	2.23692700	4.61736800	-0.39586200
C	3.57058000	4.25471000	-0.50493900
C	4.52436100	5.26591500	-0.63487400
C	4.13059400	6.59826000	-0.65166700
C	2.78076500	6.95249900	-0.54081400
C	1.82175300	5.94124400	-0.40996900
H	3.87916500	3.21812300	-0.49345100
H	4.88988700	7.36488500	-0.75471700
H	0.77017800	6.18718000	-0.32099800
Cl	1.01982900	3.36317500	-0.24002100
N	2.39823800	8.29291800	-0.49831800
H	3.04532400	8.92903600	-0.94302400
H	1.44638000	8.47469900	-0.78488200
C	6.01328800	4.90362000	-0.76239600
O	6.29190100	3.68435500	-0.74975100
O	6.81196600	5.86086600	-0.86666500

Anion-Anion-Cl DMSO

N	-2.54660600	-1.24657900	0.50715200
H	-1.55688200	-1.15758100	0.29466700
C	-3.21963600	-0.09144300	-0.08708100
C	-2.31309200	1.15680400	-0.12466000
H	-3.53344600	-0.26517600	-1.12545500

Anion-Anion-Cl Water

N	-2.42281000	-1.27741900	0.39109900
H	-1.49045800	-1.15179300	0.00729500
C	-3.21018500	-0.10477600	0.00962100
C	-2.35197700	1.17472000	-0.06607000
H	-3.68340300	-0.20745800	-0.97659800

H	-4.01285200	0.06813900	0.73007500
O	-1.11019400	1.03086500	-0.13107200
H	-2.81122100	-2.12022800	-0.01635800
O	-2.98786000	2.25549300	-0.09058000
C	2.21232300	4.63039900	-0.46109500
C	3.54563200	4.25367300	-0.51164100
C	4.51458600	5.25486100	-0.59836000
C	4.13621900	6.59139500	-0.63151900
C	2.78647900	6.95987200	-0.57944200
C	1.81222200	5.95852700	-0.49200500
H	3.84150200	3.21367900	-0.48754700
H	4.90775100	7.34949700	-0.70112400
H	0.76034100	6.21580300	-0.44988000
Cl	0.97646700	3.38843900	-0.35966400
N	2.41673800	8.30387700	-0.55192500
H	3.08883100	8.93410400	-0.96708800
H	1.47969800	8.49656000	-0.87749400
C	6.00392900	4.87820000	-0.65945900
O	6.27097400	3.65639300	-0.63322100
O	6.81503600	5.82799100	-0.72988400

H	-3.81182800	-0.22757100	0.76359300
O	-1.19349300	1.30316900	0.63634800
H	-1.61575200	-1.06713500	-0.97295000
O	-3.16831300	2.31810700	0.28840100
C	2.20121000	4.65839700	-0.39930700
C	3.52871400	4.26205400	-0.48864300
C	4.50440000	5.23249400	-0.72613100
C	4.13769600	6.56460500	-0.87598100
C	2.79900400	6.95538400	-0.78878100
C	1.82044900	5.98663500	-0.54715400
H	3.82379400	3.22776200	-0.37486100
H	4.91777500	7.29498800	-1.05903300
H	0.77634200	6.26873700	-0.47540200
N	2.43084700	8.29295300	-0.99585600
H	1.56677700	8.55949200	-0.54447400
H	3.16584900	8.95404700	-0.78570600
C	5.99253000	4.83595200	-0.81173900
O	6.24671900	3.61801100	-0.70329900
O	6.80106700	5.77577800	-0.97785300
Br	0.84151900	3.36395300	-0.04882600

Anion-Anion-Br Vacuum SP

N	-2.17954500	-1.18657400	-0.13641800
H	-1.50523600	-1.11467700	0.62190900
C	-3.07079400	-0.03175400	-0.01853700
C	-2.40591000	1.32490800	0.32808100
H	-3.63310400	0.09065000	-0.94738100

Anion-Anion-Br TCM

N	-2.17954500	-1.18657400	-0.13641800
H	-1.50523600	-1.11467700	0.62190900
C	-3.07079400	-0.03175400	-0.01853700
C	-2.40591000	1.32490800	0.32808100
H	-3.63310400	0.09065000	-0.94738100

H	-3.81182800	-0.22757100	0.76359300
O	-1.19349300	1.30316900	0.63634800
H	-1.61575200	-1.06713500	-0.97295000
O	-3.16831300	2.31810700	0.28840100
C	2.20121000	4.65839700	-0.39930700
C	3.52871400	4.26205400	-0.48864300
C	4.50440000	5.23249400	-0.72613100
C	4.13769600	6.56460500	-0.87598100
C	2.79900400	6.95538400	-0.78878100
C	1.82044900	5.98663500	-0.54715400
H	3.82379400	3.22776200	-0.37486100
H	4.91777500	7.29498800	-1.05903300
H	0.77634200	6.26873700	-0.47540200
N	2.43084700	8.29295300	-0.99585600
H	1.56677700	8.55949200	-0.54447400
H	3.16584900	8.95404700	-0.78570600
C	5.99253000	4.83595200	-0.81173900
O	6.24671900	3.61801100	-0.70329900
O	6.80106700	5.77577800	-0.97785300
Br	0.84151900	3.36395300	-0.04882600

H	-4.08382200	0.02513100	0.55222000
O	-1.14213900	1.12612200	0.18967800
H	-2.59223500	-2.03874700	-0.28689100
O	-3.05000900	2.28509100	-0.04569300
C	2.30222500	4.70922900	-0.39386700
C	3.63674500	4.33801200	-0.47675000
C	4.59938500	5.33909200	-0.62406000
C	4.21427400	6.67263300	-0.68650300
C	2.86636500	7.03701100	-0.60598200
C	1.89938100	6.03692500	-0.45505000
H	3.94448000	3.30210700	-0.42947400
H	4.98347200	7.42807500	-0.80018900
H	0.84977300	6.29750400	-0.38490700
N	2.49029400	8.38349800	-0.61274800
H	3.14789800	8.99542200	-1.07557800
H	1.54597700	8.55596200	-0.92865200
C	6.09125600	4.97042100	-0.71880300
O	6.36564500	3.75165400	-0.67938300
O	6.89043100	5.92689900	-0.82587500
Br	0.96186500	3.36628500	-0.18237700

Anion-Anion-Br DCE

N	-2.41360600	-1.25686100	0.33167700
H	-1.43305400	-1.00490900	0.23364200
C	-3.19048400	-0.08212100	-0.06890400
C	-2.38145500	1.23045400	0.04499900
H	-3.53194600	-0.13452100	-1.11053100

Anion-Anion-Br Acetone

N	-2.34665100	-1.24645300	0.13972700
H	-1.36585400	-0.99706200	0.04426800
C	-3.12281100	-0.03001100	-0.10344700
C	-2.33467700	1.25034800	0.24817700
H	-3.42332900	0.08226400	-1.15363700

H	-4.04056200	-0.03110400	0.48990800
O	-1.09660200	1.13654200	0.39848000
H	-2.55380800	-1.95330400	-0.55586000
O	-3.01152300	2.30206000	0.32025900
C	2.27430600	4.69801300	-0.32388900
C	3.60914200	4.32587000	-0.39431000
C	4.56829700	5.32032200	-0.59748300
C	4.17991000	6.64795400	-0.72794400
C	2.83074800	7.01318200	-0.66052200
C	1.86706200	6.01920700	-0.45258900
H	3.91967900	3.29470000	-0.29597700
H	4.94489400	7.40008900	-0.88385100
H	0.81710200	6.28105600	-0.39295400
N	2.45164400	8.35471900	-0.73594300
H	3.10524800	8.94739200	-1.22849100
H	1.50406400	8.51185800	-1.04996200
C	6.05861600	4.94711800	-0.67574500
O	6.33237700	3.72981500	-0.59084600
O	6.86125500	5.89647600	-0.81568000
Br	0.94218800	3.35931600	-0.04169300

H	-4.03943700	-0.03831900	0.47418800
O	-1.09843500	1.15033200	0.39711100
H	-2.56953200	-1.97476000	-0.50351300
O	-3.02296900	2.29881600	0.32287400
C	2.26805600	4.70429400	-0.33301700
C	3.60139300	4.32693700	-0.40168400
C	4.56457700	5.31866000	-0.59947000
C	4.18166400	6.64828000	-0.72576600
C	2.83345100	7.01869500	-0.65978800
C	1.86551600	6.02706500	-0.45798300
H	3.90745600	3.29427600	-0.30559400
H	4.94882900	7.39897800	-0.87736200
H	0.81649400	6.29292100	-0.39999300
N	2.45989900	8.36083600	-0.72960500
H	3.11643100	8.95563700	-1.21563400
H	1.51270900	8.52487900	-1.04124600
C	6.05262700	4.93866800	-0.67562200
O	6.32057200	3.71927500	-0.59771000
O	6.86159700	5.88387100	-0.80705300
Br	0.93195600	3.36827600	-0.05593300

Anion-Anion-Br DMSO

N	-2.33368600	-1.24261200	0.15614600
H	-1.35556200	-1.00495200	0.01681300
C	-3.11403300	-0.03325600	-0.10656800
C	-2.33798000	1.25198600	0.24816700
H	-3.40087800	0.07158200	-1.16176300

Anion-Anion-Br Water

N	-2.32545600	-1.24154800	0.15687100
H	-1.34968700	-1.00472100	0.00099600
C	-3.11125000	-0.03554100	-0.10469000
C	-2.34057200	1.25225000	0.25075600
H	-3.39933300	0.06910800	-1.15967000

H	-4.03616100	-0.04565300	0.47664100
O	-1.09980700	1.15706200	0.39440000
H	-2.57033000	-1.97926000	-0.49334400
O	-3.03025800	2.29574000	0.33119600
C	2.26498400	4.70693700	-0.33780300
C	3.59775400	4.32728700	-0.40414900
C	4.56293800	5.31766000	-0.59910900
C	4.18256400	6.64808000	-0.72461000
C	2.83475300	7.02080400	-0.66073100
C	1.86473800	6.03039500	-0.46211100
H	3.90174900	3.29401400	-0.30826100
H	4.95096600	7.39793300	-0.87398600
H	0.81606700	6.29802200	-0.40599500
N	2.46374000	8.36331700	-0.72921300
H	3.12206000	8.95843600	-1.21241800
H	1.51710600	8.53006400	-1.04109800
C	6.05016200	4.93476300	-0.67273700
O	6.31562600	3.71468000	-0.59544500
O	6.86166300	5.87812700	-0.80175200
Br	0.92669800	3.37241000	-0.06374400

H	-3.50409800	-0.59752600	0.95958600
O	-1.60152200	1.62361400	0.26893700
H	-1.61496600	-0.82188500	-1.25000600
O	-3.83194100	1.99053300	0.27255800
C	2.31331600	4.86447000	-0.32998100
C	3.63559200	4.43435600	-0.36188300
C	4.66078500	5.36558300	-0.55364800
C	4.34579400	6.71088300	-0.71093100
C	3.02146400	7.14062500	-0.68127100
C	1.99871300	6.21271800	-0.48407000
H	3.90669300	3.39255400	-0.24626600
H	5.16717000	7.40502400	-0.86113800
H	0.96541100	6.54277500	-0.45148500
N	2.71012300	8.52207300	-0.80779000
H	3.42632800	9.01447500	-1.32522100
H	1.81161900	8.66955400	-1.24848900
C	6.15169200	4.91863800	-0.60538200
O	6.35208500	3.70102400	-0.44674600
O	6.97286100	5.83950800	-0.80243100
I	0.68921700	3.49067800	-0.05564700

Anion-Anion-I Vacuum

N	-1.88940300	-1.05760000	-0.29993300
H	-1.13264700	-0.65062600	0.24932700
C	-3.06612300	-0.23966900	0.02090300
C	-2.80635500	1.28854100	0.19711800
H	-3.83262600	-0.37257400	-0.74714900

Anion-Anion-I TCM

N	-2.36018400	-1.27810200	-0.08950400
H	-1.55103200	-1.14538600	0.51247500
C	-3.16362600	-0.05938300	0.01279500
C	-2.38623500	1.28054500	0.04249200
H	-3.87869300	-0.02269800	-0.81197000

H	-3.75783300	-0.09602500	0.93193500
O	-1.14110500	1.20792100	0.17328100
H	-1.96302500	-1.31811600	-1.02357300
O	-3.08781900	2.31206800	-0.03797800
C	2.38886600	4.80642300	-0.35666100
C	3.73008200	4.44592600	-0.40848000
C	4.69545500	5.43998900	-0.58709500
C	4.30825800	6.76859500	-0.71403300
C	2.95982100	7.12911200	-0.66727800
C	1.99445900	6.13405100	-0.48203900
H	4.04960100	3.41621300	-0.31661800
H	5.08008600	7.51752600	-0.85364700
H	0.94524100	6.40514300	-0.43915700
N	2.57782400	8.47772200	-0.74750200
H	3.24089500	9.05692200	-1.24392100
H	1.64214000	8.62058200	-1.10221000
C	6.19247600	5.07595400	-0.64987600
O	6.47203500	3.86180600	-0.56059500
O	6.98453900	6.03515100	-0.78444800
I	0.87695500	3.31580600	-0.09743200

H	-4.03462800	0.05156300	0.54588800
O	-1.12430800	1.20655100	0.11338900
H	-2.51176400	-2.00455700	-0.23637800
O	-3.06033600	2.31602800	-0.13084900
C	2.39588700	4.82904800	-0.38251300
C	3.73243200	4.46024900	-0.47207900
C	4.70093800	5.45470600	-0.63006500
C	4.32204200	6.79005000	-0.69688400
C	2.97666200	7.15887200	-0.60997300
C	2.00728400	6.16195100	-0.44825600
H	4.04490900	3.42557900	-0.42390000
H	5.09356500	7.54188600	-0.81956500
H	0.96139100	6.43851600	-0.37564700
N	2.60464800	8.50814300	-0.62242500
H	3.26107300	9.11267600	-1.09684100
H	1.66014600	8.67947700	-0.93888300
C	6.18993400	5.07857600	-0.73407400
O	6.46024400	3.85856300	-0.69379100
O	6.99394200	6.03058400	-0.84916000
I	0.88612300	3.33425100	-0.14713000

Anion-Anion-I DCE

N	-2.33569600	-1.19543000	0.34694700
H	-1.36268100	-0.92912100	0.21810700
C	-3.14574200	-0.05394400	-0.08169500
C	-2.36984100	1.28032900	-0.01799900
H	-3.49704400	-0.14680300	-1.11726100

Anion-Anion-I Acetone

N	-2.33339700	-1.19169800	0.36998500
H	-1.36453700	-0.97465500	0.15235100
C	-3.13989500	-0.05770200	-0.08215000
C	-2.36351700	1.27404100	-0.02434300
H	-3.47945200	-0.16010000	-1.12163500

H	-4.03540600	0.05031600	0.53467600
O	-1.11537300	1.20103500	0.08250500
H	-2.58117900	-2.03477500	-0.13459600
O	-3.05319700	2.31277900	-0.12264300
C	2.39397600	4.83867200	-0.39640300
C	3.72953900	4.46606000	-0.48233600
C	4.70088800	5.45904700	-0.63202000
C	4.32607300	6.79577800	-0.69335300
C	2.98087800	7.16827400	-0.60896300
C	2.00813300	6.17228300	-0.45684500
H	4.03840800	3.43026500	-0.43727800
H	5.09824800	7.54782500	-0.80965100
H	0.96274700	6.45140800	-0.38755700
N	2.61331600	8.51678300	-0.61288800
H	3.27180500	9.12620400	-1.07812000
H	1.66848100	8.69593800	-0.92392000
C	6.18741400	5.07711800	-0.73107200
O	6.45305300	3.85527200	-0.69717300
O	6.99815600	6.02460300	-0.83627800
I	0.88401700	3.34297400	-0.17133200

H	-4.03477300	0.03993600	0.52846800
O	-1.11586900	1.20578100	0.07777100
H	-2.59946900	-2.04470300	-0.09797800
O	-3.05893700	2.31005000	-0.10784800
C	2.39065200	4.84497400	-0.40353400
C	3.72524000	4.46862600	-0.48655100
C	4.69930100	5.45948800	-0.63255000
C	4.32829500	6.79733000	-0.69276800
C	2.98357900	7.17351900	-0.61074400
C	2.00780600	6.17932700	-0.46293600
H	4.03093600	3.43192400	-0.44181800
H	5.10180800	7.54838500	-0.80615500
H	0.96300100	6.46110600	-0.39614700
N	2.62009600	8.52189000	-0.61194400
H	3.28055000	9.13275100	-1.07245300
H	1.67519400	8.70621800	-0.91965400
C	6.18409300	5.07243900	-0.72737600
O	6.44568600	3.84937300	-0.69438400
O	6.99967900	6.01619800	-0.82843600
I	0.87891600	3.35091200	-0.18151900

Anion-Anion-I DMSO

N	-2.32594500	-1.19089100	0.37446400
H	-1.36187000	-0.99308700	0.12159400
C	-3.13522700	-0.06150000	-0.08318500
C	-2.36523200	1.27252800	-0.02032800
H	-3.46833000	-0.16483000	-1.12502800

Anion-Anion-I Water

N	-2.32145600	-1.19181500	0.37318600
H	-1.35991000	-0.99896800	0.10756400
C	-3.13358000	-0.06377300	-0.08259600
C	-2.36710500	1.27172400	-0.01648400
H	-3.46596100	-0.16555100	-1.12494700

H	-4.03363900	0.03304500	0.52890200
O	-1.11709700	1.20823800	0.07571400
H	-2.60302600	-2.04794400	-0.09039500
O	-3.06351800	2.30819700	-0.09651300
C	2.38884400	4.84802300	-0.40635100
C	3.72293200	4.46970100	-0.48778000
C	4.69843100	5.45936400	-0.63230100
C	4.32939300	6.79774500	-0.69263800
C	2.98499400	7.17589000	-0.61207800
C	2.00767400	6.18278500	-0.46582100
H	4.02702900	3.43255600	-0.44287400
H	5.10383400	7.54800400	-0.80486200
H	0.96319200	6.46600000	-0.40024000
N	2.62349200	8.52427800	-0.61296800
H	3.28534700	9.13549500	-1.07090400
H	1.67882500	8.71094000	-0.91984900
C	6.18253700	5.06993900	-0.72492400
O	6.44225700	3.84637300	-0.69144500
O	7.00011100	6.01209200	-0.82483200
I	0.87558100	3.35540700	-0.18560300

Cation-Neutral-Cl Vacuum

N	-1.98938300	-0.99097600	0.37549700
H	-1.18245000	-0.89952700	-0.23171200
C	-3.00732600	-0.03454700	0.00313700
C	-2.36722200	1.30520700	-0.29892100
H	-3.58912800	-0.29254600	-0.89716900
H	-3.72290500	0.08796300	0.82317700
O	-1.21016800	1.44080700	-0.57164100
H	-2.33489600	-1.94038700	0.32261300
O	-3.19150500	2.37001900	-0.29922100
C	2.02457500	4.59962800	-0.62522300
C	3.36660800	4.22298200	-0.66771800
C	4.36111400	5.19110700	-0.67677300
C	4.04353200	6.54930800	-0.64361200
C	2.70493700	6.87895600	-0.60173200
C	1.67951500	5.94803800	-0.59144000
H	3.64458200	3.17550300	-0.69517200
H	4.83343500	7.29220300	-0.65171500
H	0.63428500	6.23731600	-0.55891000
Cl	0.78495900	3.41334900	-0.61791100
N	2.33111700	8.31974300	-0.55454000
H	1.92095500	8.57302800	0.35149900
H	3.15495200	8.91227800	-0.69861200
C	5.78826500	4.72925500	-0.72659900
O	6.10913800	3.58008100	-0.76019400
O	6.64536000	5.75972000	-0.72893800
H	7.54633000	5.40669400	-0.76248900
H	1.65046300	8.55367300	-1.28549400
H	-4.07961400	2.11865400	-0.02341900

Cation-Neutral-Cl TCM

N	-2.26064600	-1.16950200	0.29090900
H	-1.41441200	-1.17638500	-0.26928300

C	-3.08893900	-0.04003400	-0.08613100
C	-2.25078600	1.21825400	-0.15883000
H	-3.57664500	-0.13078800	-1.06888200
H	-3.88150600	0.10253000	0.65398700
O	-1.05332500	1.22203200	-0.21389500
H	-2.75227100	-2.03848900	0.11930900
O	-2.92839700	2.37859900	-0.21349500
C	2.09106700	4.60337700	-0.48672300
C	3.43164700	4.24916200	-0.54571400
C	4.40103000	5.24312800	-0.64044300
C	4.04746400	6.58888300	-0.67525900
C	2.70138700	6.89831300	-0.61088800
C	1.70771700	5.94081800	-0.51836700
H	3.73180200	3.20886200	-0.52206300
H	4.80498000	7.35927000	-0.75419700
H	0.65889600	6.21013200	-0.47408400
Cl	0.87621200	3.37853500	-0.37741600
N	2.30585800	8.32220500	-0.63297100
H	2.59066100	8.80603500	0.22600900
H	2.72903200	8.81943500	-1.42385600
C	5.83362000	4.81504100	-0.70864200
O	6.18863900	3.66940600	-0.66907000
O	6.66912400	5.85172500	-0.81997800
H	7.57605600	5.51492500	-0.86353700
H	1.29026400	8.42667500	-0.71779800
H	-3.87900300	2.23538500	-0.13192400

Cation-Neutral-Cl DCE

N	-2.32698500	-1.22197900	0.24367400
H	-1.51570600	-1.29242600	-0.36196200
C	-3.09182900	-0.03588000	-0.09335800
C	-2.19729900	1.18423900	-0.10198200
H	-3.57793100	-0.06353400	-1.08026800
H	-3.88160800	0.11605400	0.64775000
O	-0.99879900	1.14221900	-0.07706800
H	-2.89140000	-2.04996800	0.09164000
O	-2.82299300	2.37113700	-0.18613800
C	2.09784900	4.61266000	-0.45383700
C	3.43741800	4.25926200	-0.51892200
C	4.40286400	5.25525700	-0.63411700
C	4.04420700	6.59883100	-0.68399200
C	2.69787700	6.90787200	-0.61479700
C	1.70870800	5.94753100	-0.50138700
H	3.73976200	3.22013200	-0.48357600
H	4.79844500	7.37034600	-0.77729100
H	0.65985500	6.21474000	-0.45209400
Cl	0.88810400	3.38198000	-0.31510300
N	2.29945100	8.32806000	-0.66007600
H	2.62781600	8.83895800	0.16669400
H	2.67841200	8.80090000	-1.48753500
C	5.83571400	4.83214300	-0.70775900
O	6.19599500	3.68675800	-0.66174900
O	6.66755700	5.86872300	-0.83180700
H	7.57567100	5.53537100	-0.87836800

H	1.28098900	8.43180100	-0.69439900
H	-3.78262100	2.26634500	-0.18540800

Cation-Neutral-Cl Acetone

N	-2.34389300	-1.24081400	0.23439100
H	-1.55110500	-1.32950100	-0.39305900
C	-3.09792700	-0.04430500	-0.09244300
C	-2.19275700	1.16766700	-0.09475400
H	-3.58799400	-0.06155400	-1.07734400
H	-3.88364900	0.11031400	0.65220600
O	-0.99422600	1.11602400	-0.06101200
H	-2.92668500	-2.05905300	0.09861800
O	-2.80657300	2.35978600	-0.18151400
C	2.10106700	4.62218900	-0.44844000
C	3.43950300	4.26630100	-0.51411100
C	4.40555400	5.26144600	-0.63257900
C	4.04744000	6.60490500	-0.68531200
C	2.70161600	6.91655800	-0.61566000
C	1.71206600	5.95680200	-0.49872500
H	3.74032400	3.22688600	-0.47684700
H	4.80174500	7.37573600	-0.78101600
H	0.66367500	6.22522200	-0.44879500
Cl	0.89020800	3.39089800	-0.30615300
N	2.30573800	8.33611300	-0.66565800
H	2.64156400	8.85110400	0.15548300
H	2.67936700	8.80392300	-1.49840900
C	5.83779400	4.83795900	-0.70678400
O	6.19817200	3.69183000	-0.65962100
O	6.67012600	5.87311400	-0.83255900
H	7.57832200	5.53993000	-0.87938300
H	1.28746700	8.44293400	-0.69270000
H	-3.76741500	2.26511700	-0.19105400

Cation-Neutral-Cl DMSO

N	-2.35139900	-1.25566900	0.21940300
H	-1.57372500	-1.35035600	-0.42594000
C	-3.10253300	-0.05255100	-0.09077400
C	-2.19295300	1.15600700	-0.08712300
H	-3.59969400	-0.05882000	-1.07204500
H	-3.88249500	0.09807200	0.66059900
O	-0.99421600	1.10015300	-0.05412100
H	-2.94433400	-2.06820500	0.09276700
O	-2.80171600	2.35076800	-0.16617200
C	2.10253300	4.63058400	-0.44535300
C	3.44007200	4.27208200	-0.50947700
C	4.40737600	5.26580400	-0.63034800
C	4.05069200	6.60938200	-0.68712500
C	2.70535000	6.92371500	-0.61893300
C	1.71470000	5.96528300	-0.49955000
H	3.73917400	3.23233900	-0.46921000
H	4.80577200	7.37904000	-0.78456800
H	0.66673100	6.23528100	-0.45070900
Cl	0.88987900	3.40017700	-0.30030700
N	2.31224000	8.34317500	-0.67380900

H	2.65255800	8.86127200	0.14348800
H	2.68370500	8.80649700	-1.51003500
C	5.83902900	4.84085600	-0.70252500
O	6.19839100	3.69402200	-0.65297800
O	6.67262500	5.87432900	-0.82924800
H	7.58067400	5.54050900	-0.87472200
H	1.29422300	8.45272700	-0.69724500
H	-3.76313300	2.26105800	-0.17717400

Cation-Neutral-Cl Water

N	-2.35018300	-1.25854300	0.21027800
H	-1.57831300	-1.35158000	-0.44230600
C	-3.10254300	-0.05336500	-0.08951000
C	-2.19281700	1.15501800	-0.08364600
H	-3.60460800	-0.05440500	-1.06819600
H	-3.87878900	0.09345000	0.66640900
O	-0.99381600	1.09878000	-0.05402700
H	-2.94527400	-2.06965600	0.08429100
O	-2.80113900	2.35022800	-0.15579100
C	2.10258900	4.63159100	-0.44464000
C	3.43996400	4.27260600	-0.50737200
C	4.40739800	5.26609600	-0.62910600
C	4.05071900	6.60952800	-0.68819600
C	2.70542700	6.92444100	-0.62123000
C	1.71467500	5.96613800	-0.50105500
H	3.73878300	3.23287400	-0.46530000
H	4.80586600	7.37895200	-0.78609800
H	0.66675300	6.23635600	-0.45309200
Cl	0.88989000	3.40081800	-0.29845100
N	2.31297200	8.34370400	-0.67833800
H	2.65401500	8.86306800	0.13784700
H	2.68440200	8.80543400	-1.51545800
C	5.83903500	4.84122800	-0.69938200
O	6.19858000	3.69432300	-0.64785600
O	6.67270000	5.87437500	-0.82660600
H	7.58089300	5.54074600	-0.87069900
H	1.29505600	8.45404500	-0.70148600
H	-3.76270800	2.26128100	-0.16421700

Cation-Neutral-Br Vacuum

N	-2.29828900	-1.02110200	0.61311000
H	-1.32223100	-1.01339500	0.33818900
C	-3.04644600	-0.05246200	-0.15499400
C	-2.25513300	1.23292600	-0.27571800
H	-3.28075200	-0.34978300	-1.19089000
H	-3.99924200	0.16166900	0.34096100
O	-1.07193600	1.30179800	-0.10351700
H	-2.66689000	-1.95548300	0.49196700
O	-2.94565400	2.32474200	-0.65174600
C	2.15074700	4.71677800	-0.45504600
C	3.48878600	4.35632300	-0.61773700
C	4.46805500	5.33432500	-0.73209400
C	4.13883200	6.68907200	-0.68556300
C	2.80597600	7.00457900	-0.52344400

C	1.79667400	6.06247700	-0.40622200
H	3.78096900	3.31305500	-0.65673200
H	4.91507200	7.44081900	-0.77695100
H	0.75765200	6.34744100	-0.27815000
N	2.42080900	8.44211900	-0.46065400
H	2.03693000	8.68860600	0.45854000
H	3.23465700	9.04221700	-0.62776900
C	5.88961600	4.88736900	-0.90881900
O	6.22030600	3.74152100	-0.95948800
O	6.73099800	5.92691000	-1.00247900
H	7.62908100	5.58315200	-1.11562600
H	1.71570000	8.67231600	-1.16928400
H	-3.88711200	2.13235900	-0.72169000
Br	0.82302700	3.40067700	-0.29492800

Cation-Neutral-Br TCM

N	-2.30180900	-1.20366000	0.25312000
H	-1.43641200	-1.20353800	-0.27675700
C	-3.09878400	-0.04660100	-0.10555700
C	-2.24152500	1.19996600	-0.10393800
H	-3.55947000	-0.09179300	-1.10430800
H	-3.91005200	0.08439100	0.61651200
O	-1.04202900	1.18773200	-0.08974000
H	-2.80110000	-2.05657800	0.03046500
O	-2.89839000	2.37006100	-0.17052400
C	2.19474300	4.72210400	-0.45688400
C	3.53556600	4.36923900	-0.53033300
C	4.50385100	5.36208900	-0.65452400
C	4.14969800	6.70699200	-0.70452400
C	2.80419300	7.01666700	-0.62795700
C	1.81245700	6.05971300	-0.50680600
H	3.84254900	3.33134400	-0.49352500
H	4.90664000	7.47580200	-0.80356900
H	0.76572800	6.33527400	-0.45232100
N	2.40608500	8.43964100	-0.66901600
H	2.73305000	8.94691500	0.16060100
H	2.78596200	8.91511600	-1.49450400
C	5.93558500	4.93326500	-0.73463000
O	6.29142400	3.78808200	-0.68874000
O	6.77001900	5.96890300	-0.86386200
H	7.67641800	5.63148500	-0.91337600
H	1.38725000	8.54102100	-0.70411200
H	-3.85443200	2.23990200	-0.15481500
Br	0.87298300	3.38749200	-0.28315300

Cation-Neutral-Br DCE

N	-2.31850100	-1.23032600	0.22096100
H	-1.50382800	-1.28284300	-0.38200300
C	-3.09671200	-0.04949700	-0.10344200
C	-2.22021700	1.18302100	-0.08223100
H	-3.57260600	-0.06625700	-1.09553800
H	-3.89553700	0.07891800	0.63229700
O	-1.02057300	1.15583100	-0.04605400
H	-2.87221000	-2.06293200	0.05504600

O	-2.85867100	2.36239200	-0.15270700
C	2.19811700	4.73230600	-0.44453900
C	3.53739300	4.37674200	-0.51759800
C	4.50515300	5.36933500	-0.64959600
C	4.14975300	6.71330500	-0.70798800
C	2.80468100	7.02593800	-0.63167900
C	1.81389600	6.06864000	-0.50257000
H	3.84309300	3.33890500	-0.47460700
H	4.90525900	7.48220900	-0.81268600
H	0.76764700	6.34499200	-0.44798100
N	2.40888300	8.44668100	-0.68438700
H	2.75052500	8.96432600	0.13264800
H	2.77608700	8.91120300	-1.52176600
C	5.93639100	4.94194500	-0.72897900
O	6.29435900	3.79602100	-0.67798300
O	6.77035700	5.97569400	-0.86362100
H	7.67734300	5.63959800	-0.91242400
H	1.39021400	8.55216100	-0.70388000
H	-3.81719700	2.24778700	-0.16254400
Br	0.87709800	3.39493300	-0.26092200

Cation-Neutral-Br Acetone

N	-2.32551300	-1.24234400	0.20740400
H	-1.52834900	-1.30942000	-0.41721500
C	-3.09614200	-0.05261800	-0.10432800
C	-2.21285200	1.17457100	-0.07126500
H	-3.57430000	-0.05751700	-1.09520700
H	-3.89283400	0.07364400	0.63390400
O	-1.01318200	1.14141700	-0.02315900
H	-2.89544900	-2.06685500	0.05563100
O	-2.84324100	2.35755900	-0.14281300
C	2.19785100	4.73889200	-0.43684100
C	3.53578700	4.38031100	-0.51163900
C	4.50432700	5.37157900	-0.64863300
C	4.14985600	6.71548100	-0.71045900
C	2.80551500	7.03129600	-0.63230900
C	1.81414700	6.07510600	-0.49792400
H	3.83965300	3.34212400	-0.46632200
H	4.90556600	7.48333600	-0.81886500
H	0.76852200	6.35301100	-0.44173300
N	2.41286400	8.45155900	-0.68959900
H	2.76145000	8.97259500	0.12228200
H	2.77580800	8.91125100	-1.53150900
C	5.93473600	4.94325200	-0.72964600
O	6.29239800	3.79646900	-0.67708300
O	6.76939900	5.97512700	-0.86753900
H	7.67631700	5.63888500	-0.91720400
H	1.39456300	8.56066100	-0.70275000
H	-3.80259800	2.25006200	-0.16460100
Br	0.87589700	3.40159200	-0.24735100

Cation-Neutral-Br DMSO

N	-2.44509000	-1.24461200	0.24599400
H	-1.58264700	-1.38399900	-0.27071200

C	-3.07116100	-0.00297200	-0.17032500
C	-2.11552800	1.15668900	-0.00049400
H	-3.39723700	0.02003200	-1.22066300
H	-3.95703300	0.18804700	0.44191400
O	-0.94466500	1.04004700	0.24226400
H	-3.05479900	-2.02347800	0.02353000
O	-2.63821600	2.38006600	-0.17753800
C	2.19707200	4.71788900	-0.36192000
C	3.53475200	4.36965100	-0.47485300
C	4.48844900	5.36790900	-0.65739900
C	4.11881200	6.70710300	-0.72697300
C	2.77471500	7.01290300	-0.61055200
C	1.79768500	6.04918700	-0.42978200
H	3.84961400	3.33506300	-0.42457000
H	4.86423700	7.47922400	-0.86911500
H	0.75175800	6.31749300	-0.34320000
N	2.36738300	8.42791500	-0.67997900
H	2.77451300	8.97516600	0.08594900
H	2.66069200	8.86359200	-1.56105800
C	5.91966900	4.95296800	-0.77971700
O	6.29104600	3.81030700	-0.72290100
O	6.73835700	5.99059600	-0.95998400
H	7.64708000	5.66379800	-1.03385000
H	1.35035100	8.53192700	-0.61755100
H	-3.58566800	2.33974100	-0.35974200
Br	0.89606000	3.36877600	-0.11354900

Cation-Neutral-Br Water

N	-2.44511100	-1.24832700	0.23399800
H	-1.58931300	-1.38951200	-0.29319900
C	-3.07166600	-0.00352800	-0.17226900
C	-2.11454700	1.15449500	0.00033100
H	-3.40281300	0.02561600	-1.22078900
H	-3.95438900	0.18479200	0.44527600
O	-0.94382800	1.03625400	0.24348500
H	-3.06008700	-2.02430800	0.01585800
O	-2.63590900	2.37877300	-0.17362900
C	2.19698100	4.71957000	-0.35988900
C	3.53460900	4.37065200	-0.47033500
C	4.48875500	5.36844600	-0.65318100
C	4.11939000	6.70752300	-0.72564300
C	2.77522700	7.01405300	-0.61146400
C	1.79778900	6.05076500	-0.43039700
H	3.84906900	3.33606600	-0.41792500
H	4.86502600	7.47933000	-0.86807000
H	0.75182900	6.31947500	-0.34564500
N	2.36855700	8.42888300	-0.68394800
H	2.77750500	8.97806300	0.07962600
H	2.66048000	8.86195700	-1.56675300
C	5.92006600	4.95320700	-0.77243600
O	6.29132600	3.81047800	-0.71318100
O	6.73920300	5.99029400	-0.95287100
H	7.64805800	5.66338700	-1.02472000
H	1.35174200	8.53385400	-0.61990500

H	-3.58313400	2.34004900	-0.35761200
Br	0.89538600	3.37071800	-0.11148800

Cation-Neutral-I Vacuum

N	-2.34180600	-1.04370400	0.63123100
H	-1.36614800	-1.05234100	0.35526300
C	-3.08210700	-0.08097300	-0.15080300
C	-2.29574400	1.20675600	-0.26386600
H	-3.30038900	-0.38081700	-1.18974800
H	-4.04270600	0.13079500	0.33070600
O	-1.11329900	1.27755100	-0.07289900
H	-2.72138200	-1.97590100	0.52789300
O	-2.97703800	2.29533500	-0.65386900
C	2.29760000	4.86499600	-0.48817300
C	3.63958600	4.51703400	-0.65086100
C	4.61907300	5.49700200	-0.75815000
C	4.28662400	6.85015900	-0.70436900
C	2.95237700	7.15922200	-0.54319400
C	1.94671900	6.21155500	-0.43323300
H	3.94391500	3.47744400	-0.69619500
H	5.06045300	7.60519000	-0.78969900
H	0.90913500	6.50352800	-0.30578500
N	2.56255300	8.59579100	-0.47223500
H	2.18004800	8.83631000	0.44893900
H	3.37396800	9.19927800	-0.63839800
C	6.04156900	5.05515600	-0.93401500
O	6.37729900	3.91081000	-0.99167200
O	6.88147200	6.09746000	-1.01843000
H	7.78012600	5.75538000	-1.13119700
H	1.85499800	8.82693300	-1.17787200
H	-3.91797500	2.10613500	-0.74015500
I	0.81019900	3.37598000	-0.31183000

Cation-Neutral-I TCM

N	-2.32552500	-1.22495200	0.25207100
H	-1.47923300	-1.23887500	-0.30769900
C	-3.13124800	-0.07178100	-0.09789800
C	-2.28140800	1.17886600	-0.10215100
H	-3.60192900	-0.11705400	-1.09210500
H	-3.93565800	0.05433000	0.63252500
O	-1.08012900	1.16975300	-0.09321600
H	-2.83586200	-2.07940200	0.06243400
O	-2.93840000	2.34593800	-0.16738300
C	2.34007300	4.86885200	-0.48449800
C	3.68493800	4.52717500	-0.55435200
C	4.65298600	5.52201800	-0.67298700
C	4.29542900	6.86575400	-0.72167400
C	2.94886800	7.17002700	-0.64907500
C	1.96048600	6.20789400	-0.53329400
H	4.00346200	3.49256000	-0.51925500
H	5.05019800	7.63729600	-0.81618100
H	0.91492300	6.48971800	-0.48260000
N	2.54672500	8.59254700	-0.68815600
H	2.86359900	9.09730700	0.14686600

H	2.93345100	9.07289600	-1.50754700
C	6.08587100	5.09811000	-0.74865400
O	6.44670000	3.95419400	-0.70373500
O	6.91817500	6.13667500	-0.87306600
H	7.82540700	5.80134300	-0.92023000
H	1.52800800	8.69063600	-0.73334700
H	-3.89464600	2.21649900	-0.14914200
I	0.86385800	3.36373400	-0.29826200

Cation-Neutral-I DCE

N	-2.34466400	-1.24732300	0.22458000
H	-1.53737400	-1.30300400	-0.38788100
C	-3.13047500	-0.07161600	-0.09849500
C	-2.26185600	1.16558200	-0.08116800
H	-3.60957200	-0.09113500	-1.08908100
H	-3.92754400	0.05345700	0.63967400
O	-1.06040200	1.14161800	-0.04705700
H	-2.89817000	-2.08273200	0.07285400
O	-2.90063300	2.34174000	-0.15263000
C	2.34502800	4.87503300	-0.46777500
C	3.68858000	4.53194000	-0.53988200
C	4.65468300	5.52766600	-0.66872300
C	4.29443400	6.87008600	-0.72570600
C	2.94808900	7.17600000	-0.65105000
C	1.96192800	6.21250600	-0.52470900
H	4.00711600	3.49774500	-0.49889100
H	5.04694600	7.64230600	-0.82772300
H	0.91661500	6.49379600	-0.47199200
N	2.54637400	8.59576700	-0.70278300
H	2.88314600	9.11373500	0.11599100
H	2.91382900	9.06340900	-1.53824700
C	6.08740800	5.10674700	-0.74664500
O	6.45162600	3.96245800	-0.69745500
O	6.91785300	6.14431600	-0.87815200
H	7.82596900	5.81137000	-0.92647700
H	1.52735100	8.69660800	-0.72537000
H	-3.85935900	2.22744000	-0.16023800
I	0.87219200	3.36654400	-0.26758300

Cation-Neutral-I Acetone

N	-2.35239600	-1.25752900	0.21625600
H	-1.56408000	-1.33003800	-0.41885600
C	-3.12945000	-0.07232000	-0.09541000
C	-2.25135400	1.15791400	-0.07345500
H	-3.61426500	-0.08245200	-1.08306200
H	-3.92160400	0.05460200	0.64754800
O	-1.04984000	1.12584600	-0.03088000
H	-2.92324200	-2.08430800	0.08126600
O	-2.88019900	2.33868700	-0.14844000
C	2.34521000	4.87916800	-0.46285300
C	3.68789100	4.53435300	-0.53579900
C	4.65390400	5.52979800	-0.66806100
C	4.29336900	6.87188600	-0.72792700
C	2.94737700	7.17962000	-0.65247800

C	1.96138000	6.21621700	-0.52230400
H	4.00553600	3.50004700	-0.49299400
H	5.04541700	7.64388600	-0.83256300
H	0.91638900	6.49798700	-0.46862200
N	2.54743100	8.59854900	-0.70874700
H	2.89081600	9.12042700	0.10473100
H	2.90994200	9.06157400	-1.54895900
C	6.08628800	5.10938600	-0.74670100
O	6.45127700	3.96457200	-0.69634300
O	6.91654100	6.14600800	-0.88013400
H	7.82494600	5.81381300	-0.92887200
H	1.52864300	8.70205400	-0.72475900
H	-3.83997400	2.23280600	-0.16559500
I	0.87316400	3.36950700	-0.25860000

Cation-Neutral-I DMSO

N	-2.34980500	-1.26595200	0.19265500
H	-1.57877800	-1.33826900	-0.46348000
C	-3.12836600	-0.07479000	-0.09258400
C	-2.24902300	1.15426900	-0.05986100
H	-3.62339900	-0.06954100	-1.07499200
H	-3.91285600	0.04158600	0.66006500
O	-1.04713600	1.12121900	-0.02051800
H	-2.92872200	-2.08825100	0.06399400
O	-2.87666100	2.33627700	-0.11975100
C	2.34429600	4.88338400	-0.46030100
C	3.68636900	4.53641600	-0.53007100
C	4.65329600	5.53064400	-0.66514700
C	4.29367800	6.87262300	-0.73113800
C	2.94799000	7.18256100	-0.65850700
C	1.96112400	6.22028300	-0.52551300
H	4.00269300	3.50196700	-0.48257400
H	5.04623400	7.64365200	-0.83789200
H	0.91642300	6.50324300	-0.47401700
N	2.55030000	8.60113600	-0.72144400
H	2.89795200	9.12720600	0.08749300
H	2.91057600	9.05868100	-1.56560200
C	6.08537500	5.10931000	-0.73960800
O	6.44984900	3.96407100	-0.68438400
O	6.91653900	6.14440000	-0.87502900
H	7.82501000	5.81191200	-0.92083200
H	1.53177000	8.70712100	-0.73406400
H	-3.83674300	2.23213200	-0.13704200
I	0.87113300	3.37477100	-0.25247100

Cation-Neutral-I Water

N	-2.34554300	-1.27057400	0.17045400
H	-1.58254600	-1.33543600	-0.49580400
C	-3.12768900	-0.07669000	-0.09291400
C	-2.25049900	1.15343700	-0.04697800
H	-3.62814000	-0.05800700	-1.07234600
H	-3.90826900	0.02742200	0.66553300
O	-1.04833800	1.12230100	-0.01164400
H	-2.92592200	-2.09141800	0.03882000

O	-2.88034700	2.33488600	-0.08973200
C	2.34373600	4.88567500	-0.45791600
C	3.68557900	4.53753000	-0.52461400
C	4.65316100	5.53081300	-0.66221500
C	4.29422500	6.87265700	-0.73380700
C	2.94864600	7.18379200	-0.66390600
C	1.96115700	6.22244500	-0.52860300
H	4.00120600	3.50310600	-0.47268800
H	5.04721000	7.64295200	-0.84240700
H	0.91657200	6.50615900	-0.47944800
N	2.55212800	8.60218500	-0.73239900
H	2.90210800	9.13158900	0.07334900
H	2.91114300	9.05551100	-1.57934000
C	6.08511200	5.10864500	-0.73270000
O	6.44908200	3.96335000	-0.67243900
O	6.91697300	6.14268100	-0.87059200
H	7.82542800	5.80975400	-0.91354400
H	1.53371300	8.70933900	-0.74325400
H	-3.84037700	2.22957700	-0.10507400
I	0.86960900	3.37837700	-0.24640500

Neutral-Neutral-Cl Vacuum ModRedundant

N	-2.39534500	-0.97547000	-0.58448900
H	-1.94718800	-1.35471100	0.24274800
C	-2.94872400	0.32371000	-0.28938800
C	-1.94689700	1.35171500	0.23375100
H	-3.41768900	0.73567000	-1.18965800
H	-3.74572600	0.22188900	0.45549000
O	-0.78979400	1.12290300	0.41180200
H	-1.66394000	-0.88927800	-1.28212100
O	-2.45438500	2.57643900	0.49563500
C	2.34988100	4.68123100	-0.23885200
C	3.69766600	4.36344400	-0.30505400
C	4.59893200	5.39457500	-0.55860200
C	4.17351300	6.70524000	-0.74195200
C	2.81069000	7.00878600	-0.67622000
C	1.89806500	5.98089300	-0.41947600
H	4.05058900	3.35061600	-0.16645000
H	4.89881800	7.48710600	-0.93024800
H	0.83720500	6.19270400	-0.35416600
Cl	1.19051300	3.42394500	0.07587200
N	2.37101000	8.32288800	-0.80561700
H	2.99424700	8.94218600	-1.30072800
H	1.40971400	8.43660200	-1.08847700
C	6.04392300	5.03746200	-0.62811400
O	6.48403900	3.92895700	-0.48820200
O	6.83800300	6.10026700	-0.87063300
H	7.74575800	5.77110400	-0.89719600
H	-3.39511600	2.60750300	0.29185000

A 15 10 7 120.0 F

D 15 10 7 4 10.0 F

Neutral-Neutral-Cl TCM

N	-2.33806500	-1.16715000	-0.13586000
H	-1.72867000	-1.24424800	0.67167900
C	-3.02871200	0.10162200	-0.11448400
C	-2.12651700	1.33041600	-0.09845200
H	-3.68399100	0.17996200	-0.98764000
H	-3.67766400	0.15416900	0.76540600
O	-0.92949600	1.28791700	-0.09468700
H	-1.73645100	-1.22120600	-0.95111300
O	-2.75878500	2.51939400	-0.08700800
C	2.33729800	4.80911300	-0.44403700
C	3.66698200	4.42405200	-0.50922800
C	4.62888300	5.42811900	-0.60861600
C	4.27660400	6.77246600	-0.64119700
C	2.92859300	7.14349000	-0.57352200
C	1.95514300	6.14206000	-0.47343700
H	3.95798300	3.38270100	-0.48653300
H	5.04358900	7.53285500	-0.71864500
H	0.90521500	6.40480800	-0.41829100
Cl	1.10174400	3.58336300	-0.32619400
N	2.56402900	8.48181300	-0.54686000
H	3.23221600	9.12450400	-0.94660200
H	1.61751800	8.68527800	-0.83290700
C	6.05651100	5.00519600	-0.68326900
O	6.43043700	3.86056000	-0.65607700
O	6.90612300	6.03829100	-0.78710200
H	7.80440700	5.68166600	-0.82959800
H	-3.71716300	2.40716500	-0.09421800

Neutral-Neutral-Cl DCE

N	-2.34091900	-1.17218000	-0.13459400
H	-1.73426700	-1.24870200	0.67513300
C	-3.03416900	0.09590500	-0.11561500
C	-2.13393200	1.32524800	-0.09756400
H	-3.68666100	0.17374400	-0.99059200
H	-3.68517700	0.14856800	0.76243400
O	-0.93547300	1.28484600	-0.09154700
H	-1.73763600	-1.22632600	-0.94867000
O	-2.76413300	2.51383400	-0.08716000
C	2.34066100	4.81316800	-0.44331200
C	3.66969200	4.42654500	-0.50847700
C	4.63196900	5.43057600	-0.60891500
C	4.27990100	6.77485300	-0.64212700
C	2.93162500	7.14714100	-0.57364700
C	1.95759100	6.14563000	-0.47303600
H	3.95963400	3.38494500	-0.48553600
H	5.04637700	7.53550800	-0.72160200
H	0.90790100	6.40927600	-0.41874500
Cl	1.10418600	3.58626700	-0.32534700
N	2.56805900	8.48444100	-0.54627300
H	3.23637000	9.12798300	-0.94493800
H	1.62107400	8.68929900	-0.83050200
C	6.05976700	5.00733000	-0.68410900
O	6.43168600	3.86119200	-0.65570000
O	6.90863500	6.03859700	-0.78928800

H	7.80843900	5.68510000	-0.83328700
H	-3.72343900	2.40558800	-0.09547700

Neutral-Neutral-Cl Acetone

N	-2.34302100	-1.17464100	-0.13336500
H	-1.73815300	-1.25082000	0.67776000
C	-3.03705800	0.09338200	-0.11637400
C	-2.13724500	1.32264100	-0.09725600
H	-3.68770300	0.17086700	-0.99263200
H	-3.68953000	0.14654100	0.76041600
O	-0.93807900	1.28246800	-0.08917200
H	-1.73855100	-1.22938600	-0.94654900
O	-2.76558900	2.51138400	-0.08826800
C	2.34257500	4.81488100	-0.44266600
C	3.67130500	4.42765900	-0.50812500
C	4.63356400	5.43185400	-0.60927900
C	4.28135000	6.77601000	-0.64272400
C	2.93289900	7.14871700	-0.57351600
C	1.95875500	6.14700500	-0.47241400
H	3.96091600	3.38599700	-0.48518400
H	5.04742100	7.53693600	-0.72345100
H	0.90915900	6.41091700	-0.41826100
Cl	1.10584000	3.58713700	-0.32442600
N	2.56963300	8.48544700	-0.54566900
H	3.23790700	9.12955200	-0.94371800
H	1.62238000	8.69091500	-0.82892200
C	6.06154600	5.00872600	-0.68505400
O	6.43251800	3.86181500	-0.65688500
O	6.90988900	6.03917200	-0.79000400
H	7.81045300	5.68733900	-0.83522200
H	-3.72541900	2.40586200	-0.09753300

Neutral-Neutral-Cl DMSO

N	-2.34547900	-1.17640800	-0.13336900
H	-1.74207600	-1.25281200	0.67882900
C	-3.03994500	0.09155400	-0.11730300
C	-2.14046200	1.32078300	-0.09568200
H	-3.68878100	0.16938800	-0.99481700
H	-3.69417300	0.14435200	0.75816200
O	-0.94087800	1.28049600	-0.08432100
H	-1.73992700	-1.23120700	-0.94574600
O	-2.76752900	2.50962100	-0.08756000
C	2.34491300	4.81553800	-0.44239200
C	3.67359800	4.42844000	-0.50785700
C	4.63544200	5.43312200	-0.60940300
C	4.28260500	6.77703900	-0.64315500
C	2.93391200	7.14948700	-0.57361300
C	1.96008500	6.14728400	-0.47225400
H	3.96344300	3.38687100	-0.48474800
H	5.04815200	7.53842000	-0.72461100
H	0.91043300	6.41090700	-0.41824600
Cl	1.10847400	3.58678800	-0.32400300
N	2.57033900	8.48574100	-0.54551000
H	3.23844200	9.13050600	-0.94287700

H	1.62289300	8.69132600	-0.82819500
C	6.06374600	5.01068400	-0.68521700
O	6.43462600	3.86348800	-0.65623500
O	6.91121600	6.04085300	-0.79184100
H	7.81233600	5.69030600	-0.83765500
H	-3.72764400	2.40581100	-0.09887400

Neutral-Neutral-Cl Water

N	-2.34561300	-1.17726300	-0.13646400
H	-1.74553400	-1.25608900	0.67796600
C	-3.04094300	0.09029100	-0.11906800
C	-2.14220900	1.31983000	-0.09099800
H	-3.68686300	0.17039800	-0.99848000
H	-3.69785100	0.14039200	0.75448100
O	-0.94249800	1.28051000	-0.07598400
H	-1.73694400	-1.22922400	-0.94670200
O	-2.76969300	2.50840100	-0.08194300
C	2.34573400	4.81628800	-0.44069400
C	3.67440800	4.42911900	-0.50584700
C	4.63616700	5.43374700	-0.60919900
C	4.28321000	6.77758600	-0.64499200
C	2.93445000	7.15009800	-0.57561000
C	1.96069800	6.14791700	-0.47245000
H	3.96427600	3.38759000	-0.48127200
H	5.04861400	7.53891600	-0.72806800
H	0.91106700	6.41164300	-0.41863400
Cl	1.10940800	3.58753500	-0.32007200
N	2.57075800	8.48624200	-0.54930000
H	3.23880800	9.13051100	-0.94765800
H	1.62329600	8.69130300	-0.83246500
C	6.06448100	5.01126100	-0.68459500
O	6.43537100	3.86405700	-0.65386600
O	6.91182000	6.04137100	-0.79199100
H	7.81316800	5.69122900	-0.83727800
H	-3.72983200	2.40471500	-0.09731200

Neutral-Neutral-Br Vacuum ModRedundant

N	-2.46689600	-1.21359800	0.09287800
H	-1.49315800	-1.11858000	-0.17691300
C	-3.16027500	0.03678800	-0.12891700
C	-2.20268100	1.20266600	0.04121800
H	-3.58871100	0.15284700	-1.13672000
H	-3.98328100	0.15017200	0.58627500
O	-1.01424200	1.09059000	0.01329000
H	-2.88118200	-1.97108700	-0.43303200
O	-2.77446500	2.41431300	0.17867000
C	2.30436000	4.68429400	-0.44877300
C	3.64674100	4.33965800	-0.50113100
C	4.57767100	5.36201000	-0.67281500
C	4.18638800	6.69083400	-0.78978600
C	2.83018400	7.02301000	-0.73394300
C	1.88750700	6.00325300	-0.56478300
H	3.97790000	3.31404100	-0.41207600
H	4.93280700	7.46335300	-0.92780600

H	0.83067000	6.24081600	-0.52744800
N	2.41608000	8.34162800	-0.90312800
H	1.51091400	8.56597700	-0.51879800
H	3.10836200	9.04285500	-0.68768200
C	6.01581600	4.97616500	-0.72558100
O	6.42876900	3.85189400	-0.63934000
O	6.83915700	6.03313100	-0.88298700
H	7.73969400	5.68468800	-0.90774700
H	-3.73279000	2.33749200	0.22882900
Br	1.00046500	3.32879200	-0.21544600

A 15 10 7 120.0 F

D 15 10 7 4 0.0 F

Neutral-Neutral-Br TCM

N	-2.45223100	-1.24698900	0.03049200
H	-1.56032900	-1.23229100	-0.45356500
C	-3.13769400	0.01567900	-0.16970300
C	-2.17219900	1.16798700	0.00880400
H	-3.57966300	0.14834300	-1.16900600
H	-3.94870400	0.12090000	0.55716200
O	-0.97959800	1.04730300	0.00626300
H	-2.99925800	-2.01004600	-0.34945600
O	-2.72495400	2.38708600	0.12618200
C	2.28829400	4.72961200	-0.38589400
C	3.62453700	4.36318200	-0.43885600
C	4.57105600	5.37601300	-0.58923500
C	4.19829500	6.71165700	-0.68404600
C	2.84526100	7.06519000	-0.62896600
C	1.88689800	6.05464900	-0.47686800
H	3.93706600	3.33044700	-0.36755300
H	4.95373000	7.47883700	-0.79912000
H	0.83476700	6.31008300	-0.42881600
N	2.46054900	8.39787200	-0.66363600
H	3.11737300	9.03121800	-1.09568800
H	1.51009700	8.57341400	-0.95490100
C	6.00508700	4.97245800	-0.64590000
O	6.39685000	3.83595900	-0.57199900
O	6.83893400	6.01376700	-0.79008500
H	7.74253800	5.66938000	-0.81720900
H	-3.68821400	2.33700400	0.14056400
Br	0.96731900	3.37928800	-0.18265400

Neutral-Neutral-Br DCE

N	-2.43790100	-1.25275800	0.01606400
H	-1.59236000	-1.26104300	-0.54551600
C	-3.13047800	0.01006300	-0.16255300
C	-2.17126300	1.16535200	0.02209000
H	-3.58588600	0.15103700	-1.15425800
H	-3.93319700	0.10150900	0.57468200
O	-0.97699000	1.05042800	0.04118800
H	-3.02269700	-2.01628500	-0.30342400
O	-2.72829800	2.38320700	0.12323800
C	2.28893400	4.73782300	-0.37900200

C	3.62394200	4.36774800	-0.43363900
C	4.57207400	5.37869200	-0.58916500
C	4.20137300	6.71461900	-0.68685300
C	2.84872400	7.07157300	-0.62934100
C	1.88853100	6.06277600	-0.47264800
H	3.93401900	3.33446500	-0.36039500
H	4.95727800	7.48054600	-0.80691000
H	0.83710700	6.32074700	-0.42423400
N	2.46683600	8.40381800	-0.66572600
H	3.12357700	9.03567300	-1.10059200
H	1.51562300	8.58114800	-0.95426200
C	6.00554500	4.97237800	-0.64831200
O	6.39364100	3.83395000	-0.57110500
O	6.83995500	6.01006600	-0.79818400
H	7.74447500	5.66737700	-0.82806000
H	-3.69223500	2.33399200	0.11339300
Br	0.96547900	3.38910300	-0.17016700

Neutral-Neutral-Br Acetone

N	-2.46043200	-1.26379100	0.00837900
H	-1.65044400	-1.31098800	-0.60153500
C	-3.12990300	0.01272400	-0.16373000
C	-2.15353600	1.15218800	0.02710200
H	-3.58610700	0.16489800	-1.15311700
H	-3.92914200	0.11323000	0.57578800
O	-0.96114700	1.01933900	0.06948800
H	-3.08420300	-2.01540500	-0.26272500
O	-2.69174900	2.37973200	0.10906200
C	2.29495500	4.73848000	-0.37245200
C	3.63078000	4.37161800	-0.42603300
C	4.57585000	5.38506000	-0.58522200
C	4.20104500	6.71941900	-0.68731600
C	2.84708100	7.07293200	-0.63055200
C	1.88979200	6.06156900	-0.47032400
H	3.94368100	3.33946700	-0.34957400
H	4.95434300	7.48738200	-0.81066700
H	0.83765400	6.31668200	-0.42322800
N	2.46137300	8.40330200	-0.67076800
H	3.11604400	9.03637300	-1.10717700
H	1.50931600	8.57727300	-0.95895800
C	6.01070700	4.98289900	-0.64340100
O	6.40133000	3.84519400	-0.56188900
O	6.84144300	6.02177600	-0.79718500
H	7.74774700	5.68337300	-0.82714900
H	-3.65627100	2.34773300	0.07870400
Br	0.97560000	3.38554300	-0.15921000

Neutral-Neutral-Br DMSO

N	-2.54447300	-1.23409100	0.18658200
H	-1.66463200	-1.38958400	-0.29511800
C	-3.10787000	0.04024300	-0.22162000
C	-2.11208300	1.15646800	0.00410800
H	-3.39750000	0.09836800	-1.28126400
H	-4.00555300	0.25257200	0.36564100

O	-0.95296000	0.98536900	0.26735800
H	-3.16957200	-1.98446900	-0.08536600
O	-2.58285600	2.40447200	-0.14748300
C	2.29695500	4.72091200	-0.31662300
C	3.63055000	4.36000200	-0.42991300
C	4.56472700	5.37980000	-0.61192400
C	4.18130300	6.71396300	-0.67777500
C	2.82952200	7.06120300	-0.56045000
C	1.88295800	6.04345500	-0.37766500
H	3.94979400	3.32799900	-0.38260200
H	4.92609200	7.48704500	-0.81933300
H	0.83276400	6.29337700	-0.28424900
N	2.43782500	8.39009600	-0.56360400
H	3.07186700	9.03272500	-1.01627700
H	1.47415900	8.56441800	-0.81044600
C	5.99750500	4.98454900	-0.73648900
O	6.39463100	3.84694900	-0.68766300
O	6.81688000	6.02848100	-0.91058400
H	7.72309800	5.69593700	-0.98282600
H	-3.52774400	2.40743300	-0.34612800
Br	0.99041600	3.36031200	-0.07197400

Neutral-Neutral-Br Water

N	-2.54172000	-1.24019600	0.17365300
H	-1.67772200	-1.39776100	-0.33528000
C	-3.11045600	0.03895900	-0.21169400
C	-2.10891600	1.15173400	0.00548800
H	-3.42089300	0.10711300	-1.26475400
H	-3.99610300	0.24740700	0.39492900
O	-0.94682500	0.97727200	0.25376700
H	-3.17861900	-1.98558200	-0.08438600
O	-2.57867200	2.40135200	-0.13486600
C	2.29786600	4.72248000	-0.32089400
C	3.63157400	4.36155300	-0.43277600
C	4.56596800	5.38151300	-0.61292800
C	4.18260200	6.71571100	-0.67832800
C	2.83062600	7.06293200	-0.56242100
C	1.88380800	6.04499100	-0.38146300
H	3.95066000	3.32949000	-0.38584200
H	4.92748700	7.48893100	-0.81863300
H	0.83350500	6.29487600	-0.28928300
N	2.43900800	8.39167400	-0.56501900
H	3.07359000	9.03479200	-1.01626100
H	1.47554600	8.56638400	-0.81240900
C	5.99892700	4.98638200	-0.73602700
O	6.39588200	3.84862400	-0.68751800
O	6.81837200	6.03038300	-0.90824700
H	7.72479800	5.69821000	-0.97992100
H	-3.52564200	2.40739100	-0.32355000
Br	0.99115500	3.36138900	-0.07902600

Neutral-Neutral-I Vacuum

N	-2.48415300	-1.16816700	0.42325800
H	-1.47719400	-1.05919700	0.36006500

C	-3.14059100	-0.05075400	-0.21950900
C	-2.30434100	1.20528000	-0.06329900
H	-3.29333400	-0.16645100	-1.30446400
H	-4.12606400	0.12177300	0.22811100
O	-1.14208300	1.19257000	0.21704700
H	-2.74680400	-2.04921400	0.00260700
O	-2.93275800	2.36690100	-0.31523400
C	2.41164700	4.89220800	-0.40598000
C	3.73813700	4.51139600	-0.55007200
C	4.69442700	5.50850700	-0.73589000
C	4.34395200	6.85320200	-0.77627000
C	3.00632200	7.22566600	-0.62747300
C	2.04014600	6.22931600	-0.44499100
H	4.04622000	3.47486600	-0.52233300
H	5.10753800	7.60660000	-0.92649800
H	0.99863100	6.50968500	-0.33638500
N	2.62915400	8.56342600	-0.71661800
H	1.75324800	8.79847900	-0.27507800
H	3.35508800	9.23151900	-0.50648000
C	6.11231900	5.07813000	-0.89068300
O	6.49096200	3.93847700	-0.87220300
O	6.96143700	6.11297700	-1.05895800
H	7.84634400	5.73653200	-1.15089700
H	-3.86888000	2.22294800	-0.48821300
I	0.92012700	3.41053200	-0.11568500

Neutral-Neutral-I TCM

N	-2.39743100	-1.21872000	0.27236900
H	-1.48540700	-1.19733200	-0.17225000
C	-3.15897300	-0.04723700	-0.11675300
C	-2.29499500	1.19145200	-0.02724100
H	-3.54459100	-0.06709700	-1.14753900
H	-4.02004400	0.07622200	0.54673100
O	-1.09859800	1.16539100	0.06333000
H	-2.87014300	-2.06212700	-0.02983000
O	-2.93621800	2.36741300	-0.10508100
C	2.42011400	4.89963700	-0.46576300
C	3.75131500	4.51942000	-0.55730200
C	4.71092600	5.51927500	-0.71694300
C	4.35682300	6.86179700	-0.78435800
C	3.01179000	7.23340300	-0.69020600
C	2.04214800	6.23357500	-0.53168600
H	4.05824400	3.48354400	-0.50775400
H	5.12049000	7.61918000	-0.91141400
H	0.99714100	6.51336800	-0.46255900
N	2.63503100	8.56446200	-0.81152700
H	1.74367200	8.80561300	-0.40347300
H	3.35103100	9.24073400	-0.58954200
C	6.13666500	5.09497900	-0.81218400
O	6.51355800	3.95186900	-0.76265200
O	6.98328200	6.12552200	-0.96158000
H	7.88041000	5.76762100	-1.01595600
H	-3.89219500	2.24623000	-0.15476400
I	0.92545200	3.40901500	-0.21620200

Neutral-Neutral-I DCE

N	-2.50301400	-1.20063400	0.27062900
H	-1.53738100	-1.27415100	-0.03329100
C	-3.09570700	0.00757500	-0.27229100
C	-2.21037300	1.19984000	0.01324100
H	-3.24587200	-0.00089500	-1.36257200
H	-4.07455600	0.17929900	0.18427000
O	-1.06878800	1.11519700	0.37808600
H	-2.99473700	-2.01428400	-0.08037800
O	-2.75000200	2.40682500	-0.21041700
C	2.41395200	4.87934800	-0.29364400
C	3.74141500	4.50497500	-0.44335400
C	4.68733700	5.50999800	-0.64830200
C	4.32326600	6.85043900	-0.70116400
C	2.98128200	7.21571100	-0.54831700
C	2.02526400	6.21082200	-0.34236400
H	4.05495200	3.47052100	-0.40786800
H	5.07617800	7.61270300	-0.85885100
H	0.98399200	6.48590300	-0.22089000
N	2.60770400	8.55168500	-0.53991200
H	3.23863800	9.18404000	-1.01072900
H	1.64118900	8.73791700	-0.76558200
C	6.10927200	5.09288600	-0.81323500
O	6.49230300	3.95038200	-0.77908600
O	6.94085000	6.12575100	-1.00794200
H	7.83811700	5.77626100	-1.10463900
H	-3.67233800	2.33835800	-0.48660000
I	0.93655300	3.38074000	0.01307600

Neutral-Neutral-I Acetone

N	-2.44467600	-1.25847700	0.07160700
H	-1.63787800	-1.31886300	-0.54121100
C	-3.14803300	-0.01081000	-0.16121500
C	-2.20918100	1.16455200	-0.00837100
H	-3.59856200	0.08767800	-1.16003300
H	-3.95728100	0.09752100	0.56619800
O	-1.01369100	1.06830100	0.06927700
H	-3.05109900	-2.03909400	-0.15318500
O	-2.77994700	2.37822100	-0.00494900
C	2.43328900	4.88366200	-0.38776900
C	3.77058500	4.52057200	-0.45591100
C	4.71814100	5.53306700	-0.61072400
C	4.34592300	6.86954300	-0.69504500
C	2.99374800	7.22376000	-0.62417300
C	2.03605500	6.21102800	-0.46829700
H	4.09033400	3.48932100	-0.39426900
H	5.09975900	7.63757200	-0.81542200
H	0.98694000	6.47739900	-0.41163100
N	2.60904200	8.55596000	-0.64629200
H	3.26039900	9.19128300	-1.08461100
H	1.65548500	8.73245300	-0.92827500
C	6.15135800	5.12875100	-0.68453900
O	6.54137800	3.98954500	-0.61944200

O	6.98360600	6.16772800	-0.83260200
H	7.88873000	5.82733400	-0.87322200
H	-3.74223800	2.31956600	-0.06066600
I	0.95730900	3.36963700	-0.15735100

Neutral-Neutral-I DMSO

N	-2.49900200	-1.16139300	0.46103800
H	-1.59410100	-1.33906400	0.03682800
C	-3.13776200	-0.03747700	-0.19926300
C	-2.24310900	1.18040400	-0.15881000
H	-3.38077400	-0.20164100	-1.25946500
H	-4.07477400	0.20538800	0.30942000
O	-1.08828800	1.15910000	0.17526200
H	-3.05932700	-1.99581700	0.32824800
O	-2.79556100	2.33231500	-0.56525200
C	2.42742900	4.90235700	-0.35994900
C	3.75177000	4.52274100	-0.52298600
C	4.70834100	5.52792800	-0.67172400
C	4.35720900	6.87281500	-0.65584700
C	3.01783300	7.24327700	-0.48917800
C	2.05110800	6.23807000	-0.34011500
H	4.05441800	3.48454800	-0.53931400
H	5.11735000	7.63525000	-0.77289900
H	1.01200200	6.51669300	-0.20933200
N	2.65771200	8.57996800	-0.41065700
H	3.29684100	9.23001300	-0.84550600
H	1.69385300	8.78822100	-0.62945500
C	6.12721100	5.10600200	-0.85221200
O	6.49805100	3.95841200	-0.87363200
O	6.96859500	6.13798700	-0.99166600
H	7.86375500	5.78757100	-1.10559900
H	-3.72590800	2.21917900	-0.79874200
I	0.93462200	3.40436300	-0.13131600

Neutral-Neutral-I Water

N	-2.49691500	-1.23877400	0.22051200
H	-1.64284900	-1.38159900	-0.30901400
C	-3.12953500	0.00031500	-0.19299400
C	-2.17940100	1.16440900	-0.02555700
H	-3.45967500	0.02256200	-1.24205500
H	-4.01383900	0.18751900	0.42260500
O	-1.00824500	1.05272100	0.22249500
H	-3.11023100	-2.01865900	0.01179500
O	-2.70439200	2.38430800	-0.20966400
C	2.43253800	4.87796900	-0.34605300
C	3.76636300	4.51627200	-0.46701400
C	4.70761400	5.53178100	-0.64081700
C	4.33233000	6.86908500	-0.69158000
C	2.98341500	7.22161600	-0.56708600
C	2.03188100	6.20592900	-0.39248500
H	4.08792900	3.48429600	-0.43247900
H	5.08099400	7.63962600	-0.82720200
H	0.98550900	6.47065500	-0.29459000
N	2.59810300	8.55329200	-0.55484800

H	3.23345700	9.19586400	-1.00600900
H	1.63501500	8.73356200	-0.80011800
C	6.13744700	5.12956500	-0.77335500
O	6.52906300	3.98923900	-0.73800400
O	6.96287900	6.17047700	-0.93826800
H	7.86685100	5.83319600	-1.01650400
H	-3.65071000	2.34085900	-0.39759600
I	0.96389900	3.36112500	-0.08624100

Anion-Neutral-Cl Vacuum SP

N	-2.70583100	-1.21378400	0.46891600
H	-1.80639300	-1.40259200	0.03770300
C	-3.24543500	0.02461500	-0.06200500
C	-2.14298400	1.05440900	-0.20504800
H	-3.70080200	-0.06446700	-1.05978900
H	-4.01422900	0.41872900	0.60930000
O	-0.97584500	0.78697100	-0.19649100
H	-3.32154900	-1.98912100	0.25592700
O	-2.54551500	2.32223900	-0.40035700
C	2.27026300	4.57942300	-0.52932800
C	3.61555500	4.26332500	-0.62840400
C	4.53750700	5.30717400	-0.72551900
C	4.09821900	6.62500400	-0.71972500
C	2.73780400	6.93138000	-0.61571200
C	1.81050700	5.88918500	-0.52228800
H	3.96116000	3.23834100	-0.63034500
H	4.83714000	7.41448600	-0.79846700
H	0.74947000	6.09697200	-0.44789700
Cl	1.09173100	3.28248500	-0.41070200
N	2.29925200	8.25995400	-0.66594900
H	1.41984600	8.42969200	-0.19829200
H	2.99755400	8.93389100	-0.38479800
C	6.04575000	4.99922600	-0.83901300
O	6.36056200	3.79126600	-0.82137100
O	6.80096500	5.98991200	-0.93717200
H	-3.50554000	2.39802500	-0.34992000

Anion-Neutral-Cl TCM ModRedundant

N	-2.70583100	-1.21378400	0.46891600
H	-1.80639300	-1.40259200	0.03770300
C	-3.24543500	0.02461500	-0.06200500
C	-2.14298400	1.05440900	-0.20504800
H	-3.70080200	-0.06446700	-1.05978900
H	-4.01422900	0.41872900	0.60930000
O	-0.97584500	0.78697100	-0.19649100
H	-3.32154900	-1.98912100	0.25592700
O	-2.54551500	2.32223900	-0.40035700
C	2.27026300	4.57942300	-0.52932800
C	3.61555500	4.26332500	-0.62840400
C	4.53750700	5.30717400	-0.72551900
C	4.09821900	6.62500400	-0.71972500
C	2.73780400	6.93138000	-0.61571200
C	1.81050700	5.88918500	-0.52228800
H	3.96116000	3.23834100	-0.63034500

H	4.83714000	7.41448600	-0.79846700
H	0.74947000	6.09697200	-0.44789700
Cl	1.09173100	3.28248500	-0.41070200
N	2.29925200	8.25995400	-0.66594900
H	1.41984600	8.42969200	-0.19829200
H	2.99755400	8.93389100	-0.38479800
C	6.04575000	4.99922600	-0.83901300
O	6.36056200	3.79126600	-0.82137100
O	6.80096500	5.98991200	-0.93717200
H	-3.50554000	2.39802500	-0.34992000

A 15 10 7 120.0 F

D 15 10 7 4 5.0 F

D 9 4 7 19 5.0 F

Anion-Neutral-Cl DCE

N	-2.61135600	-1.22830600	0.40473100
H	-1.88090300	-1.47493400	-0.25542000
C	-3.21007500	0.03653900	0.01908900
C	-2.13256100	1.06061800	-0.26680500
H	-3.83314600	-0.00563500	-0.88681300
H	-3.84499800	0.41011800	0.82757900
O	-0.97386000	0.79259800	-0.41665100
H	-3.30751600	-1.96412300	0.37843500
O	-2.55085500	2.33086500	-0.39940200
C	2.25704100	4.58172100	-0.59265700
C	3.60411300	4.26011300	-0.63680200
C	4.53204900	5.30184900	-0.68683900
C	4.09857100	6.62151900	-0.69044100
C	2.73496800	6.93316200	-0.64314800
C	1.80124000	5.89242000	-0.59575300
H	3.94366100	3.23321900	-0.63239600
H	4.84102400	7.41021800	-0.73203700
H	0.73891000	6.10404200	-0.56443500
Cl	1.07050500	3.28785200	-0.53446300
N	2.30464300	8.26038600	-0.70613600
H	1.39933900	8.43349500	-0.29197800
H	2.98766800	8.93565000	-0.39224000
C	6.03902800	4.98859200	-0.73944700
O	6.35121700	3.77861700	-0.73584900
O	6.80692000	5.97434900	-0.78146600
H	-3.49646900	2.41179800	-0.22539800

Anion-Neutral-Cl Acetone

N	-2.57097300	-1.23629200	0.37546100
H	-1.90845200	-1.49934100	-0.34707200
C	-3.18497500	0.03466700	0.03522900
C	-2.12210400	1.06709900	-0.27182400
H	-3.84405900	0.00696100	-0.84513100
H	-3.78767700	0.39154400	0.87510800
O	-0.96406500	0.81039300	-0.45061800
H	-3.27946400	-1.96026200	0.41196500
O	-2.55151800	2.33484700	-0.38644000
C	2.23751300	4.59358600	-0.60821600

C	3.58215900	4.25985300	-0.63915000
C	4.51953600	5.29353300	-0.67698100
C	4.09842700	6.61728900	-0.68331900
C	2.73670700	6.94125000	-0.65070100
C	1.79347500	5.90803300	-0.61397500
H	3.91199600	3.22987900	-0.63360800
H	4.84690400	7.40066400	-0.71509100
H	0.73291300	6.12949500	-0.59214800
Cl	1.04033600	3.30931300	-0.56263800
N	2.31926100	8.27056400	-0.71781900
H	1.40684100	8.45238300	-0.32351500
H	3.00173300	8.94239600	-0.39545200
C	6.02236000	4.96561700	-0.71249700
O	6.32473600	3.75246500	-0.70785400
O	6.80265400	5.94241100	-0.74335400
H	-3.49510000	2.40839400	-0.19710500

Anion-Neutral-Cl DMSO

N	-2.55505800	-1.23770900	0.36223500
H	-1.91549200	-1.50561200	-0.37903300
C	-3.17219300	0.03594800	0.03713000
C	-2.11297100	1.07192600	-0.26905800
H	-3.83872800	0.01460900	-0.83760400
H	-3.76824900	0.38527200	0.88481200
O	-0.95386200	0.81960100	-0.45076400
H	-3.26712000	-1.95725800	0.41700000
O	-2.54510600	2.33879900	-0.37829600
C	2.22697300	4.59769500	-0.60779700
C	3.57038100	4.25849400	-0.63653800
C	4.51187600	5.28841600	-0.67401600
C	4.09631000	6.61396800	-0.68281300
C	2.73554200	6.94350000	-0.65298200
C	1.78816700	5.91372100	-0.61585700
H	3.89574700	3.22715700	-0.62958500
H	4.84698100	7.39521000	-0.71429300
H	0.72854800	6.13976100	-0.59524800
Cl	1.02568800	3.31746100	-0.56160700
N	2.32368200	8.27343900	-0.72352600
H	1.40925400	8.46000200	-0.33607200
H	3.00667200	8.94459600	-0.40077000
C	6.01238000	4.95347400	-0.70620800
O	6.31035800	3.73885100	-0.69762900
O	6.79859200	5.92567900	-0.73865800
H	-3.48921200	2.40974100	-0.18956800

Anion-Neutral-Cl Water

N	-2.58652300	-1.19186500	0.50052600
H	-1.83171500	-1.49753100	-0.10546800
C	-3.19043200	0.01297700	-0.04016300
C	-2.14009800	1.08098300	-0.25293100
H	-3.69183700	-0.11864000	-1.01019600
H	-3.94044100	0.39428000	0.65783700
O	-0.95729800	0.88121300	-0.21508800
H	-3.27381400	-1.93690600	0.51950900

O	-2.60048000	2.30978500	-0.54097200
C	2.23741800	4.60610300	-0.53605700
C	3.57649600	4.26517900	-0.64251200
C	4.51662200	5.29391800	-0.72489900
C	4.10333700	6.62015500	-0.70040500
C	2.74716400	6.95150600	-0.59077600
C	1.80124700	5.92267000	-0.50874300
H	3.89926900	3.23316400	-0.66132500
H	4.85162100	7.40138700	-0.76894400
H	0.74504600	6.15022500	-0.42562100
Cl	1.03901500	3.32704500	-0.43384300
N	2.33490000	8.28222500	-0.62650300
H	1.44230000	8.46686900	-0.19033900
H	3.03518800	8.94997800	-0.33567000
C	6.01199900	4.95564600	-0.84335800
O	6.30701000	3.74019300	-0.85587400
O	6.79870100	5.92542100	-0.91616900
H	-3.56553400	2.34075900	-0.52876100

Anion-Neutral-Br Vacuum SP

N	-2.72537600	-1.25010600	0.15114500
H	-1.75633500	-1.36529900	-0.12828200
C	-3.18592400	0.07094600	-0.23479600
C	-2.11310600	1.10137100	0.05094500
H	-3.42539800	0.17991400	-1.30342700
H	-4.08760800	0.33449100	0.32597100
O	-0.96374000	0.82927300	0.25095100
H	-3.26979900	-1.96511100	-0.31580300
O	-2.50781600	2.38544600	0.02076900
C	2.35178000	4.67837900	-0.32386900
C	3.69309800	4.35413300	-0.45236000
C	4.61082900	5.38957400	-0.64249200
C	4.17229300	6.70617700	-0.69841800
C	2.81588800	7.02075700	-0.57113100
C	1.89264500	5.98789500	-0.37946800
H	4.04346800	3.33177000	-0.41200900
H	4.90912100	7.48794200	-0.84480600
H	0.83708300	6.20816500	-0.27204700
N	2.38917700	8.35418500	-0.57479300
H	3.01536100	8.98400100	-1.05670400
H	1.43454400	8.48841600	-0.87734700
C	6.11365100	5.07260800	-0.79696400
O	6.42962600	3.86698500	-0.72366800
O	6.86343900	6.05501800	-0.98196400
H	-3.45805400	2.45783000	-0.12730900
Br	1.07326600	3.28153000	-0.06493300

Anion-Neutral-Br TCM ModRedundant

N	-2.72537600	-1.25010600	0.15114500
H	-1.75633500	-1.36529900	-0.12828200
C	-3.18592400	0.07094600	-0.23479600
C	-2.11310600	1.10137100	0.05094500
H	-3.42539800	0.17991400	-1.30342700
H	-4.08760800	0.33449100	0.32597100

O	-0.96374000	0.82927300	0.25095100
H	-3.26979900	-1.96511100	-0.31580300
O	-2.50781600	2.38544600	0.02076900
C	2.35178000	4.67837900	-0.32386900
C	3.69309800	4.35413300	-0.45236000
C	4.61082900	5.38957400	-0.64249200
C	4.17229300	6.70617700	-0.69841800
C	2.81588800	7.02075700	-0.57113100
C	1.89264500	5.98789500	-0.37946800
H	4.04346800	3.33177000	-0.41200900
H	4.90912100	7.48794200	-0.84480600
H	0.83708300	6.20816500	-0.27204700
N	2.38917700	8.35418500	-0.57479300
H	3.01536100	8.98400100	-1.05670400
H	1.43454400	8.48841600	-0.87734700
C	6.11365100	5.07260800	-0.79696400
O	6.42962600	3.86698500	-0.72366800
O	6.86343900	6.05501800	-0.98196400
H	-3.45805400	2.45783000	-0.12730900
Br	1.07326600	3.28153000	-0.06493300

A 15 10 7 120.0 F

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D 9 4 7 26 -15.0 F

Anion-Neutral-Br DCE ModRedundant

N	-2.68382000	-1.25184800	0.13835300
H	-1.76039100	-1.38798800	-0.26076200
C	-3.17575800	0.06760500	-0.21474100
C	-2.11249700	1.11126000	0.05187300
H	-3.45625200	0.18687400	-1.27201100
H	-4.06107500	0.30784200	0.38082100
O	-0.95753800	0.85602900	0.25096900
H	-3.29111000	-1.96380900	-0.25049200
O	-2.51908100	2.39067400	0.01226300
C	2.34875500	4.68120200	-0.33147800
C	3.69051800	4.35432600	-0.45106400
C	4.61030500	5.38856800	-0.63736800
C	4.17492000	6.70613400	-0.69789000
C	2.81733800	7.02359100	-0.57898400
C	1.89153800	5.99063800	-0.39293100
H	4.03716500	3.33104200	-0.40631800
H	4.91144300	7.48862300	-0.84077400
H	0.83556800	6.21284800	-0.29451100
N	2.39369900	8.35448300	-0.58352400
H	3.01773200	8.98905900	-1.06188800
H	1.43558600	8.49406600	-0.87245500
C	6.11011400	5.06757300	-0.78046900
O	6.42480600	3.85971400	-0.71794700
O	6.87069800	6.04602600	-0.94671700
H	-3.46893500	2.45610000	-0.14493400
Br	1.06838100	3.28566000	-0.07983000

A 15 10 7 120.0 F

D 15 10 7 4 15.0 F

D 9 4 7 26 -15.0 F

Anion-Neutral-Br Acetone

N	-2.64506500	-1.24346600	0.21002500
H	-1.73803500	-1.41185800	-0.21345800
C	-3.15362700	0.04703400	-0.21897600
C	-2.12974800	1.13053000	0.04072300
H	-3.40221700	0.11286400	-1.28868400
H	-4.06445900	0.28789700	0.33603400
O	-0.98419600	0.91992900	0.32998600
H	-3.26597800	-1.97864500	-0.10869100
O	-2.55809300	2.39423800	-0.11231100
C	2.33031500	4.69956700	-0.34089300
C	3.66608300	4.35549600	-0.47944700
C	4.59878700	5.37971100	-0.65702300
C	4.18215300	6.70440500	-0.69115500
C	2.83019500	7.03936600	-0.55260000
C	1.89156200	6.01606900	-0.37328600
H	3.99816200	3.32670600	-0.45419800
H	4.92665900	7.48025100	-0.82841000
H	0.84011600	6.25187100	-0.25973200
N	2.42621400	8.37447200	-0.52947800
H	3.05277700	9.01091600	-1.00205200
H	1.46560500	8.53437000	-0.79910800
C	6.09081300	5.03811200	-0.81680700
O	6.38743400	3.82384700	-0.78772800
O	6.86928000	6.00635000	-0.96088100
H	-3.49739000	2.42809400	-0.33266900
Br	1.03476400	3.31816500	-0.09199100

Anion-Neutral-Br DMSO

N	-2.62862900	-1.25043500	0.20438900
H	-1.74349400	-1.42533700	-0.26068600
C	-3.15308000	0.03885100	-0.20925900
C	-2.13042200	1.12774800	0.03079300
H	-3.42692200	0.10589500	-1.27259500
H	-4.05249000	0.27303900	0.36669700
O	-0.97844500	0.92432800	0.30129200
H	-3.26629800	-1.98455800	-0.08232500
O	-2.56725800	2.38879300	-0.11682900
C	2.32581200	4.70897900	-0.34427500
C	3.66077700	4.35950500	-0.47822500
C	4.59793500	5.38003700	-0.65347200
C	4.18687700	6.70645100	-0.69006300
C	2.83556000	7.04693500	-0.55610300
C	1.89233300	6.02697900	-0.37919600
H	3.98833800	3.32933700	-0.45106000
H	4.93419000	7.47983900	-0.82565300
H	0.84143400	6.26717600	-0.26999600
N	2.43691200	8.38268700	-0.53466100
H	3.06609900	9.01797700	-1.00530900
H	1.47658100	8.54706600	-0.80268000
C	6.08819700	5.03210900	-0.80728000

O	6.37963500	3.81604800	-0.78527300
O	6.87364000	5.99655300	-0.93984100
H	-3.51036800	2.41843600	-0.32159600
Br	1.02519700	3.33185300	-0.09960400

Anion-Neutral-Br Water

N	-2.61822700	-1.25534300	0.19503400
H	-1.74676300	-1.42930100	-0.29552300
C	-3.15401300	0.03473800	-0.20136900
C	-2.13122900	1.12595000	0.02724500
H	-3.44738100	0.10690800	-1.25908700
H	-4.04377900	0.26270800	0.39184000
O	-0.97515500	0.92572700	0.28294200
H	-3.26375000	-1.98843700	-0.07643100
O	-2.57344900	2.38591900	-0.11239800
C	2.32379600	4.71344700	-0.34780800
C	3.65862100	4.36154200	-0.47718000
C	4.59805800	5.38036300	-0.65017100
C	4.18949600	6.70748000	-0.68924100
C	2.83826300	7.05044700	-0.55989700
C	1.89270700	6.03210100	-0.38522600
H	3.98416500	3.33079500	-0.44807500
H	4.93837700	7.47962900	-0.82312800
H	0.84187700	6.27426500	-0.27984200
N	2.44193500	8.38658200	-0.54062300
H	3.07324800	9.02096100	-1.00964800
H	1.48230500	8.55275400	-0.81005800
C	6.08796700	5.02975200	-0.79836200
O	6.37724900	3.81303400	-0.77744000
O	6.87625500	5.99263700	-0.92568100
H	-3.51897900	2.41328500	-0.30626800
Br	1.02051900	3.33835000	-0.10641400

Anion-Neutral-I Vacuum ModRedundant

N	-2.83443200	-1.39211100	-0.09088100
H	-2.37957200	-1.54926900	0.80269500
C	-3.31393800	-0.03077200	-0.15244200
C	-2.24348200	1.03912600	0.06282700
H	-3.78252900	0.14828400	-1.12630400
H	-4.09581600	0.11711300	0.60053600
O	-1.09741700	0.79199400	0.27910700
H	-2.10998900	-1.52664700	-0.78899800
O	-2.67623000	2.31482800	-0.00829300
C	2.49246100	4.86641100	-0.42156900
C	3.82873000	4.52590800	-0.53947200
C	4.75871300	5.54427500	-0.76674300
C	4.33071800	6.86080000	-0.86859900
C	2.98112000	7.18973500	-0.74606000
C	2.04361900	6.17827600	-0.52523200
H	4.19215000	3.50933200	-0.46270400
H	5.08839900	7.61936700	-1.04107900
H	0.98956100	6.41682100	-0.44211700
N	2.54912400	8.52864900	-0.89438900
H	1.74647400	8.75048000	-0.32145600

H	3.29423000	9.18895500	-0.71903000
C	6.27651700	5.20824300	-0.89658100
O	6.55527000	4.00045100	-0.80484500
O	7.01326600	6.19618800	-1.07491000
H	-3.61553600	2.34772800	-0.21610800
I	1.03916100	3.32950500	-0.08119900

A 15 10 7 120.0 F

D 15 10 7 4 15.0 F

D 9 4 7 26 -15.0 F

Anion-Neutral-I TCM

N	-2.58756200	-1.22042500	0.30721700
H	-1.57985000	-1.23055600	0.18532400
C	-3.13235800	0.00325000	-0.25095100
C	-2.25965500	1.18170900	0.12513700
H	-3.19813100	0.01921500	-1.34946000
H	-4.14157000	0.17557800	0.13520500
O	-1.14328200	1.07517100	0.54970200
H	-2.96591400	-2.02704900	-0.17442100
O	-2.78523900	2.39871400	-0.08682900
C	2.43298400	4.86195300	-0.36515100
C	3.75674600	4.49223700	-0.54831300
C	4.70126100	5.49147500	-0.79602200
C	4.30643100	6.82133400	-0.85656300
C	2.96989000	7.18505800	-0.67056000
C	2.02064700	6.18732200	-0.42259300
H	4.08274900	3.46187500	-0.50576200
H	5.06290600	7.57416100	-1.04803600
H	0.97998900	6.45419100	-0.27985600
N	2.57158300	8.52311000	-0.78714100
H	1.73917900	8.75836200	-0.26457200
H	3.31199800	9.18673900	-0.60584300
C	6.18581500	5.12051900	-0.99787200
O	6.45795200	3.90264300	-0.95609500
O	6.96750400	6.07798100	-1.18179400
H	-3.68922000	2.34011100	-0.41843400
I	0.96571500	3.35899200	0.01983800

Anion-Neutral-I DCE

N	-2.50181100	-1.28629000	0.08315100
H	-1.65103000	-1.28843000	-0.47058400
C	-3.20538700	-0.03142800	-0.10760900
C	-2.25721300	1.13383100	0.06912700
H	-3.65907400	0.09767300	-1.10171500
H	-4.01079800	0.05941900	0.62673900
O	-1.06154600	1.02841400	0.08958900
H	-3.07575300	-2.05743600	-0.23765100
O	-2.82366600	2.34697400	0.16084800
C	2.46004500	4.87679100	-0.47962000
C	3.80000300	4.52141700	-0.53168500
C	4.75286900	5.52945600	-0.69897700
C	4.35256400	6.85422500	-0.81492700
C	2.99934100	7.20399100	-0.76515300

C	2.04203200	6.19624400	-0.59441800
H	4.12818800	3.49468200	-0.44406500
H	5.11321200	7.61562200	-0.94580900
H	0.98983800	6.45362700	-0.55537100
N	2.59904200	8.53118300	-0.94348800
H	1.70901000	8.76453000	-0.52586700
H	3.30498100	9.21382100	-0.70508500
C	6.25050900	5.17386600	-0.75054600
O	6.53355000	3.95828400	-0.68432800
O	7.04227900	6.13626800	-0.85263300
H	-3.78714900	2.29024900	0.14876500
I	0.98653400	3.35668800	-0.21253500

Anion-Neutral-I Acetone

N	-2.53377000	-1.17924900	0.53087900
H	-1.61693800	-1.33667700	0.12463600
C	-3.17990200	-0.06346900	-0.13578400
C	-2.28477700	1.15518200	-0.11505700
H	-3.42889400	-0.23832700	-1.19301700
H	-4.11413500	0.18262600	0.37659800
O	-1.12315000	1.13299600	0.19058900
H	-3.07545600	-2.02372000	0.38589900
O	-2.84849300	2.30693100	-0.50942300
C	2.44166500	4.90344200	-0.46484300
C	3.76470300	4.52582700	-0.64315900
C	4.72919800	5.52388400	-0.80453900
C	4.35651800	6.86188700	-0.78666000
C	3.02020800	7.23490600	-0.60692800
C	2.05152200	6.23608600	-0.44481900
H	4.07114100	3.48875200	-0.65891400
H	5.12284400	7.61789700	-0.91486200
H	1.01261600	6.51114200	-0.30504300
N	2.64509400	8.57885000	-0.64818100
H	1.78835400	8.79701700	-0.15869000
H	3.38186900	9.22642200	-0.40530900
C	6.20633700	5.13869600	-0.99971600
O	6.46153200	3.91480000	-1.02823900
O	7.01658200	6.08506700	-1.11084300
H	-3.78472400	2.19245300	-0.71609700
I	0.95062600	3.40024600	-0.20232300

Anion-Neutral-I DMSO

N	-2.52407800	-1.18342500	0.52053900
H	-1.62767900	-1.35951100	0.07799500
C	-3.17757500	-0.06021900	-0.12653700
C	-2.27720800	1.15448500	-0.11699000
H	-3.45038700	-0.22826400	-1.17886500
H	-4.09950800	0.18775600	0.40668900
O	-1.11214500	1.12918000	0.17701500
H	-3.08566600	-2.01876900	0.39958200
O	-2.84009400	2.30802900	-0.50613600
C	2.44007000	4.90420500	-0.46621800
C	3.76375900	4.52601700	-0.63971400
C	4.72887200	5.52367000	-0.79980300

C	4.35673500	6.86197300	-0.78519800
C	3.01965800	7.23571100	-0.61049200
C	2.05027200	6.23684800	-0.44972100
H	4.06930200	3.48866000	-0.65269500
H	5.12300200	7.61820500	-0.91240400
H	1.01108600	6.51260200	-0.31354400
N	2.64493500	8.57855200	-0.65618100
H	1.78352000	8.79857800	-0.17586200
H	3.37925600	9.22846800	-0.41229600
C	6.20537800	5.13743200	-0.99104800
O	6.46117600	3.91322400	-1.01678000
O	7.01757300	6.08226100	-1.10300500
H	-3.77866800	2.19733800	-0.70487700
I	0.94898500	3.40066300	-0.20730000

Anion-Neutral-I Water

N	-2.55960700	-1.25853200	0.22043000
H	-1.70040600	-1.40919900	-0.29856600
C	-3.17026700	-0.00864800	-0.19429700
C	-2.20234800	1.13976400	-0.01802200
H	-3.49256200	0.02098300	-1.24558900
H	-4.05597000	0.19057900	0.41544000
O	-1.03368700	1.00817200	0.22967900
H	-3.18005700	-2.02907800	-0.00135500
O	-2.70942000	2.36893700	-0.19470500
C	2.45379700	4.87537500	-0.36302100
C	3.78847200	4.51781300	-0.48980100
C	4.73805700	5.52872200	-0.65877600
C	4.34101000	6.85928900	-0.69670700
C	2.99272500	7.21203200	-0.57031500
C	2.03875700	6.19992200	-0.39971500
H	4.11345000	3.48669800	-0.46268700
H	5.09645900	7.62565800	-0.82755500
H	0.99163300	6.45980100	-0.29772500
N	2.60636500	8.55194800	-0.54991500
H	3.24315300	9.18095400	-1.01896500
H	1.64899800	8.72480500	-0.82346400
C	6.22544100	5.16650900	-0.80383800
O	6.50608400	3.94757800	-0.78512800
O	7.02175200	6.12353400	-0.92678300
H	-3.65667600	2.34026800	-0.38042800
I	0.98541900	3.34978500	-0.10203800

Cation-Cation-Cl Vacuum SP

N	-2.35370200	-1.25360800	0.15320900
H	-1.48521400	-1.15212100	-0.38893700
C	-3.19664800	-0.04110300	-0.04083700
C	-2.25762700	1.15265100	-0.17043700
H	-3.76770300	-0.15417300	-0.96257700
H	-3.88153300	0.05520200	0.79991200
O	-1.07870600	0.99610400	-0.31261300
H	-2.83480700	-2.10860600	-0.13705600
O	-2.81332000	2.35199600	-0.14805800
C	2.08814900	4.62178800	-0.50180400

C	3.42691800	4.26196000	-0.53921500
C	4.40003200	5.25305200	-0.62579900
C	4.04958000	6.59885100	-0.67421300
C	2.70355700	6.91265100	-0.62952900
C	1.70550200	5.95849400	-0.54532100
H	3.72478200	3.22140400	-0.50630100
H	4.80917100	7.36817900	-0.74838100
H	0.65695800	6.23115300	-0.51778000
Cl	0.86988200	3.39401300	-0.40800500
N	2.31612800	8.33763900	-0.66777900
H	2.60947200	8.83140800	0.18289800
H	2.73933800	8.82052900	-1.46769400
C	5.83245700	4.81837300	-0.66924500
O	6.17884100	3.67095100	-0.60938700
O	6.67187300	5.84958300	-0.78275100
H	7.57926600	5.51183000	-0.81072000
H	1.30099500	8.44927500	-0.74896500
H	-3.76899400	2.32894600	-0.00598000
H	-2.07685100	-1.36661700	1.13293700

Cation-Cation-Cl TCM

N	-2.35370200	-1.25360800	0.15320900
H	-1.48521400	-1.15212100	-0.38893700
C	-3.19664800	-0.04110300	-0.04083700
C	-2.25762700	1.15265100	-0.17043700
H	-3.76770300	-0.15417300	-0.96257700
H	-3.88153300	0.05520200	0.79991200
O	-1.07870600	0.99610400	-0.31261300
H	-2.83480700	-2.10860600	-0.13705600
O	-2.81332000	2.35199600	-0.14805800
C	2.08814900	4.62178800	-0.50180400
C	3.42691800	4.26196000	-0.53921500
C	4.40003200	5.25305200	-0.62579900
C	4.04958000	6.59885100	-0.67421300
C	2.70355700	6.91265100	-0.62952900
C	1.70550200	5.95849400	-0.54532100
H	3.72478200	3.22140400	-0.50630100
H	4.80917100	7.36817900	-0.74838100
H	0.65695800	6.23115300	-0.51778000
Cl	0.86988200	3.39401300	-0.40800500
N	2.31612800	8.33763900	-0.66777900
H	2.60947200	8.83140800	0.18289800
H	2.73933800	8.82052900	-1.46769400
C	5.83245700	4.81837300	-0.66924500
O	6.17884100	3.67095100	-0.60938700
O	6.67187300	5.84958300	-0.78275100
H	7.57926600	5.51183000	-0.81072000
H	1.30099500	8.44927500	-0.74896500
H	-3.76899400	2.32894600	-0.00598000
H	-2.07685100	-1.36661700	1.13293700

Cation-Cation-Cl DCE

N	-2.30416400	-1.22671100	0.09972500
H	-1.44268800	-1.13505300	-0.44985100

C	-3.17560400	-0.03912200	-0.10324200
C	-2.30007900	1.20077500	-0.01895600
H	-3.63784500	-0.10933500	-1.08778900
H	-3.95259000	-0.03690800	0.66023800
O	-1.11076400	1.11582300	0.09902200
H	-2.77823500	-2.09214500	-0.17069200
O	-2.91714500	2.36924500	-0.10019100
C	2.09289400	4.61383700	-0.43214900
C	3.42921300	4.25078700	-0.49715400
C	4.39983100	5.23999100	-0.62819600
C	4.04860200	6.58477200	-0.69316100
C	2.70420400	6.90252700	-0.62317300
C	1.70972200	5.94937700	-0.49591600
H	3.72643500	3.21081200	-0.44889200
H	4.80665200	7.35128200	-0.79815300
H	0.66268900	6.22363600	-0.44729700
Cl	0.87552600	3.39220500	-0.26768400
N	2.31399000	8.32396200	-0.68146700
H	2.65531200	8.84302100	0.13496000
H	2.68626300	8.78411800	-1.51908700
C	5.83000500	4.80601900	-0.69956000
O	6.18080400	3.65832400	-0.63951200
O	6.66778100	5.83490400	-0.83798500
H	7.57424100	5.49646700	-0.88197900
H	1.29587200	8.43420700	-0.70451000
H	-3.87620200	2.28967700	-0.19610500
H	-2.01692200	-1.31669200	1.07832900

Cation-Cation-Cl Acetone

N	-2.30134900	-1.22790600	0.09968200
H	-1.43691800	-1.13625000	-0.44472300
C	-3.16996900	-0.03911400	-0.10279200
C	-2.29567500	1.20027800	-0.01275100
H	-3.62855700	-0.10509200	-1.08934800
H	-3.94998700	-0.03815300	0.65752400
O	-1.10533700	1.11891800	0.10254400
H	-2.77515800	-2.09094300	-0.17825600
O	-2.91430000	2.36883800	-0.08693500
C	2.08966000	4.61757900	-0.41998900
C	3.42457000	4.25107300	-0.48990400
C	4.39603900	5.23820800	-0.63088100
C	4.04628400	6.58303000	-0.70101400
C	2.70301100	6.90457000	-0.62615600
C	1.70802700	5.95323500	-0.48868100
H	3.71933900	3.21065000	-0.43778200
H	4.80477800	7.34766900	-0.81309200
H	0.66187500	6.22951900	-0.43580900
Cl	0.87084500	3.39814100	-0.24345500
N	2.31584600	8.32551000	-0.69075800
H	2.66877300	8.84991500	0.11714200
H	2.67885500	8.77856500	-1.53625300
C	5.82500500	4.80318600	-0.70682700
O	6.17639300	3.65499300	-0.64455500
O	6.66353700	5.83018600	-0.85175400

H	7.56954100	5.49083300	-0.89779500
H	1.29799100	8.43915100	-0.70179400
H	-3.87400800	2.28792200	-0.17562900
H	-2.02131200	-1.32470800	1.07961400

Cation-Cation-Cl DMSO

N	-2.35203700	-1.24548500	-0.02940200
H	-1.46330900	-1.11173200	-0.52495300
C	-3.16239600	-0.00093000	-0.08994300
C	-2.22086000	1.17931800	0.08535500
H	-3.64367300	0.05602700	-1.06640500
H	-3.92464800	-0.03618600	0.68654400
O	-1.03030400	1.03594600	0.08780000
H	-2.84447100	-2.03938400	-0.44570700
O	-2.78005300	2.37340100	0.20720600
C	2.08591900	4.60998100	-0.41993400
C	3.42431000	4.25156300	-0.45574300
C	4.39074100	5.24189100	-0.60835100
C	4.03206000	6.58104300	-0.72441700
C	2.68557700	6.89500500	-0.68128900
C	1.69554200	5.93994500	-0.53322800
H	3.72523300	3.21549500	-0.36689500
H	4.78678600	7.34805000	-0.84371200
H	0.64671800	6.20957100	-0.50577800
Cl	0.87467700	3.38448700	-0.22934800
N	2.29031200	8.31033500	-0.78952100
H	2.62126000	8.85662200	0.01321800
H	2.67028100	8.74541100	-1.63674500
C	5.82416600	4.81757600	-0.64131400
O	6.18417500	3.67483400	-0.53591400
O	6.65752100	5.84656900	-0.79980200
H	7.56696500	5.51380100	-0.81530400
H	1.27228600	8.41670500	-0.82682200
H	-3.74670000	2.34631300	0.20482700
H	-2.11827900	-1.49637000	0.93515000

Cation-Cation-Cl Water

N	-2.35097000	-1.24556300	-0.02855300
H	-1.46280500	-1.11507800	-0.52574500
C	-3.15994300	-0.00048100	-0.09219500
C	-2.21854200	1.17919200	0.08594300
H	-3.63801900	0.05643000	-1.07017500
H	-3.92484700	-0.03473800	0.68173000
O	-1.02795900	1.03547800	0.09334300
H	-2.84519900	-2.04004200	-0.44161800
O	-2.77743700	2.37376400	0.20496600
C	2.08425400	4.61140500	-0.41382000
C	3.42218400	4.25166200	-0.45239700
C	4.38900500	5.24101900	-0.60863400
C	4.03099700	6.58024900	-0.72583400
C	2.68494900	6.89560900	-0.68007300
C	1.69456300	5.94148800	-0.52785800
H	3.72225600	3.21539800	-0.36308400
H	4.78606700	7.34634800	-0.84814000

H	0.64603600	6.21189800	-0.49806600
Cl	0.87251900	3.38678700	-0.21945700
N	2.29079800	8.31094400	-0.78992300
H	2.61813600	8.85701900	0.01443100
H	2.67494300	8.74601800	-1.63525300
C	5.82198400	4.81584100	-0.64466500
O	6.18171800	3.67283200	-0.53960300
O	6.65571400	5.84409900	-0.80538200
H	7.56492300	5.51078700	-0.82283800
H	1.27304000	8.41780000	-0.83216000
H	-3.74411800	2.34733200	0.19812400
H	-2.11644700	-1.49369700	0.93650800

Cation-Cation-Br Vacuum SP

N	-2.33226300	-1.23475000	0.09826600
H	-1.45207400	-1.11348100	-0.41891600
C	-3.18602700	-0.02821500	-0.08091000
C	-2.26773900	1.18718800	-0.08304100
H	-3.70334200	-0.10268400	-1.03789900
H	-3.91714700	0.01465500	0.72545200
O	-1.07681400	1.06023500	-0.12724500
H	-2.79813800	-2.08622200	-0.22550200
O	-2.85108100	2.37227200	-0.05952400
C	2.19196900	4.71724700	-0.46322100
C	3.53258600	4.36366100	-0.51441300
C	4.50068500	5.35685600	-0.63740600
C	4.14469400	6.69998400	-0.70858300
C	2.79775400	7.00915600	-0.65272900
C	1.80539600	6.05213700	-0.53364500
H	3.84174600	3.32732900	-0.46114700
H	4.90162400	7.46941000	-0.80646000
H	0.75782900	6.32714800	-0.49605400
N	2.40031500	8.43086500	-0.71492100
H	2.73557000	8.95254500	0.10263000
H	2.77425700	8.89101700	-1.55189100
C	5.93424300	4.92692400	-0.68978500
O	6.28618600	3.78193900	-0.61683800
O	6.76862200	5.95959900	-0.82650200
H	7.67690300	5.62459400	-0.85800000
H	1.38145000	8.53455500	-0.74310800
H	-3.81409500	2.32291300	0.00655200
H	-2.07660800	-1.37124500	1.08052400
Br	0.87197000	3.37766600	-0.28965000

Cation-Cation-Br TCM

N	-2.33226300	-1.23475000	0.09826600
H	-1.45207400	-1.11348100	-0.41891600
C	-3.18602700	-0.02821500	-0.08091000
C	-2.26773900	1.18718800	-0.08304100
H	-3.70334200	-0.10268400	-1.03789900
H	-3.91714700	0.01465500	0.72545200
O	-1.07681400	1.06023500	-0.12724500
H	-2.79813800	-2.08622200	-0.22550200
O	-2.85108100	2.37227200	-0.05952400

C	2.19196900	4.71724700	-0.46322100
C	3.53258600	4.36366100	-0.51441300
C	4.50068500	5.35685600	-0.63740600
C	4.14469400	6.69998400	-0.70858300
C	2.79775400	7.00915600	-0.65272900
C	1.80539600	6.05213700	-0.53364500
H	3.84174600	3.32732900	-0.46114700
H	4.90162400	7.46941000	-0.80646000
H	0.75782900	6.32714800	-0.49605400
N	2.40031500	8.43086500	-0.71492100
H	2.73557000	8.95254500	0.10263000
H	2.77425700	8.89101700	-1.55189100
C	5.93424300	4.92692400	-0.68978500
O	6.28618600	3.78193900	-0.61683800
O	6.76862200	5.95959900	-0.82650200
H	7.67690300	5.62459400	-0.85800000
H	1.38145000	8.53455500	-0.74310800
H	-3.81409500	2.32291300	0.00655200
H	-2.07660800	-1.37124500	1.08052400
Br	0.87197000	3.37766600	-0.28965000

Cation-Cation-Br DCE

N	-2.28358900	-1.21558700	0.09042600
H	-1.42723500	-1.12306200	-0.46710400
C	-3.16025200	-0.03128400	-0.10820600
C	-2.28897800	1.21187000	-0.03643600
H	-3.63122000	-0.10525900	-1.08833600
H	-3.93034400	-0.02877600	0.66211500
O	-1.09707000	1.13111100	0.06765500
H	-2.75773500	-2.08296100	-0.17360200
O	-2.90942600	2.37753900	-0.11383800
C	2.17899100	4.72416300	-0.41283800
C	3.51479800	4.35832400	-0.48679000
C	4.48755200	5.34336800	-0.63839400
C	4.13969400	6.68829900	-0.71442000
C	2.79681800	7.01025000	-0.63541800
C	1.80072800	6.06091100	-0.48879200
H	3.81533300	3.31978800	-0.42938700
H	4.89906600	7.45146400	-0.83383800
H	0.75658500	6.34480300	-0.43417900
N	2.40944400	8.43214700	-0.70274600
H	2.76662000	8.95895500	0.10176700
H	2.76751200	8.88247000	-1.55179000
C	5.91588100	4.90459200	-0.71700900
O	6.26423400	3.75651200	-0.64995200
O	6.75560600	5.92998200	-0.86977500
H	7.66083700	5.58863000	-0.91651600
H	1.39131400	8.54473000	-0.70812100
H	-3.86979800	2.29566700	-0.19402700
H	-1.98779600	-1.30211600	1.06683200
Br	0.85090200	3.39676600	-0.20124600

Cation-Cation-Br Acetone

N	-2.34539500	-1.23135600	-0.03979400

H	-1.45538000	-1.08587600	-0.53032100
C	-3.16589900	0.00709600	-0.09499700
C	-2.23293900	1.19471400	0.07735000
H	-3.65211400	0.06187400	-1.06930900
H	-3.92452700	-0.03542100	0.68468100
O	-1.04077900	1.05908500	0.07089600
H	-2.82885400	-2.02656400	-0.46415100
O	-2.79853800	2.38372400	0.20499100
C	2.19467200	4.70579000	-0.41455400
C	3.53618700	4.35702500	-0.45517800
C	4.49684900	5.35221600	-0.61767400
C	4.13064300	6.68874400	-0.73899200
C	2.78211800	6.99429700	-0.69151600
C	1.79806200	6.03395600	-0.53379700
H	3.84978600	3.32509700	-0.36228500
H	4.88128000	7.45906600	-0.86497400
H	0.74903200	6.30301700	-0.50316600
N	2.37599000	8.40654900	-0.80985600
H	2.76166900	8.97497000	-0.04825200
H	2.69248800	8.81827400	-1.69406500
C	5.93263600	4.93500000	-0.65424600
O	6.29864000	3.79493600	-0.54549000
O	6.75995200	5.96815800	-0.82004900
H	7.67097700	5.63980300	-0.83725600
H	1.35749400	8.51065900	-0.77721400
H	-3.76498300	2.35202400	0.21130300
H	-2.11359300	-1.48704400	0.92403800
Br	0.88299900	3.36348500	-0.19009000

Cation-Cation-Br DMSO

N	-2.34219100	-1.23238900	-0.03810500
H	-1.45408500	-1.09242500	-0.53308300
C	-3.16156000	0.00610200	-0.09790100
C	-2.23033100	1.19393600	0.07716000
H	-3.64381900	0.05999800	-1.07408500
H	-3.92335400	-0.03492200	0.67877400
O	-1.03770400	1.06031000	0.07834800
H	-2.82885100	-2.02918600	-0.45571700
O	-2.79743500	2.38309100	0.19935100
C	2.19049800	4.70943000	-0.41020600
C	3.53096500	4.35733500	-0.45322600
C	4.49331100	5.35056300	-0.61790700
C	4.12922800	6.68761500	-0.73927100
C	2.78164000	6.99664300	-0.68941400
C	1.79604100	6.03825800	-0.52892000
H	3.84193900	3.32460300	-0.36072300
H	4.88070700	7.45649200	-0.86742300
H	0.74771100	6.30950400	-0.49620300
N	2.37946100	8.40940000	-0.80779000
H	2.76363000	8.97615200	-0.04414900
H	2.70078300	8.82126000	-1.69017500
C	5.92809100	4.93147500	-0.65713000
O	6.29338400	3.79065300	-0.54898700
O	6.75675500	5.96305300	-0.82453400

H	7.66730200	5.63348600	-0.84347400
H	1.36121700	8.51644500	-0.77936300
H	-3.76394900	2.35038700	0.19803900
H	-2.10755400	-1.48297100	0.92631000
Br	0.87664200	3.36900000	-0.18415900

Cation-Cation-Br Water

N	-2.34142400	-1.23148000	-0.03664800
H	-1.45434500	-1.09436100	-0.53406100
C	-3.15974200	0.00751400	-0.09846800
C	-2.22825300	1.19480600	0.07739900
H	-3.63994300	0.06133100	-1.07563400
H	-3.92297300	-0.03247800	0.67682900
O	-1.03560300	1.06104400	0.08081900
H	-2.83006500	-2.02885900	-0.45080400
O	-2.79526900	2.38439000	0.19765600
C	2.18965500	4.70891900	-0.40895800
C	3.52997600	4.35654300	-0.45303300
C	4.49224300	5.34969900	-0.61853500
C	4.12801800	6.68669400	-0.73977400
C	2.78056500	6.99607700	-0.68884100
C	1.79504500	6.03773400	-0.52729000
H	3.84075600	3.32373400	-0.36081300
H	4.87933600	7.45549800	-0.86871800
H	0.74678200	6.30902900	-0.49362800
N	2.37889300	8.40879600	-0.80716100
H	2.76243300	8.97521500	-0.04294200
H	2.70142600	8.82087600	-1.68900300
C	5.92696900	4.93088600	-0.65903900
O	6.29264400	3.78991600	-0.55196500
O	6.75543200	5.96250000	-0.82622100
H	7.66604300	5.63316000	-0.84613100
H	1.36068800	8.51629700	-0.77995300
H	-3.76180400	2.35128000	0.19533900
H	-2.10514400	-1.47949900	0.92799900
Br	0.87613600	3.36804000	-0.18238700

Cation-Cation-I Vacuum SP

N	-2.31895300	-1.24431400	0.05366500
H	-1.60041200	-1.20385600	-0.67743600
C	-3.21805500	-0.06207000	-0.02832800
C	-2.34907500	1.18542500	-0.03936800
H	-3.80214400	-0.12935300	-0.94611700
H	-3.88986100	-0.07002000	0.82943800
O	-1.15224100	1.10519400	-0.03316300
H	-2.83909900	-2.12021400	-0.04787400
O	-2.97792100	2.34606300	-0.06946400
C	2.33820500	4.86885500	-0.48067600
C	3.68179600	4.52177500	-0.51785400
C	4.65207800	5.51354600	-0.64512700
C	4.29620000	6.85537800	-0.73364800
C	2.94877700	7.16290600	-0.69001600
C	1.95700100	6.20472300	-0.56893800
H	3.99966400	3.48886300	-0.44947700

H	5.05301400	7.62488500	-0.83277300
H	0.91116100	6.48859000	-0.54281800
N	2.55042500	8.58399200	-0.76615100
H	2.88289300	9.11307100	0.04768500
H	2.92641200	9.03715400	-1.60577800
C	6.08594200	5.08436400	-0.68034700
O	6.43938400	3.94089200	-0.59005900
O	6.92135100	6.11592400	-0.82308200
H	7.82974600	5.78047100	-0.84215900
H	1.53153200	8.68626600	-0.79799000
H	-3.94108000	2.26047200	-0.07363700
H	-1.81993900	-1.27294000	0.94821400
I	0.86059200	3.36829100	-0.27652800

Cation-Cation-I TCM

N	-2.31895300	-1.24431400	0.05366500
H	-1.60041200	-1.20385600	-0.67743600
C	-3.21805500	-0.06207000	-0.02832800
C	-2.34907500	1.18542500	-0.03936800
H	-3.80214400	-0.12935300	-0.94611700
H	-3.88986100	-0.07002000	0.82943800
O	-1.15224100	1.10519400	-0.03316300
H	-2.83909900	-2.12021400	-0.04787400
O	-2.97792100	2.34606300	-0.06946400
C	2.33820500	4.86885500	-0.48067600
C	3.68179600	4.52177500	-0.51785400
C	4.65207800	5.51354600	-0.64512700
C	4.29620000	6.85537800	-0.73364800
C	2.94877700	7.16290600	-0.69001600
C	1.95700100	6.20472300	-0.56893800
H	3.99966400	3.48886300	-0.44947700
H	5.05301400	7.62488500	-0.83277300
H	0.91116100	6.48859000	-0.54281800
N	2.55042500	8.58399200	-0.76615100
H	2.88289300	9.11307100	0.04768500
H	2.92641200	9.03715400	-1.60577800
C	6.08594200	5.08436400	-0.68034700
O	6.43938400	3.94089200	-0.59005900
O	6.92135100	6.11592400	-0.82308200
H	7.82974600	5.78047100	-0.84215900
H	1.53153200	8.68626600	-0.79799000
H	-3.94108000	2.26047200	-0.07363700
H	-1.81993900	-1.27294000	0.94821400
I	0.86059200	3.36829100	-0.27652800

Cation-Cation-I DCE

N	-2.37389300	-1.25282800	-0.04331600
H	-1.48768100	-1.09647000	-0.53823400
C	-3.20500200	-0.02015700	-0.08570800
C	-2.27883800	1.17480500	0.07403700
H	-3.70521100	0.03190700	-1.05335800
H	-3.95190200	-0.06956200	0.70481100
O	-1.08524800	1.04511500	0.04845400
H	-2.85331700	-2.04976800	-0.46934100

O	-2.84703800	2.35924800	0.20943600
C	2.34500200	4.85129200	-0.44190000
C	3.69118700	4.51576200	-0.47647700
C	4.64999000	5.51467000	-0.63314200
C	4.27913000	6.84969000	-0.75483500
C	2.92888500	7.14672000	-0.71330000
C	1.94892800	6.18022700	-0.56199000
H	4.01858400	3.48790200	-0.38348700
H	5.02730700	7.62361300	-0.87598300
H	0.90051300	6.45362100	-0.53755900
N	2.51507100	8.55838900	-0.83156900
H	2.89488100	9.12812200	-0.06804700
H	2.83143500	8.97305900	-1.71441300
C	6.08778400	5.10291100	-0.66312800
O	6.45781600	3.96504500	-0.55091100
O	6.91169700	6.13968900	-0.82819800
H	7.82384300	5.81435800	-0.84150500
H	1.49577800	8.65576500	-0.80176900
H	-3.81309800	2.32522400	0.23384400
H	-2.13398500	-1.51216200	0.91763600
I	0.88477200	3.33814600	-0.19985400

Cation-Cation-I Acetone

N	-2.31561500	-1.24050700	0.04642600
H	-1.59916900	-1.21386900	-0.68624300
C	-3.20664100	-0.05510800	-0.04130400
C	-2.33592500	1.18880300	-0.04520400
H	-3.78454500	-0.11975900	-0.96291800
H	-3.88449600	-0.06146100	0.81131100
O	-1.13761000	1.11226000	-0.03361400
H	-2.84344900	-2.11166900	-0.05116500
O	-2.96034700	2.35323300	-0.07363400
C	2.33272100	4.86743700	-0.46706400
C	3.67434400	4.51610200	-0.51500800
C	4.64497800	5.50731900	-0.64578800
C	4.28939000	6.84946600	-0.72834200
C	2.94343500	7.16235100	-0.67553000
C	1.95229500	6.20388200	-0.54877400
H	3.98811900	3.48171800	-0.45310200
H	5.04496100	7.61846100	-0.83128600
H	0.90755300	6.48936000	-0.51415700
N	2.54947700	8.58154300	-0.75138000
H	2.88759300	9.11131400	0.05932700
H	2.92227000	9.03318600	-1.59316600
C	6.07719800	5.08071100	-0.69405600
O	6.43605000	3.93545100	-0.61773200
O	6.91267500	6.11196100	-0.83124000
H	7.82089000	5.77674600	-0.85908000
H	1.53130000	8.68935400	-0.77790800
H	-3.92384500	2.26985200	-0.07859700
H	-1.81936300	-1.27073300	0.94180000
I	0.85314700	3.36692700	-0.26237600

Cation-Cation-I DMSO

N	-2.31550400	-1.24049200	0.04837100
H	-1.59678700	-1.21626500	-0.68190800
C	-3.20497400	-0.05469400	-0.04379600
C	-2.33391100	1.18860700	-0.04534200
H	-3.77909400	-0.11963300	-0.96776300
H	-3.88620500	-0.06018700	0.80606300
O	-1.13533400	1.11274300	-0.03276000
H	-2.84428600	-2.11086500	-0.05024500
O	-2.95731000	2.35395900	-0.07234900
C	2.33133000	4.86846800	-0.46383000
C	3.67236800	4.51560700	-0.51367600
C	4.64346000	5.50615500	-0.64637800
C	4.28845600	6.84838400	-0.72929400
C	2.94297100	7.16304800	-0.67475300
C	1.95153500	6.20509300	-0.54548300
H	3.98491500	3.48087000	-0.45186100
H	5.04426700	7.61663600	-0.83391800
H	0.90714000	6.49131000	-0.50910300
N	2.55070700	8.58206900	-0.75216100
H	2.89180000	9.11291600	0.05652700
H	2.92186200	9.03177700	-1.59569100
C	6.07521900	5.07950600	-0.69674700
O	6.43457800	3.93379900	-0.62265800
O	6.91108200	6.11031700	-0.83305000
H	7.81921200	5.77499600	-0.86232000
H	1.53272000	8.69168300	-0.77613700
H	-3.92084800	2.27119800	-0.07729800
H	-1.82316100	-1.27094500	0.94574000
I	0.85118600	3.36827100	-0.25798500

Cation-Cation-I Water

N	-2.31497400	-1.24142200	0.04923100
H	-1.59483300	-1.21787400	-0.67962500
C	-3.20417100	-0.05577600	-0.04572400
C	-2.33321800	1.18753400	-0.04565300
H	-3.77559600	-0.12109800	-0.97134400
H	-3.88782200	-0.06117700	0.80216400
O	-1.13452700	1.11205100	-0.03187500
H	-2.84363000	-2.11175400	-0.04999500
O	-2.95628400	2.35307200	-0.07283800
C	2.33087100	4.86927600	-0.46217600
C	3.67169500	4.51600900	-0.51354700
C	4.64281300	5.50645400	-0.64688100
C	4.28788400	6.84872300	-0.72906100
C	2.94255400	7.16386600	-0.67322600
C	1.95112500	6.20598700	-0.54303400
H	3.98393900	3.48114000	-0.45255000
H	5.04372300	7.61676700	-0.83429900
H	0.90683800	6.49232300	-0.50544700
N	2.55077100	8.58285000	-0.75061500
H	2.89338500	9.11393500	0.05726500
H	2.92081100	9.03211100	-1.59489200
C	6.07441200	5.07987200	-0.69915000
O	6.43400400	3.93398400	-0.62660700

O	6.91023700	6.11063200	-0.83536000
H	7.81833400	5.77533600	-0.86599200
H	1.53283600	8.69310600	-0.77308800
H	-3.91986900	2.27085100	-0.07719700
H	-1.82468900	-1.27140500	0.94769900
I	0.85077300	3.36895800	-0.25598800

Neutral-Cation-Cl Vacuum SP

N	-2.49975200	-1.23034500	0.10174600
H	-1.61291100	-1.29478400	-0.41062700
C	-3.14971300	0.08164900	-0.16282000
C	-2.08640700	1.15958500	0.00726600
H	-3.53163800	0.08131700	-1.18368800
H	-3.97550100	0.21448300	0.53500600
O	-0.94320600	0.86821100	0.20794800
H	-3.09953300	-2.01273500	-0.17096700
O	-2.49228200	2.41421400	-0.09278700
C	2.16795000	4.59996600	-0.34459700
C	3.49880000	4.23113900	-0.44826500
C	4.43973700	5.24673300	-0.61290400
C	4.06467200	6.58318500	-0.67082700
C	2.71379700	6.93702800	-0.56392500
C	1.76028100	5.92415200	-0.39871000
H	3.80837800	3.19601500	-0.40519900
H	4.81618300	7.35242200	-0.79722200
H	0.70916200	6.17219800	-0.30997200
Cl	0.95994100	3.35535900	-0.13745900
N	2.33074200	8.26825300	-0.56147900
H	2.97753500	8.91424000	-0.98953900
H	1.37171100	8.45549500	-0.81377900
C	5.87082900	4.84187000	-0.72731800
O	6.25924700	3.70249800	-0.68581600
O	6.69972500	5.88314900	-0.88426500
H	7.60248100	5.54105500	-0.94920100
H	-3.44089800	2.49939500	-0.25510900
H	-2.26706500	-1.33699400	1.09342800

Neutral-Cation-Cl TCM

N	-2.49975200	-1.23034500	0.10174600
H	-1.61291100	-1.29478400	-0.41062700
C	-3.14971300	0.08164900	-0.16282000
C	-2.08640700	1.15958500	0.00726600
H	-3.53163800	0.08131700	-1.18368800
H	-3.97550100	0.21448300	0.53500600
O	-0.94320600	0.86821100	0.20794800
H	-3.09953300	-2.01273500	-0.17096700
O	-2.49228200	2.41421400	-0.09278700
C	2.16795000	4.59996600	-0.34459700
C	3.49880000	4.23113900	-0.44826500
C	4.43973700	5.24673300	-0.61290400
C	4.06467200	6.58318500	-0.67082700
C	2.71379700	6.93702800	-0.56392500
C	1.76028100	5.92415200	-0.39871000
H	3.80837800	3.19601500	-0.40519900

H	4.81618300	7.35242200	-0.79722200
H	0.70916200	6.17219800	-0.30997200
Cl	0.95994100	3.35535900	-0.13745900
N	2.33074200	8.26825300	-0.56147900
H	2.97753500	8.91424000	-0.98953900
H	1.37171100	8.45549500	-0.81377900
C	5.87082900	4.84187000	-0.72731800
O	6.25924700	3.70249800	-0.68581600
O	6.69972500	5.88314900	-0.88426500
H	7.60248100	5.54105500	-0.94920100
H	-3.44089800	2.49939500	-0.25510900
H	-2.26706500	-1.33699400	1.09342800

Neutral-Cation-Cl DCE

N	-2.52448700	-1.22920900	0.10504200
H	-1.63810900	-1.31942400	-0.40292300
C	-3.14634400	0.09242400	-0.17037900
C	-2.07468400	1.15684700	0.01121300
H	-3.51371600	0.09655500	-1.19639900
H	-3.98040900	0.23982700	0.51423300
O	-0.93474600	0.86101800	0.22962200
H	-3.14035400	-1.99850700	-0.16895800
O	-2.46698000	2.41622200	-0.09943600
C	2.18093200	4.58717200	-0.33266500
C	3.51419300	4.22779500	-0.44168800
C	4.44677500	5.25004600	-0.61362500
C	4.06126900	6.58362000	-0.67333800
C	2.70813400	6.92792700	-0.56034200
C	1.76298000	5.90808200	-0.38790700
H	3.83068700	3.19479100	-0.39768300
H	4.80580900	7.35841500	-0.80635700
H	0.71050700	6.14887000	-0.29574500
Cl	0.98292000	3.33391700	-0.11809900
N	2.31496400	8.25602900	-0.55827000
H	2.95250200	8.90425600	-0.99728000
H	1.35265900	8.43330300	-0.80672600
C	5.88056900	4.85682300	-0.73352500
O	6.27821600	3.71985800	-0.69021300
O	6.69993000	5.90330300	-0.89699500
H	7.60610700	5.57054100	-0.96619000
H	-3.41291200	2.50738900	-0.27533800
H	-2.30414900	-1.33914400	1.09889100

Neutral-Cation-Cl Acetone

N	-2.53080700	-1.22708900	0.10664500
H	-1.64391500	-1.32482800	-0.39845000
C	-3.14538900	0.09612500	-0.17418400
C	-2.07468100	1.15866100	0.01562200
H	-3.50364900	0.10107200	-1.20341000
H	-3.98557700	0.24620900	0.50216200
O	-0.93525000	0.86502700	0.24261200
H	-3.14995800	-1.99306500	-0.16907700
O	-2.46524200	2.41893800	-0.09755000
C	2.18689000	4.58077700	-0.33056100

C	3.52123100	4.22552000	-0.44122800
C	4.45031300	5.25082700	-0.61445700
C	4.06032400	6.58319800	-0.67386000
C	2.70611200	6.92329600	-0.55897400
C	1.76446400	5.90023900	-0.38518100
H	3.84060600	3.19337600	-0.39775100
H	4.80190900	7.36052100	-0.80846200
H	0.71136800	6.13784500	-0.29225700
Cl	0.99304300	3.32344800	-0.11498700
N	2.30850300	8.24990100	-0.55609500
H	2.94230900	8.89958200	-0.99861500
H	1.34494400	8.42308700	-0.80329400
C	5.88535900	4.86274700	-0.73601800
O	6.28678700	3.72667600	-0.69293700
O	6.70070500	5.91148700	-0.90033600
H	7.60841100	5.58295400	-0.97134300
H	-3.40992700	2.51013100	-0.28076000
H	-2.31661800	-1.33791300	1.10166700

Neutral-Cation-Cl DMSO

N	-2.53129200	-1.22671600	0.10884400
H	-1.64473000	-1.32898600	-0.39555900
C	-3.14404200	0.09568600	-0.17803600
C	-2.07660800	1.15967400	0.01811600
H	-3.49434700	0.09921000	-1.21002700
H	-3.98991400	0.24601700	0.49105600
O	-0.93736900	0.86981500	0.25250600
H	-3.15157600	-1.99251400	-0.16474200
O	-2.46850800	2.41956600	-0.09829400
C	2.18818300	4.58019100	-0.32901800
C	3.52251100	4.22521000	-0.44131700
C	4.45115600	5.25086300	-0.61533400
C	4.06068200	6.58318500	-0.67393900
C	2.70644900	6.92294000	-0.55739500
C	1.76527100	5.89951500	-0.38274100
H	3.84192500	3.19303900	-0.39862700
H	4.80170500	7.36087600	-0.80942800
H	0.71224100	6.13695800	-0.28892500
Cl	0.99466300	3.32258800	-0.11253000
N	2.30839000	8.24937600	-0.55348900
H	2.94067500	8.89874900	-0.99881300
H	1.34423900	8.42158700	-0.79955100
C	5.88625900	4.86348800	-0.73853300
O	6.28809100	3.72730600	-0.69588900
O	6.70087700	5.91231100	-0.90318900
H	7.60894900	5.58486400	-0.97547900
H	-3.41273000	2.50856900	-0.28530900
H	-2.31888300	-1.33461600	1.10456100

Neutral-Cation-Cl Water

N	-2.53168900	-1.22681400	0.10967100
H	-1.64517500	-1.33035700	-0.39444700
C	-3.14376500	0.09548200	-0.17864400
C	-2.07673200	1.15955300	0.01787500

H	-3.49290000	0.09844500	-1.21103300
H	-3.99048700	0.24636100	0.48922300
O	-0.93730000	0.87059200	0.25308300
H	-3.15234400	-1.99237100	-0.16367600
O	-2.46877000	2.41945800	-0.09895900
C	2.18842000	4.58024000	-0.32872500
C	3.52274900	4.22524700	-0.44128900
C	4.45135500	5.25094800	-0.61538700
C	4.06082900	6.58328700	-0.67382900
C	2.70659100	6.92303900	-0.55695500
C	1.76545600	5.89954200	-0.38219600
H	3.84207000	3.19303300	-0.39883400
H	4.80174500	7.36103600	-0.80954500
H	0.71244800	6.13702000	-0.28832300
Cl	0.99487200	3.32258700	-0.11241900
N	2.30846200	8.24939200	-0.55280500
H	2.94047600	8.89873400	-0.99860800
H	1.34418500	8.42141900	-0.79865700
C	5.88646400	4.86370100	-0.73890200
O	6.28834100	3.72744500	-0.69647700
O	6.70091400	5.91248900	-0.90379500
H	7.60908200	5.58533900	-0.97657100
H	-3.41295500	2.50821400	-0.28644500
H	-2.32007600	-1.33430900	1.10558800

Neutral-Cation-Br Vacuum SP

N	-2.37147100	-1.22752700	-0.02768900
H	-1.47078000	-1.05410100	-0.49243100
C	-3.19839900	0.00998200	-0.07366100
C	-2.25590200	1.19374600	0.11031000
H	-3.68353500	0.07059100	-1.04845700
H	-3.95609000	-0.04113500	0.70646100
O	-1.06823900	1.03855700	0.09956700
H	-2.83586500	-2.01849200	-0.48002400
O	-2.81181200	2.38375600	0.25403800
C	2.26199800	4.75457200	-0.44218600
C	3.59003600	4.36150700	-0.47830200
C	4.55371500	5.35363600	-0.65859700
C	4.20322900	6.69061900	-0.79905600
C	2.85579000	7.06947300	-0.75905700
C	1.87920300	6.08051600	-0.57957500
H	3.88544600	3.32718500	-0.37032000
H	4.97106600	7.44096800	-0.94138000
H	0.83086500	6.35396400	-0.55158500
N	2.48826100	8.39112800	-0.95401800
H	1.58515500	8.65786000	-0.59096100
H	3.20135400	9.07853500	-0.75898000
C	5.98126400	4.92231000	-0.69237200
O	6.34857500	3.78109200	-0.57718300
O	6.83326400	5.94218900	-0.86553900
H	7.73177800	5.58354900	-0.87816800
H	-3.77797500	2.36292500	0.25746300
H	-2.15500700	-1.49852700	0.93601700
Br	0.91815500	3.43139700	-0.19519300

Neutral-Cation-Br TCM

N	-2.37147100	-1.22752700	-0.02768900
H	-1.47078000	-1.05410100	-0.49243100
C	-3.19839900	0.00998200	-0.07366100
C	-2.25590200	1.19374600	0.11031000
H	-3.68353500	0.07059100	-1.04845700
H	-3.95609000	-0.04113500	0.70646100
O	-1.06823900	1.03855700	0.09956700
H	-2.83586500	-2.01849200	-0.48002400
O	-2.81181200	2.38375600	0.25403800
C	2.26199800	4.75457200	-0.44218600
C	3.59003600	4.36150700	-0.47830200
C	4.55371500	5.35363600	-0.65859700
C	4.20322900	6.69061900	-0.79905600
C	2.85579000	7.06947300	-0.75905700
C	1.87920300	6.08051600	-0.57957500
H	3.88544600	3.32718500	-0.37032000
H	4.97106600	7.44096800	-0.94138000
H	0.83086500	6.35396400	-0.55158500
N	2.48826100	8.39112800	-0.95401800
H	1.58515500	8.65786000	-0.59096100
H	3.20135400	9.07853500	-0.75898000
C	5.98126400	4.92231000	-0.69237200
O	6.34857500	3.78109200	-0.57718300
O	6.83326400	5.94218900	-0.86553900
H	7.73177800	5.58354900	-0.87816800
H	-3.77797500	2.36292500	0.25746300
H	-2.15500700	-1.49852700	0.93601700
Br	0.91815500	3.43139700	-0.19519300

Neutral-Cation-Br DCE

N	-2.32593300	-1.17764100	-0.20078800
H	-1.46400100	-1.01565600	-0.73233100
C	-3.15221900	0.05768000	-0.15853200
C	-2.24269300	1.20982400	0.23872800
H	-3.57833800	0.22744000	-1.14744300
H	-3.95534900	-0.08270600	0.56334000
O	-1.06554100	1.04654200	0.39357800
H	-2.83296500	-1.95654100	-0.62862100
O	-2.81491100	2.39333300	0.39031900
C	2.25632500	4.73678400	-0.30322300
C	3.58638000	4.35029800	-0.34472400
C	4.54173700	5.34301700	-0.56257600
C	4.18148900	6.67405600	-0.73360400
C	2.83185000	7.04609100	-0.69084800
C	1.86396400	6.05647200	-0.47006900
H	3.88814400	3.32037600	-0.21445900
H	4.94336800	7.42545800	-0.89939200
H	0.81511500	6.32585200	-0.43038300
N	2.46108000	8.37573500	-0.80468700
H	3.12272100	8.97904300	-1.27117400
H	1.51003200	8.54664600	-1.09722800
C	5.97143200	4.91993500	-0.60588800

O	6.34680700	3.78231300	-0.47375300
O	6.81461300	5.94023300	-0.80871700
H	7.71635400	5.58916200	-0.82386800
H	-3.76924400	2.38005300	0.23647400
H	-2.03886400	-1.46587400	0.73876500
Br	0.92272500	3.41235200	-0.00977600

Neutral-Cation-Br Acetone

N	-2.37720900	-1.22587700	-0.02434700
H	-1.48926300	-1.08318300	-0.51950500
C	-3.18964400	0.01855900	-0.06991000
C	-2.24551500	1.19766500	0.10404900
H	-3.67975100	0.08123100	-1.04175900
H	-3.94430700	-0.02228600	0.71368600
O	-1.05536400	1.05060200	0.09416500
H	-2.86819400	-2.01638700	-0.44865300
O	-2.80139600	2.39095900	0.23850800
C	2.26345600	4.74633200	-0.44589600
C	3.59305400	4.35694000	-0.48142800
C	4.55448400	5.35234300	-0.65745100
C	4.20026300	6.68892900	-0.79500700
C	2.85133200	7.06423400	-0.75700300
C	1.87723000	6.07161200	-0.58048000
H	3.88955000	3.32261100	-0.37613100
H	4.96538200	7.44276200	-0.93269000
H	0.82834200	6.34266700	-0.55169400
N	2.48039000	8.38448900	-0.95188100
H	1.57468100	8.64678400	-0.59084100
H	3.18984200	9.07368100	-0.74823200
C	5.98365000	4.92682900	-0.69083600
O	6.35485000	3.78568500	-0.57466400
O	6.83129600	5.94810200	-0.86486400
H	7.73282300	5.59604600	-0.87729300
H	-3.76798000	2.36621500	0.24624300
H	-2.14058500	-1.48613800	0.93710900
Br	0.92266500	3.41886900	-0.20407200

Neutral-Cation-Br DMSO

N	-2.37639700	-1.22817400	-0.02880200
H	-1.66695800	-1.20977400	-0.76835000
C	-3.20120000	0.00743000	-0.05885500
C	-2.26126400	1.20078200	-0.07138200
H	-3.81618400	-0.00448900	-0.95812000
H	-3.84698600	0.01925300	0.81802300
O	-1.07104300	1.05948200	-0.10842600
H	-2.95178400	-2.06508600	-0.15442600
O	-2.82292400	2.39981000	-0.04866400
C	2.27519300	4.74227700	-0.40617000
C	3.60649800	4.35825800	-0.43964400
C	4.56651100	5.36220600	-0.56854200
C	4.20971200	6.70216200	-0.66006500
C	2.85911100	7.07224800	-0.62296500
C	1.88661600	6.07074300	-0.49379900
H	3.90481600	3.32130400	-0.37082200

H	4.97413500	7.46243100	-0.76089800
H	0.83695500	6.33796700	-0.46290500
N	2.49109300	8.40701500	-0.65186100
H	3.16215400	9.03880300	-1.06474200
H	1.54655800	8.59859900	-0.95338600
C	5.99732100	4.94260900	-0.60533900
O	6.37134000	3.79878200	-0.52804200
O	6.84296900	5.97177700	-0.73406100
H	7.74599600	5.62359300	-0.75145000
H	-3.78900300	2.36885300	-0.02083300
H	-1.87364800	-1.32192500	0.85842200
Br	0.93449200	3.40334100	-0.23477600

Neutral-Cation-Br Water

N	-2.37616100	-1.22845000	-0.02904400
H	-1.66588100	-1.21009700	-0.76768000
C	-3.20064700	0.00715500	-0.05896200
C	-2.26150300	1.20085100	-0.07065900
H	-3.81513200	-0.00438300	-0.95854100
H	-3.84696900	0.01847400	0.81746900
O	-1.07092300	1.06107500	-0.10665800
H	-2.95192800	-2.06482000	-0.15637300
O	-2.82395700	2.39965600	-0.04876800
C	2.27509800	4.74275100	-0.40519700
C	3.60635000	4.35849100	-0.43895800
C	4.56654900	5.36222300	-0.56842800
C	4.20995300	6.70223800	-0.66026300
C	2.85940000	7.07257600	-0.62283300
C	1.88675200	6.07127600	-0.49302800
H	3.90439500	3.32146000	-0.37001300
H	4.97440500	7.46239600	-0.76170700
H	0.83718000	6.33879600	-0.46201100
N	2.49152600	8.40739400	-0.65191500
H	3.16223500	9.03867000	-1.06622700
H	1.54679900	8.59864200	-0.95321200
C	5.99727800	4.94241800	-0.60558100
O	6.37106700	3.79842400	-0.52830900
O	6.84297600	5.97132600	-0.73470000
H	7.74607100	5.62326000	-0.75257100
H	-3.79012200	2.36830100	-0.02198800
H	-1.87497000	-1.32381900	0.85881900
Br	0.93423800	3.40399400	-0.23354100

Neutral-Cation-I Vacuum SP

N	-2.33376100	-1.21953100	0.12003500
H	-1.47321100	-1.11497400	-0.42996700
C	-3.22307900	-0.04442000	-0.08948000
C	-2.36055700	1.20598100	0.00047000
H	-3.67735500	-0.12232100	-1.07726000
H	-4.00449300	-0.05312900	0.66958500
O	-1.17196400	1.12258100	0.12976500
H	-2.79396100	-2.09448200	-0.14396100
O	-2.98265200	2.36747500	-0.08727500
C	2.41009600	4.90505500	-0.43891400

C	3.73629000	4.51143900	-0.52746000
C	4.70100600	5.50392000	-0.70401700
C	4.35468600	6.84663300	-0.78971400
C	3.01168900	7.22942200	-0.69821500
C	2.03536300	6.23819400	-0.52303600
H	4.03710000	3.47482200	-0.46384700
H	5.12278600	7.59748000	-0.92850800
H	0.99203800	6.52437000	-0.45734000
N	2.64480400	8.55884300	-0.83834300
H	1.75621900	8.81778100	-0.43581700
H	3.36765100	9.23630200	-0.64437400
C	6.12409600	5.06723000	-0.79690700
O	6.48922100	3.92109500	-0.73201000
O	6.97639900	6.08839700	-0.96279900
H	7.87203100	5.72602600	-1.01498000
H	-3.93975600	2.28593100	-0.19654000
H	-2.04143900	-1.29566600	1.09859300
I	0.90852400	3.42502700	-0.16700000

Neutral-Cation-I TCM

N	-2.33376100	-1.21953100	0.12003500
H	-1.47321100	-1.11497400	-0.42996700
C	-3.22307900	-0.04442000	-0.08948000
C	-2.36055700	1.20598100	0.00047000
H	-3.67735500	-0.12232100	-1.07726000
H	-4.00449300	-0.05312900	0.66958500
O	-1.17196400	1.12258100	0.12976500
H	-2.79396100	-2.09448200	-0.14396100
O	-2.98265200	2.36747500	-0.08727500
C	2.41009600	4.90505500	-0.43891400
C	3.73629000	4.51143900	-0.52746000
C	4.70100600	5.50392000	-0.70401700
C	4.35468600	6.84663300	-0.78971400
C	3.01168900	7.22942200	-0.69821500
C	2.03536300	6.23819400	-0.52303600
H	4.03710000	3.47482200	-0.46384700
H	5.12278600	7.59748000	-0.92850800
H	0.99203800	6.52437000	-0.45734000
N	2.64480400	8.55884300	-0.83834300
H	1.75621900	8.81778100	-0.43581700
H	3.36765100	9.23630200	-0.64437400
C	6.12409600	5.06723000	-0.79690700
O	6.48922100	3.92109500	-0.73201000
O	6.97639900	6.08839700	-0.96279900
H	7.87203100	5.72602600	-1.01498000
H	-3.93975600	2.28593100	-0.19654000
H	-2.04143900	-1.29566600	1.09859300
I	0.90852400	3.42502700	-0.16700000

Neutral-Cation-I DCE

N	-2.33516900	-1.21738400	0.11726900
H	-1.47597900	-1.12023200	-0.43507500
C	-3.21612900	-0.03686600	-0.08508000
C	-2.35152700	1.20995300	0.00008900

H	-3.67682800	-0.10931400	-1.07021200
H	-3.99352500	-0.04103000	0.67792300
O	-1.15995900	1.13222900	0.11470900
H	-2.80354000	-2.08657400	-0.15079800
O	-2.97474900	2.37289800	-0.07681200
C	2.40857700	4.89841300	-0.44957800
C	3.73637300	4.50766400	-0.53325300
C	4.70053400	5.50204400	-0.70327600
C	4.35227000	6.84458200	-0.78797300
C	3.00802500	7.22498800	-0.70194100
C	2.03265900	6.23143400	-0.53250400
H	4.03762100	3.47108100	-0.47045500
H	5.11909500	7.59764200	-0.92134400
H	0.98885800	6.51645700	-0.46931200
N	2.63928500	8.55382700	-0.84244800
H	1.74753500	8.80880000	-0.44358600
H	3.35893600	9.23171700	-0.63707600
C	6.12500700	5.06910400	-0.79051900
O	6.49248900	3.92295900	-0.72382200
O	6.97518000	6.09119300	-0.95323400
H	7.87298300	5.73309600	-1.00205400
H	-3.93390000	2.28905900	-0.16780300
H	-2.04429900	-1.30375300	1.09517000
I	0.90794900	3.41549600	-0.18632200

Neutral-Cation-I Acetone

N	-2.33585300	-1.21654900	0.11487500
H	-1.47861000	-1.12234800	-0.44047200
C	-3.21400000	-0.03405100	-0.08240200
C	-2.34849200	1.21146600	-0.00200600
H	-3.67967600	-0.10408600	-1.06535800
H	-3.98795700	-0.03669800	0.68399600
O	-1.15491900	1.13652300	0.09871400
H	-2.80799200	-2.08339100	-0.15387400
O	-2.97249300	2.37521000	-0.06840000
C	2.40837600	4.89534500	-0.45597500
C	3.73702000	4.50604400	-0.53625500
C	4.70091400	5.50145700	-0.70230000
C	4.35166400	6.84387400	-0.78677400
C	3.00669500	7.22305900	-0.70450700
C	2.03177300	6.22824600	-0.53857100
H	4.03849800	3.46950000	-0.47359600
H	5.11792800	7.59803800	-0.91683500
H	0.98770300	6.51263200	-0.47724100
N	2.63702600	8.55143400	-0.84542400
H	1.74329700	8.80466500	-0.44953100
H	3.35489600	9.22987900	-0.63517200
C	6.12616700	5.07045600	-0.78561600
O	6.49476500	3.92432000	-0.71780000
O	6.97532400	6.09306200	-0.94615800
H	7.87424000	5.73711700	-0.99253700
H	-3.93307000	2.29083800	-0.14372100
H	-2.04357400	-1.30741300	1.09187600
I	0.90812500	3.41085500	-0.19825700

Neutral-Cation-I DMSO

N	-2.33751400	-1.21662400	0.11186000
H	-1.48171600	-1.12389900	-0.44566900
C	-3.21344800	-0.03221600	-0.08071400
C	-2.34629100	1.21184000	-0.00255100
H	-3.68246700	-0.09936300	-1.06230200
H	-3.98507200	-0.03441300	0.68798400
O	-1.15141300	1.13736200	0.08635400
H	-2.81240400	-2.08158300	-0.15791900
O	-2.96985100	2.37670400	-0.05839000
C	2.40877000	4.89328900	-0.46059400
C	3.73805100	4.50519200	-0.53795400
C	4.70159000	5.50146400	-0.70131900
C	4.35141500	6.84367400	-0.78625300
C	3.00585800	7.22176900	-0.70714100
C	2.03140500	6.22598100	-0.54357300
H	4.03995700	3.46878500	-0.47490900
H	5.11720000	7.59867500	-0.91410300
H	0.98706100	6.50969800	-0.48403000
N	2.63530300	8.54972000	-0.84898500
H	1.74006200	8.80169800	-0.45548300
H	3.35171900	9.22876500	-0.63540500
C	6.12748000	5.07198800	-0.78128400
O	6.49700000	3.92599000	-0.71224200
O	6.97582800	6.09510900	-0.94026500
H	7.87552700	5.74068700	-0.98453000
H	-3.93140800	2.29298200	-0.12129500
H	-2.04389800	-1.31127300	1.08807800
I	0.90903000	3.40748500	-0.20668400

Neutral-Cation-I Water

N	-2.33867300	-1.21688900	0.11018900
H	-1.48318000	-1.12455100	-0.44778500
C	-3.21338900	-0.03139600	-0.08026500
C	-2.34512400	1.21175900	-0.00219600
H	-3.68347000	-0.09684200	-1.06148000
H	-3.98432200	-0.03356500	0.68911200
O	-1.14984000	1.13683100	0.08221400
H	-2.81467600	-2.08090300	-0.16060400
O	-2.96799000	2.37732500	-0.05336000
C	2.40906800	4.89248400	-0.46201100
C	3.73861000	4.50493000	-0.53821900
C	4.70191300	5.50157300	-0.70084200
C	4.35126700	6.84364900	-0.78625900
C	3.00546400	7.22123400	-0.70838300
C	2.03128300	6.22503500	-0.54544300
H	4.04078500	3.46862200	-0.47479100
H	5.11680900	7.59899400	-0.91348500
H	0.98680900	6.50841100	-0.48663400
N	2.63445100	8.54895800	-0.85087600
H	1.73863600	8.80049600	-0.45832200
H	3.35026900	9.22835800	-0.63631500
C	6.12807600	5.07277000	-0.77948500

O	6.49802900	3.92687500	-0.70975300
O	6.97603500	6.09612300	-0.93811100
H	7.87603700	5.74230700	-0.98152100
H	-3.92989900	2.29432600	-0.11167300
H	-2.04488100	-1.31352700	1.08615800
I	0.90967700	3.40609800	-0.20917600

Anion-Cation-Cl Vacuum SP

N	-2.38186800	-1.20036200	-0.03809800
H	-1.48100400	-1.01175500	-0.49742900
C	-3.21760500	0.03180700	-0.07265500
C	-2.27802700	1.21749400	0.12204000
H	-3.70252500	0.09774900	-1.04708100
H	-3.97419200	-0.03058500	0.70759000
O	-1.09181700	1.06293600	0.10876800
H	-2.83773100	-1.98988500	-0.50076300
O	-2.83814800	2.40493800	0.27882000
C	2.18780100	4.59726400	-0.41623200
C	3.51944200	4.22241600	-0.45869100
C	4.47952700	5.21645300	-0.65620500
C	4.08905200	6.54024300	-0.80784500
C	2.73891900	6.90437600	-0.76479800
C	1.77218400	5.91273100	-0.56704700
H	3.82930100	3.19299600	-0.34139800
H	4.85844600	7.28885900	-0.96001100
H	0.71850000	6.16408900	-0.53433300
Cl	0.95949700	3.36440600	-0.16525700
N	2.35152800	8.23148600	-0.97640900
H	1.47514600	8.48958700	-0.54540300
H	3.07276000	8.90924900	-0.77278500
C	5.97613400	4.84250200	-0.69921700
O	6.23767300	3.62583400	-0.59268700
O	6.77275200	5.79420600	-0.83404500
H	-3.80387700	2.37963800	0.27429400
H	-2.16443700	-1.47966200	0.92294000

Anion-Cation-Cl TCM ModRedundant

N	-2.38186800	-1.20036200	-0.03809800
H	-1.48100400	-1.01175500	-0.49742900
C	-3.21760500	0.03180700	-0.07265500
C	-2.27802700	1.21749400	0.12204000
H	-3.70252500	0.09774900	-1.04708100
H	-3.97419200	-0.03058500	0.70759000
O	-1.09181700	1.06293600	0.10876800
H	-2.83773100	-1.98988500	-0.50076300
O	-2.83814800	2.40493800	0.27882000
C	2.18780100	4.59726400	-0.41623200
C	3.51944200	4.22241600	-0.45869100
C	4.47952700	5.21645300	-0.65620500
C	4.08905200	6.54024300	-0.80784500
C	2.73891900	6.90437600	-0.76479800
C	1.77218400	5.91273100	-0.56704700
H	3.82930100	3.19299600	-0.34139800
H	4.85844600	7.28885900	-0.96001100

H	0.71850000	6.16408900	-0.53433300
Cl	0.95949700	3.36440600	-0.16525700
N	2.35152800	8.23148600	-0.97640900
H	1.47514600	8.48958700	-0.54540300
H	3.07276000	8.90924900	-0.77278500
C	5.97613400	4.84250200	-0.69921700
O	6.23767300	3.62583400	-0.59268700
O	6.77275200	5.79420600	-0.83404500
H	-3.80387700	2.37963800	0.27429400
H	-2.16443700	-1.47966200	0.92294000

A 15 10 7 120.0 F

D 15 10 7 4 0.0 F

Anion-Cation-Cl DCE

N	-2.38899800	-1.23029500	-0.02293000
H	-1.49034800	-1.07157900	-0.49464500
C	-3.20784600	0.01078000	-0.07341900
C	-2.26546800	1.19042600	0.12218900
H	-3.68387600	0.07614600	-1.05202600
H	-3.97305600	-0.03794600	0.69937300
O	-1.07754600	1.03877300	0.12863100
H	-2.86275300	-2.02000900	-0.46735100
O	-2.82369500	2.38277300	0.25902800
C	2.16339800	4.63454000	-0.42829600
C	3.48982700	4.23789100	-0.47113300
C	4.46725300	5.21681200	-0.65972400
C	4.10075900	6.54885800	-0.80274300
C	2.75646900	6.93595800	-0.75963900
C	1.77319900	5.95844100	-0.56920700
H	3.77839200	3.20189600	-0.35878600
H	4.88023200	7.28799100	-0.94827400
H	0.72429700	6.22903800	-0.53463700
Cl	0.91844400	3.41997900	-0.18392000
N	2.39248000	8.26803700	-0.96459500
H	1.51100200	8.53727600	-0.55085600
H	3.11903000	8.93694000	-0.75082500
C	5.95417400	4.81736800	-0.70277000
O	6.19983200	3.59617500	-0.59784500
O	6.77276600	5.75204300	-0.83648700
H	-3.78985900	2.35871500	0.24597000
H	-2.17067700	-1.49801900	0.94097700

Anion-Cation-Cl Acetone

N	-2.40654800	-1.23907600	-0.02000300
H	-1.51530000	-1.09816900	-0.50973200
C	-3.21403200	0.00859200	-0.06866700
C	-2.26488700	1.18254000	0.11746900
H	-3.69562200	0.07565400	-1.04437000
H	-3.97524800	-0.03164300	0.70858900
O	-1.07654400	1.02893200	0.11909500
H	-2.89760800	-2.02746100	-0.44797400
O	-2.81731700	2.37861000	0.25107200
C	2.17251800	4.63410600	-0.43344400

C	3.50056500	4.24147300	-0.47439200
C	4.47519600	5.22418300	-0.65834400
C	4.10528500	6.55566300	-0.79888100
C	2.75930100	6.93872300	-0.75836800
C	1.77883800	5.95706000	-0.57219900
H	3.79076400	3.20574500	-0.36412800
H	4.88147000	7.29885500	-0.94081800
H	0.72911100	6.22448000	-0.53879200
Cl	0.93137500	3.41548700	-0.19445500
N	2.39218900	8.26867800	-0.96214200
H	1.50426300	8.53401800	-0.55974600
H	3.11319400	8.94177000	-0.74289000
C	5.96197600	4.82959200	-0.70017800
O	6.21359000	3.60863400	-0.60104200
O	6.78045500	5.76598300	-0.82788000
H	-3.78388900	2.35744900	0.24581700
H	-2.17566400	-1.50087000	0.94246300

Anion-Cation-Cl DMSO

N	-2.53467800	-1.22093800	-0.21669900
H	-1.79280000	-1.21723300	-0.92317200
C	-3.17811500	0.11425300	-0.11264500
C	-2.09240200	1.13630100	0.17917000
H	-3.67761700	0.33556100	-1.05552800
H	-3.91538200	0.08396900	0.68906900
O	-0.94152900	0.81818900	0.27857100
H	-3.21434800	-1.94231200	-0.46999600
O	-2.48525800	2.39451600	0.31560100
C	2.19101900	4.57311700	-0.33719100
C	3.53430900	4.23293100	-0.33866800
C	4.47393600	5.25112000	-0.51039500
C	4.05612900	6.56579200	-0.67470400
C	2.69500500	6.89554200	-0.67506800
C	1.74947000	5.87785600	-0.50061700
H	3.86119200	3.21010000	-0.21158400
H	4.80487500	7.33860200	-0.80555100
H	0.68992000	6.10477700	-0.49316800
Cl	0.99465000	3.30673100	-0.11911200
N	2.28457600	8.22326400	-0.78430400
H	2.94531000	8.83224500	-1.24643600
H	1.34850200	8.35405600	-1.14174100
C	5.97425800	4.91276100	-0.51693600
O	6.27072000	3.70360600	-0.39539100
O	6.76167200	5.87633400	-0.64203800
H	-3.43868700	2.51137700	0.20613600
H	-2.09729300	-1.49350800	0.66845900

Anion-Cation-Cl Water

N	-2.53933700	-1.22137400	-0.21840100
H	-1.79713900	-1.21886500	-0.92451000
C	-3.17854800	0.11547700	-0.11216500
C	-2.09022800	1.13437200	0.17971500
H	-3.67811600	0.33964000	-1.05433200
H	-3.91543800	0.08644400	0.68992100

O	-0.93941200	0.81454100	0.27567200
H	-3.22121400	-1.93994500	-0.47370100
O	-2.48053800	2.39303500	0.32017900
C	2.19304200	4.57184000	-0.33834100
C	3.53682100	4.23330200	-0.33843700
C	4.47530500	5.25260000	-0.50987600
C	4.05608800	6.56674100	-0.67520300
C	2.69448600	6.89490300	-0.67656700
C	1.75009000	5.87595500	-0.50259100
H	3.86460000	3.21087800	-0.21049800
H	4.80375800	7.34061400	-0.80585900
H	0.69026700	6.10159600	-0.49630200
Cl	0.99812700	3.30410400	-0.12101100
N	2.28261100	8.22180400	-0.78615400
H	2.94212100	8.83199800	-1.24839500
H	1.34572200	8.35192500	-1.14166400
C	5.97574100	4.91604500	-0.51450100
O	6.27404900	3.70777300	-0.38772900
O	6.76256800	5.87978900	-0.64320900
H	-3.43412300	2.51143300	0.21348900
H	-2.10386900	-1.49761800	0.66653400

Anion-Cation-Br Vacuum SP

N	-2.37048300	-1.23222400	-0.01947800
H	-1.45404100	-1.03480300	-0.44297100
C	-3.21711600	-0.00917600	-0.09027100
C	-2.29887100	1.18821300	0.13153000
H	-3.66803800	0.04670000	-1.08131200
H	-4.00088800	-0.07556800	0.66208200
O	-1.11067500	1.04764400	0.16249200
H	-2.79900100	-2.02717000	-0.49878100
O	-2.87656900	2.36979800	0.26160800
C	2.25953600	4.76235300	-0.43722100
C	3.58211500	4.35512700	-0.48426900
C	4.56650900	5.32686700	-0.67695000
C	4.20873100	6.66085200	-0.81948400
C	2.86839300	7.05801900	-0.77087400
C	1.87725500	6.08931900	-0.57713400
H	3.87134900	3.31921400	-0.37315900
H	4.99590600	7.39141500	-0.96849200
H	0.83187200	6.37248300	-0.54091100
N	2.51329400	8.39541100	-0.97295800
H	1.64314100	8.67199500	-0.54077600
H	3.25076100	9.05446200	-0.76621400
C	6.05354200	4.91478300	-0.72365100
O	6.28439500	3.69270400	-0.60985100
O	6.87311700	5.84521400	-0.86777800
H	-3.84130500	2.33507800	0.22389400
H	-2.18896300	-1.50790100	0.95003900
Br	0.89641400	3.44775600	-0.16911300

Anion-Cation-Br TCM

N	-2.37048300	-1.23222400	-0.01947800
H	-1.45404100	-1.03480300	-0.44297100

C	-3.21711600	-0.00917600	-0.09027100
C	-2.29887100	1.18821300	0.13153000
H	-3.66803800	0.04670000	-1.08131200
H	-4.00088800	-0.07556800	0.66208200
O	-1.11067500	1.04764400	0.16249200
H	-2.79900100	-2.02717000	-0.49878100
O	-2.87656900	2.36979800	0.26160800
C	2.25953600	4.76235300	-0.43722100
C	3.58211500	4.35512700	-0.48426900
C	4.56650900	5.32686700	-0.67695000
C	4.20873100	6.66085200	-0.81948400
C	2.86839300	7.05801900	-0.77087400
C	1.87725500	6.08931900	-0.57713400
H	3.87134900	3.31921400	-0.37315900
H	4.99590600	7.39141500	-0.96849200
H	0.83187200	6.37248300	-0.54091100
N	2.51329400	8.39541100	-0.97295800
H	1.64314100	8.67199500	-0.54077600
H	3.25076100	9.05446200	-0.76621400
C	6.05354200	4.91478300	-0.72365100
O	6.28439500	3.69270400	-0.60985100
O	6.87311700	5.84521400	-0.86777800
H	-3.84130500	2.33507800	0.22389400
H	-2.18896300	-1.50790100	0.95003900
Br	0.89641400	3.44775600	-0.16911300

Anion-Cation-Br DCE

N	-2.40686000	-1.24319900	-0.02223500
H	-1.51022400	-1.08326100	-0.49739200
C	-3.22938100	-0.00459300	-0.07181600
C	-2.29063900	1.17864400	0.11689000
H	-3.70963100	0.05763800	-1.04861400
H	-3.99130800	-0.05384800	0.70417900
O	-1.10157900	1.03127100	0.11709700
H	-2.88018200	-2.03474800	-0.46388600
O	-2.85162800	2.36904700	0.25320800
C	2.27934700	4.75042500	-0.45415000
C	3.60754700	4.35744200	-0.49064800
C	4.58329100	5.34068900	-0.66907100
C	4.21376200	6.67204700	-0.80857700
C	2.86827000	7.05536100	-0.77219600
C	1.88597900	6.07417400	-0.59190000
H	3.90345100	3.32321000	-0.38216400
H	4.99206900	7.41387900	-0.94679700
H	0.83752200	6.34680700	-0.56360400
N	2.50197800	8.38716400	-0.97414600
H	1.61676000	8.65245700	-0.56592000
H	3.22511200	9.05744300	-0.75326600
C	6.07201800	4.94599100	-0.70553400
O	6.32115600	3.72531400	-0.60418600
O	6.88776000	5.88421500	-0.83119200
H	-3.81782700	2.34201100	0.24871700
H	-2.18481600	-1.50905100	0.94130400
Br	0.92843500	3.42203400	-0.20410600

Anion-Cation-Br Acetone

N	-2.42098700	-1.24873500	-0.06848200
H	-1.53071000	-1.10591600	-0.55943100
C	-3.23203900	-0.00346200	-0.11661100
C	-2.28683600	1.17376800	0.06661700
H	-3.71551200	0.06177000	-1.09156800
H	-3.99187300	-0.04523800	0.66191700
O	-1.09744600	1.02390900	0.06527200
H	-2.91055000	-2.03851200	-0.49563900
O	-2.84201100	2.36788100	0.19993200
C	2.29051900	4.75031600	-0.38400900
C	3.62087300	4.36318800	-0.42290400
C	4.59327700	5.35370800	-0.57724600
C	4.21996700	6.68696400	-0.68786000
C	2.87256200	7.06466400	-0.64968900
C	1.89366000	6.07549100	-0.49319400
H	3.91874300	3.32732600	-0.33774600
H	4.99550400	7.43491800	-0.80693400
H	0.84462300	6.34457300	-0.45762700
N	2.50900400	8.40994700	-0.70326100
H	3.18390200	9.01030800	-1.15608800
H	1.57263300	8.58742200	-1.03887000
C	6.08181800	4.96557100	-0.62477500
O	6.33846400	3.74396600	-0.55113000
O	6.89613500	5.90814400	-0.73199100
H	-3.80856400	2.34404900	0.19903900
H	-2.18837400	-1.50972900	0.89377600
Br	0.94360000	3.41227200	-0.17149700

Anion-Cation-Br DMSO

N	-2.31610700	-1.15144100	-0.26017800
H	-1.65388800	-1.08936800	-1.03851900
C	-3.16201900	0.06619600	-0.16293100
C	-2.27996900	1.21619800	0.29171800
H	-3.61013300	0.26309400	-1.13554200
H	-3.94992400	-0.11543900	0.56778000
O	-1.13332200	1.04452200	0.59660600
H	-2.88277100	-1.99247600	-0.39616100
O	-2.84791200	2.41152100	0.34773400
C	2.25735100	4.71974200	-0.26021900
C	3.58798500	4.33293000	-0.29251700
C	4.55467000	5.31152200	-0.53393400
C	4.17587900	6.63297500	-0.73327100
C	2.82797800	7.01062600	-0.69843700
C	1.85474400	6.03306500	-0.45596700
H	3.88939200	3.30618700	-0.13817400
H	4.94638400	7.37280000	-0.91785700
H	0.80561100	6.30203100	-0.42341400
N	2.45980200	8.34735200	-0.84052600
H	3.12382900	8.91729900	-1.34573000
H	1.51586900	8.50043300	-1.16693700
C	6.04221800	4.92185400	-0.57750700
O	6.30508500	3.71432600	-0.38500400

O	6.85268200	5.84773700	-0.80031400
H	-3.77268500	2.40828500	0.06486200
H	-1.75794400	-1.27000700	0.59157600
Br	0.91757900	3.39659900	0.06286400

Anion-Cation-Br Water

N	-2.56833600	-1.25386700	0.10331100
H	-1.68729400	-1.35153600	-0.41153000
C	-3.19670800	0.06116300	-0.18259300
C	-2.13854500	1.13666900	-0.00207700
H	-3.55786200	0.05768100	-1.21085200
H	-4.03703200	0.20577400	0.49459300
O	-0.99221300	0.86014000	0.21551200
H	-3.18515200	-2.02661200	-0.15835600
O	-2.54534100	2.39199100	-0.11350700
C	2.31906500	4.69790200	-0.34971900
C	3.65570800	4.34963400	-0.46639400
C	4.59245100	5.37146900	-0.63617900
C	4.17916600	6.69667000	-0.68479900
C	2.82553800	7.03530400	-0.56819800
C	1.88230900	6.01421000	-0.39654000
H	3.98463700	3.32028100	-0.42989800
H	4.92634800	7.47089100	-0.81613300
H	0.82967500	6.25249000	-0.30114700
N	2.42416700	8.36977600	-0.55853200
H	3.05693000	9.00468400	-1.02487100
H	1.46603400	8.53145700	-0.83584300
C	6.08498700	5.02586100	-0.76982900
O	6.37827900	3.81027700	-0.74175500
O	6.87053800	5.99127800	-0.89362900
H	-3.49356300	2.47138000	-0.28400200
H	-2.34291300	-1.35429100	1.09693800
Br	1.01951300	3.31788600	-0.11397400

Anion-Cation-I Vacuum SP

N	-2.41011400	-1.25358800	-0.01550500
H	-1.49681500	-1.05710300	-0.44599100
C	-3.26052300	-0.03327600	-0.08550700
C	-2.34701400	1.16828400	0.12823100
H	-3.71587800	0.01905500	-1.07480800
H	-4.04085100	-0.10022100	0.67032200
O	-1.15695000	1.03349600	0.15086300
H	-2.84024200	-2.05125300	-0.48900200
O	-2.92711500	2.34734200	0.25899700
C	2.42856300	4.90272700	-0.45253500
C	3.75698800	4.51349300	-0.50234100
C	4.73032400	5.49677400	-0.69743800
C	4.35744600	6.82610900	-0.84048100
C	3.01302500	7.20722800	-0.79005500
C	2.03356800	6.22641800	-0.59308200
H	4.06653500	3.48327000	-0.39303700
H	5.13631700	7.56516700	-0.99181200
H	0.98706100	6.50580600	-0.55640500
N	2.64162400	8.54050400	-0.99343800

H	1.76841300	8.80645100	-0.56064100
H	3.37091200	9.20823200	-0.78519500
C	6.22237600	5.10281900	-0.74679500
O	6.46883200	3.88312600	-0.64088700
O	7.03006100	6.04455200	-0.88517000
H	-3.89212600	2.31064300	0.22877900
H	-2.22239200	-1.52552000	0.95389200
I	0.92682100	3.41540600	-0.15199900

Anion-Cation-I TCM

N	-2.41011400	-1.25358800	-0.01550500
H	-1.49681500	-1.05710300	-0.44599100
C	-3.26052300	-0.03327600	-0.08550700
C	-2.34701400	1.16828400	0.12823100
H	-3.71587800	0.01905500	-1.07480800
H	-4.04085100	-0.10022100	0.67032200
O	-1.15695000	1.03349600	0.15086300
H	-2.84024200	-2.05125300	-0.48900200
O	-2.92711500	2.34734200	0.25899700
C	2.42856300	4.90272700	-0.45253500
C	3.75698800	4.51349300	-0.50234100
C	4.73032400	5.49677400	-0.69743800
C	4.35744600	6.82610900	-0.84048100
C	3.01302500	7.20722800	-0.79005500
C	2.03356800	6.22641800	-0.59308200
H	4.06653500	3.48327000	-0.39303700
H	5.13631700	7.56516700	-0.99181200
H	0.98706100	6.50580600	-0.55640500
N	2.64162400	8.54050400	-0.99343800
H	1.76841300	8.80645100	-0.56064100
H	3.37091200	9.20823200	-0.78519500
C	6.22237600	5.10281900	-0.74679500
O	6.46883200	3.88312600	-0.64088700
O	7.03006100	6.04455200	-0.88517000
H	-3.89212600	2.31064300	0.22877900
H	-2.22239200	-1.52552000	0.95389200
I	0.92682100	3.41540600	-0.15199900

Anion-Cation-I DCE

N	-2.42778900	-1.25309900	-0.02198700
H	-1.53564300	-1.08957700	-0.50425900
C	-3.25882600	-0.02025000	-0.06761500
C	-2.32916300	1.17038500	0.11376400
H	-3.74551300	0.03787800	-1.04155500
H	-4.01572300	-0.07397400	0.71299100
O	-1.13796100	1.03242300	0.10620300
H	-2.89975300	-2.04831300	-0.45864500
O	-2.89641900	2.35636700	0.25123000
C	2.43504100	4.88721100	-0.46777500
C	3.76846000	4.50967600	-0.50671500
C	4.73610900	5.50108900	-0.68814300
C	4.35513900	6.82885200	-0.82912200
C	3.00671700	7.19943000	-0.79152500
C	2.03356400	6.20887000	-0.60750700

H	4.08174800	3.48047500	-0.39879000
H	5.12666600	7.57741500	-0.96972300
H	0.98485200	6.48111300	-0.57912700
N	2.62726200	8.52791500	-0.99584200
H	1.74070900	8.78492900	-0.58503100
H	3.34416300	9.20493800	-0.77478200
C	6.22812900	5.11950200	-0.72656000
O	6.48872300	3.90069300	-0.63071000
O	7.03564500	6.06551600	-0.84837800
H	-3.86252000	2.32404800	0.25385400
H	-2.19744800	-1.51632700	0.94028600
I	0.94267600	3.38875700	-0.18557600

Anion-Cation-I Acetone

N	-2.43073600	-1.25299500	-0.01952700
H	-1.54537500	-1.10288700	-0.51715700
C	-3.25548800	-0.01676400	-0.06435200
C	-2.32368700	1.17167500	0.10965400
H	-3.74636100	0.04139600	-1.03609400
H	-4.00943500	-0.06527200	0.71946700
O	-1.13164700	1.03572600	0.09916000
H	-2.91522600	-2.04863400	-0.44164100
O	-2.88955400	2.35929200	0.24414300
C	2.43503800	4.88366400	-0.47314000
C	3.76964100	4.50826100	-0.51030800
C	4.73653600	5.50133700	-0.68677700
C	4.35471800	6.82942300	-0.82477700
C	3.00542400	7.19838500	-0.78956300
C	2.03327000	6.20541500	-0.61027200
H	4.08256900	3.47875300	-0.40445500
H	5.12429000	7.58064300	-0.96138800
H	0.98433100	6.47686800	-0.58281100
N	2.62513900	8.52560100	-0.99196900
H	1.73266400	8.77974700	-0.59222500
H	3.33748500	9.20530800	-0.76458000
C	6.22756000	5.12146200	-0.72403700
O	6.49165300	3.90251600	-0.63275100
O	7.03704900	6.06715700	-0.84110600
H	-3.85587400	2.32671500	0.25088000
H	-2.18925200	-1.51013800	0.94152200
I	0.94411300	3.38328700	-0.19693500

Anion-Cation-I DMSO

N	-2.43386800	-1.25751400	-0.06934600
H	-1.55001400	-1.11431700	-0.57091900
C	-3.25600300	-0.02028700	-0.11859000
C	-2.32583500	1.16774600	0.06090500
H	-3.74150000	0.03863200	-1.09290400
H	-4.01463700	-0.06780100	0.66078300
O	-1.13310800	1.03415100	0.05917000
H	-2.92250700	-2.05384400	-0.48549600
O	-2.89349800	2.35539100	0.19075500
C	2.44254400	4.88786300	-0.39541100
C	3.77817800	4.51547300	-0.43623200

C	4.74364600	5.51318900	-0.59317000
C	4.36053200	6.84350000	-0.70520500
C	3.01038200	7.20984000	-0.66579000
C	2.03982100	6.21169600	-0.50629800
H	4.09176100	3.48422300	-0.35098600
H	5.12906000	7.59838900	-0.82636300
H	0.99084000	6.48168300	-0.47162000
N	2.63517000	8.55183100	-0.72068400
H	3.30179000	9.15712100	-1.17936000
H	1.69529100	8.72019300	-1.05150500
C	6.23415400	5.13635800	-0.64149300
O	6.50197100	3.91648700	-0.57225900
O	7.04319700	6.08451300	-0.74489200
H	-3.85993800	2.32152100	0.19064900
H	-2.19089300	-1.51068400	0.89235800
I	0.95231100	3.38058600	-0.15713300

Anion-Cation-I Water

N	-2.43177600	-1.25183800	-0.01625500
H	-1.55196900	-1.11273200	-0.52587500
C	-3.25209900	-0.01348200	-0.06336000
C	-2.31962800	1.17367600	0.10729100
H	-3.74343500	0.04396000	-1.03482600
H	-4.00602600	-0.05782600	0.72075900
O	-1.12688700	1.03939200	0.09853300
H	-2.92561900	-2.04875200	-0.42514100
O	-2.88516900	2.36241800	0.23723700
C	2.43502900	4.88016300	-0.47650200
C	3.77050600	4.50650400	-0.51345600
C	4.73656000	5.50104900	-0.68655000
C	4.35386400	6.82936300	-0.82158900
C	3.00385200	7.19694300	-0.78714400
C	2.03274400	6.20197700	-0.61098000
H	4.08352400	3.47681200	-0.40981000
H	5.12177900	7.58272000	-0.95534700
H	0.98362400	6.47265000	-0.58324200
N	2.62266000	8.52315800	-0.98740100
H	1.72569300	8.77481100	-0.59611900
H	3.33139800	9.20498300	-0.75516600
C	6.22675000	5.12258800	-0.72431400
O	6.49361900	3.90355600	-0.63674700
O	7.03754700	6.06811400	-0.83864300
H	-3.85167900	2.32954700	0.24316600
H	-2.18151200	-1.50198400	0.94432900
I	0.94549400	3.37817000	-0.20388800

Neutral-Cation-Cl oxocarbenium^{+} DCE

C	-4.51802900	-3.28805900	0.00174300
C	-3.00166800	-3.33665000	0.17443300
C	-2.45273500	-1.91366300	0.19507800
C	-3.32821000	-0.94023600	0.85378000
C	-5.13526800	-2.49666100	1.12708700
H	-1.46699600	-1.81609200	0.66338700
H	-2.75091600	-3.84000300	1.11048400

H	-2.53390300	-3.89424100	-0.63494300
H	-4.78530000	-2.83785400	-0.95832100
H	-4.95064600	-4.28890500	0.02937900
H	-3.00346300	0.08847200	1.01124500
H	-5.00130800	-2.95542900	2.10630700
H	-6.17933400	-2.23893800	0.97449600
H	-2.31138400	-1.49656200	-0.81508500
O	-4.48448700	-1.16476600	1.26437000
C	-6.46256000	1.92164900	4.46892500
C	-5.67936400	3.01236500	4.80590900
C	-6.17593100	3.88530500	5.77356200
C	-7.40889700	3.67594500	6.37866700
C	-8.18678000	2.56587700	6.02222900
C	-7.69726600	1.68216300	5.05111200
H	-4.71759200	3.18869700	4.34438400
H	-7.77177000	4.37213000	7.12451700
H	-8.28041800	0.81799400	4.75599900
N	-9.44159300	2.37652300	6.57289100
H	-9.80913200	1.43711300	6.53647100
H	-9.61023600	2.82692600	7.46045100
C	-5.32814600	5.05832300	6.13537700
O	-4.25151700	5.29177000	5.64641700
O	-5.88469000	5.83951100	7.06864500
H	-5.28207700	6.57529500	7.24807000
Cl	-5.87436200	0.79781000	3.26386200

Neutral-Cation-Br oxocarbenium^{+} DCE

C	-4.52525600	-3.34953900	0.03244000
C	-2.99947900	-3.37402700	-0.01322400
C	-2.47432700	-1.94190800	0.00167800
C	-3.26029400	-1.02086300	0.82734200
C	-4.98612100	-2.62927700	1.27413800
H	-1.43325600	-1.84575400	0.32987500
H	-2.61131500	-3.91499800	0.85237300
H	-2.64338000	-3.88239700	-0.90722300
H	-4.93230100	-2.85861800	-0.85571700
H	-4.93550800	-4.35946500	0.06883600
H	-2.93093000	0.00561500	0.98827500
H	-4.70202600	-3.13308700	2.19762200
H	-6.04521900	-2.38903400	1.28797800
H	-2.48426000	-1.47372000	-0.99628700
O	-4.34335600	-1.29010700	1.38531900
C	-6.50354000	2.06108800	4.62576200
C	-5.72107000	3.13920200	5.00352400
C	-6.25749000	4.02608700	5.93736300
C	-7.52666100	3.84132200	6.47142200
C	-8.30168700	2.74251200	6.07695500
C	-7.77374700	1.84574900	5.13733700
H	-4.73080500	3.29990500	4.60063800
H	-7.91839400	4.54744300	7.19310400
H	-8.35829000	0.99182200	4.81699100
N	-9.58777600	2.57338800	6.55854900
H	-9.96420900	1.63811300	6.50547200
H	-9.79675600	3.02687700	7.43597300

C	-5.40999200	5.18454600	6.34449100
O	-4.30031500	5.39280000	5.92297000
O	-6.00746700	5.98339400	7.23677300
H	-5.40111400	6.70678800	7.45048600
Br	-5.80638700	0.81952600	3.36156600

Neutral-Cation-I oxocarbenium^{+} DCE

C	-4.50405000	-3.38827400	-0.00636600
C	-2.97820200	-3.41850900	-0.04254200
C	-2.44855100	-1.98820800	-0.04171800
C	-3.23548200	-1.05456600	0.76774100
C	-4.96971900	-2.65319400	1.22452100
H	-1.40909200	-1.89088200	0.29151800
H	-2.59723900	-3.95006200	0.83204800
H	-2.61842800	-3.93886800	-0.92814500
H	-4.90452000	-2.90631500	-0.90238800
H	-4.91792100	-4.39635400	0.03951300
H	-2.90282400	-0.02733400	0.91689700
H	-4.69197700	-3.14667300	2.15555600
H	-6.02811400	-2.40902200	1.22925400
H	-2.45052000	-1.53172400	-1.04523000
O	-4.32263300	-1.31363300	1.32419500
C	-6.59117300	2.21067400	4.81068800
C	-5.81491600	3.29490600	5.18593500
C	-6.36050800	4.19238400	6.10513700
C	-7.63427300	4.01276200	6.62968700
C	-8.40398600	2.90926300	6.24021000
C	-7.86610200	2.00269000	5.31443700
H	-4.82060300	3.45952800	4.79453200
H	-8.03315100	4.72656700	7.33990700
H	-8.45430300	1.14781000	5.00292300
N	-9.69492800	2.74355500	6.71158600
H	-10.06834200	1.80662000	6.66578700
H	-9.91078500	3.20406900	7.58373900
C	-5.51819400	5.35672300	6.50592000
O	-4.40445700	5.56138500	6.09323900
O	-6.12548400	6.16661200	7.38181600
H	-5.52192300	6.89347300	7.59165000
I	-5.79731600	0.81269300	3.41845900

Neutral-Cation-Cl dimethyloxidanium^{+} DCE

O	-0.23176500	0.32046700	-0.00016900
C	1.24211200	0.30167200	0.01371600
H	1.52780600	-0.74504200	-0.00603800
H	1.60218900	0.85025100	-0.85294400
H	1.52717800	0.77233200	0.94937000
C	-0.86977700	1.64743800	0.05315500
H	-0.56682500	2.21283700	-0.82466600
H	-1.93864100	1.46210300	0.08065300
H	-0.52134000	2.09793200	0.97721300
H	-0.60231300	-0.23792300	-0.70562700
C	-1.61134000	-1.69436500	4.21673300
C	-1.19220800	-1.11574900	5.40163800
C	-1.64535000	-1.68927200	6.58948100

C	-2.48388600	-2.79669600	6.58976700
C	-2.89333800	-3.36901300	5.37774600
C	-2.44590500	-2.80007400	4.17796700
H	-0.54152100	-0.25257700	5.41793600
H	-2.82349600	-3.21886000	7.52731400
H	-2.75219600	-3.21869700	3.22684200
N	-3.77091100	-4.43818700	5.36196700
H	-3.77188800	-5.00370200	4.52563000
H	-3.81215500	-4.99056100	6.20606700
C	-1.19292600	-1.06350800	7.86631700
O	-0.46125800	-0.10796500	7.92925400
O	-1.68420700	-1.67290400	8.95172200
H	-1.35032700	-1.21371300	9.73552300
Cl	-1.07411500	-1.00443200	2.69941900

Neutral-Cation-Br dimethyloxidanium^{+} DCE

O	-0.21501900	0.38066100	-0.05882400
C	1.23878700	0.32129100	0.17969300
H	1.53293700	-0.70161200	-0.03407700
H	1.72436700	1.04186700	-0.47310700
H	1.36769900	0.55949000	1.23107200
C	-0.86640600	1.68020000	0.18716100
H	-0.42744500	2.41796900	-0.47989500
H	-1.92336500	1.52328500	-0.00103500
H	-0.68060000	1.90372800	1.23318500
H	-0.46208300	0.00503000	-0.92140200
C	-1.71335600	-1.92385100	4.20731100
C	-1.24662500	-1.25952900	5.32803200
C	-1.66421500	-1.73286900	6.57246300
C	-2.51357600	-2.82551700	6.68802400
C	-2.97290200	-3.48430200	5.53951400
C	-2.56084500	-3.01813900	4.28328300
H	-0.58489200	-0.40750700	5.26007100
H	-2.82430500	-3.16978300	7.66653600
H	-2.90468900	-3.51106900	3.38202500
N	-3.86405600	-4.53712000	5.63871600
H	-3.90817600	-5.16283000	4.84775100
H	-3.87800100	-5.02421900	6.52275400
C	-1.16228600	-1.01513100	7.78076400
O	-0.42539300	-0.06225700	7.74483400
O	-1.61650700	-1.53758000	8.92602200
H	-1.25279600	-1.02344800	9.66096400
Br	-1.17298200	-1.31710700	2.48360800

Neutral-Cation-I dimethyloxidanium^{+} DCE

O	0.03144000	0.26302500	-0.15166300
C	1.34344600	0.38200400	0.51191900
H	1.82631300	-0.58210200	0.38874600
H	1.89431000	1.19183700	0.03994400
H	1.11957000	0.58281900	1.55530200
C	-0.83609300	1.45388300	-0.08383600
H	-0.32271400	2.28134400	-0.56703500
H	-1.75602700	1.18088200	-0.59084600
H	-1.00264900	1.62943900	0.97458000

H	0.11113200	-0.07938200	-1.05924000
C	-1.87956800	-2.17958600	4.27418600
C	-1.30593200	-1.48576300	5.32609800
C	-1.65070000	-1.88002700	6.62006100
C	-2.53473400	-2.92590400	6.85085400
C	-3.10447100	-3.61550100	5.77283800
C	-2.76508900	-3.22853500	4.46789400
H	-0.61338500	-0.66949600	5.17591700
H	-2.78697600	-3.20897100	7.86526700
H	-3.20045800	-3.75216100	3.62524800
N	-4.03094900	-4.61962200	5.98768200
H	-4.16465700	-5.27504400	5.23181000
H	-3.99860500	-5.06739100	6.89189800
C	-1.02824800	-1.13204000	7.75142800
O	-0.25281100	-0.21956400	7.61496800
O	-1.41851700	-1.57819400	8.95119700
H	-0.97717300	-1.04982900	9.63158700
I	-1.38590900	-1.62928400	2.27871900

Neutral-Cation-Cl Me-gua$^+$ DCE

C	0.01225200	0.55994100	-0.03909800
N	0.11177600	0.70853600	1.28258400
N	1.09130800	0.28094600	-0.76247800
N	-1.16922300	0.69780400	-0.63625600
H	-0.70030400	0.91831800	1.84124500
H	1.01353300	0.78714500	1.72627500
H	1.95488200	0.10228100	-0.27158100
H	-1.29715500	0.45834700	-1.60661900
H	-1.98910000	0.95438700	-0.10893800
C	1.31850100	5.17815100	-0.72165200
C	0.13369000	5.79579100	-1.08574800
C	0.04257300	7.19431300	-1.04097900
C	2.33181400	7.27381300	-0.26350700
C	2.43651400	5.88336100	-0.30650300
H	-0.71654000	5.20234600	-1.40025400
H	3.34913200	5.37606900	-0.02935300
C	1.08341700	0.18154000	-2.21730600
H	2.11012300	0.05486000	-2.54809900
H	0.50122900	-0.67942800	-2.55137600
H	0.68843700	1.09934200	-2.65734300
C	1.15972900	7.92650600	-0.62197300
H	1.12023600	9.00827300	-0.57303700
C	3.48512200	8.11499100	0.17195500
O	3.46289000	9.31783600	0.23478700
O	4.56551000	7.39196400	0.49230300
H	5.26833400	7.99971500	0.76316700
N	-1.14767700	7.82934300	-1.34714200
H	-1.78530300	7.32011100	-1.94143600
H	-1.07646100	8.80420800	-1.59987400
Cl	1.40556200	3.42927700	-0.78702400

Neutral-Cation-Br Me-gua$^+$ DCE

C	-0.00975500	0.16134600	-0.02915000
N	0.04011400	0.16725100	1.30253300

N	1.10253900	-0.00809900	-0.73841700
N	-1.17411800	0.33229200	-0.64948500
H	-0.79023800	0.31813600	1.85290700
H	0.92087100	0.11471400	1.78919500
H	1.95598100	-0.20348100	-0.23552900
H	-1.24665900	0.29224200	-1.65340800
H	-2.01845100	0.50751600	-0.12771100
C	1.30064200	5.14451900	-0.64493900
C	0.11803900	5.75683000	-1.02599300
C	0.04078400	7.15733900	-1.04321300
C	2.33873500	7.24943600	-0.29374300
C	2.42997000	5.85713400	-0.27321400
H	-0.74320300	5.16309000	-1.30822100
H	3.34286000	5.35888400	0.01879800
C	1.13107700	-0.05362000	-2.19630900
H	2.16767600	-0.15188100	-2.50520300
H	0.56982700	-0.91033800	-2.57407100
H	0.73576200	0.87377800	-2.61553500
C	1.16905700	7.89662500	-0.66937900
H	1.14055400	8.97982800	-0.66956600
C	3.50487300	8.09883300	0.08901400
O	3.49309900	9.30336700	0.09836400
O	4.58369200	7.38148400	0.42654800
H	5.29489600	7.99468500	0.66080000
N	-1.14660800	7.78923700	-1.36605700
H	-1.79598700	7.25874700	-1.92806000
H	-1.06943700	8.75052200	-1.66478800
Br	1.37798400	3.23967600	-0.63143000

Neutral-Cation-I Me-gua^{+} DCE

C	-0.06295200	-0.02141600	-0.04035700
N	-0.01657700	-0.01748900	1.29097200
N	1.05798700	-0.16095500	-0.74600100
N	-1.22701300	0.12792500	-0.66502500
H	-0.85057800	0.11976800	1.83956500
H	0.86435500	-0.04806100	1.77950300
H	1.90439900	-0.37857500	-0.23956900
H	-1.29445600	0.08963100	-1.66946800
H	-2.07566400	0.29389000	-0.14695200
C	1.36328600	5.31398200	-0.61897600
C	0.17502400	5.91632900	-1.00013800
C	0.08407900	7.31649100	-1.02813100
C	2.38284300	7.43498000	-0.28901600
C	2.48645000	6.04299400	-0.25802400
H	-0.68688200	5.32041400	-1.27654500
H	3.40852900	5.56297300	0.03596200
C	1.08698100	-0.24135300	-2.20320600
H	2.12635600	-0.31204700	-2.51076300
H	0.55177100	-1.12317000	-2.56058000
H	0.66362300	0.66391700	-2.64287900
C	1.20608900	8.06910600	-0.66477600
H	1.16748900	9.15206300	-0.67318600
C	3.54250700	8.29771300	0.08304300
O	3.52008300	9.50227300	0.08332300

O	4.62926500	7.59311900	0.42246400
H	5.33549400	8.21476200	0.64930100
N	-1.11129100	7.93413800	-1.35187000
H	-1.75629200	7.39164800	-1.90757800
H	-1.04316200	8.89231500	-1.66271800
I	1.46564300	3.18855300	-0.58938700

Cation-Neutral-Cl Me-gua TCM ModRedundant

C	-0.36330800	0.19288300	-0.32641800
N	-1.07220900	0.28988200	0.74195800
N	1.01352100	0.16323300	-0.37618600
N	-0.98490200	0.21855400	-1.56409200
H	-0.47464500	0.36050800	1.56195000
H	1.46109600	-0.08333700	0.49280700
H	-0.57625400	-0.35100300	-2.29109600
H	-1.98449700	0.09681700	-1.48555300
C	1.11131700	4.91152400	-0.50176400
C	-0.07628500	5.62932100	-0.55388900
C	0.00255200	7.01212700	-0.60672600
C	2.37557700	6.95053500	-0.55930800
C	2.34100900	5.56209400	-0.50587000
H	-1.02797100	5.11151600	-0.55251800
H	3.25974700	4.99182000	-0.46462300
Cl	1.06235700	3.18304200	-0.42113900
C	1.77244800	-0.08452700	-1.59060600
H	2.83010800	0.03799700	-1.36378900
H	1.62235100	-1.09262500	-1.99289700
H	1.50738600	0.64977300	-2.35367200
C	1.19971500	7.69572600	-0.60936900
H	1.25212300	8.77764700	-0.64901500
C	3.66760200	7.70607100	-0.56333100
O	3.73124300	8.90544400	-0.60235100
O	4.72905200	6.90179800	-0.52027100
H	5.53226200	7.44308800	-0.52635200
N	-1.25675400	7.78064600	-0.68592700
H	-1.63411300	7.78745900	-1.64008900
H	-1.97975000	7.39104800	-0.07226400
H	-1.11755500	8.75658000	-0.40598800

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Cation-Neutral-Cl Me-gua DCE

C	-0.40305400	0.36563400	-0.36857800
N	-1.09833200	0.50078700	0.70761000
N	0.94266100	0.09240200	-0.42311000
N	-0.99661500	0.59616600	-1.59730000
H	-0.50580300	0.39774800	1.52779800
H	1.33964800	-0.27688300	0.42662400
H	-0.67168300	0.03969400	-2.37497300
H	-2.00375400	0.63463500	-1.53362800
C	1.32917700	4.85235100	-0.41061900
C	0.08199900	5.45671900	-0.48245100
C	0.03703200	6.83934800	-0.57782400

C	2.40822100	6.98924900	-0.52363500
C	2.49787200	5.60535600	-0.42925900
H	-0.82103100	4.85818500	-0.46764100
H	3.46230100	5.11859900	-0.37004600
Cl	1.41636000	3.12474700	-0.29955200
C	1.66557600	-0.17401600	-1.65549400
H	2.72155300	-0.28238100	-1.41547600
H	1.33182200	-1.08984500	-2.15544500
H	1.56238800	0.66804400	-2.34285700
C	1.17055800	7.62451100	-0.59993500
H	1.12807700	8.70487300	-0.67423600
C	3.62847500	7.85407500	-0.54871100
O	3.58933000	9.05352900	-0.62666300
O	4.75671600	7.14861400	-0.47606800
H	5.50994200	7.75710100	-0.49809600
N	-1.28553700	7.48443500	-0.67968300
H	-1.74085200	7.27301500	-1.57484900
H	-1.91668800	7.17501900	0.06646600
H	-1.21313800	8.50393100	-0.61075700

Cation-Neutral-Cl Me-gua Acetone

C	-0.38129600	0.26472100	-0.30539200
N	-1.04315800	0.26758900	0.80137700
N	0.97419900	0.08423400	-0.42520000
N	-1.03499700	0.55207000	-1.49030200
H	-0.41411900	0.13860400	1.58999200
H	1.43152700	-0.30680600	0.38342200
H	-0.70314500	0.08913200	-2.32423900
H	-2.03953100	0.51811100	-1.39300800
C	1.28036000	4.85631200	-0.39393400
C	0.04665400	5.48137400	-0.50671300
C	0.02852100	6.86278300	-0.62652500
C	2.40090900	6.97008100	-0.52160700
C	2.46292300	5.58655900	-0.39852200
H	-0.86754200	4.90032400	-0.50304800
H	3.41653200	5.08384000	-0.30712000
Cl	1.33449700	3.12830800	-0.24874700
C	1.67216000	-0.02063400	-1.69532700
H	2.74118600	-0.05740400	-1.49481700
H	1.39702400	-0.91808800	-2.25982000
H	1.47500200	0.86306300	-2.30563200
C	1.17735700	7.62617400	-0.63779300
H	1.15506400	8.70545200	-0.73336700
C	3.63813100	7.81003100	-0.53493300
O	3.62611500	9.00850400	-0.63911600
O	4.75039400	7.08489600	-0.42029400
H	5.51581600	7.67823300	-0.43700500
N	-1.27832800	7.53020200	-0.76387100
H	-1.70947100	7.33563400	-1.67466400
H	-1.93776500	7.22491500	-0.04077200
H	-1.19180100	8.54742800	-0.68140900

Cation-Neutral-Cl Me-gua DMSO

C	0.13512000	0.14034200	0.11703300

N	0.32230100	0.05923100	1.39069800
N	1.11948500	0.09428900	-0.83840700
N	-1.13574700	0.38370100	-0.37160300
H	1.31489500	-0.02184100	1.59743600
H	2.00720200	-0.26616000	-0.52531700
H	-1.37495300	-0.03244500	-1.26006700
H	-1.85052000	0.25559600	0.33022600
C	1.31284300	4.88236100	-0.68957500
C	0.16242300	5.51546500	-1.13758800
C	0.13321300	6.90148300	-1.10782800
C	2.33363200	6.99683200	-0.21294700
C	2.40336800	5.60848200	-0.22596100
H	-0.68259900	4.93900500	-1.49438800
H	3.29223300	5.09766600	0.11943700
Cl	1.38378400	3.14808000	-0.70706000
C	0.86594500	0.06784600	-2.26921400
H	1.82358600	0.11209300	-2.78454900
H	0.34352500	-0.83923000	-2.59193100
H	0.28421800	0.94282900	-2.56626100
C	1.19183500	7.66105200	-0.65594500
H	1.15774400	8.74355600	-0.63681800
C	3.47397200	7.83240500	0.27367100
O	3.45041400	9.03491000	0.30640800
O	4.51602300	7.09924300	0.66435500
H	5.22028400	7.69087500	0.96769100
N	-1.08656500	7.57999200	-1.57914400
H	-1.31023400	7.32680300	-2.54742400
H	-1.90091400	7.34255200	-1.00246500
H	-0.98329200	8.59862900	-1.55085100

Cation-Neutral-Cl Me-gua Water

C	0.13675500	0.13960800	0.11730600
N	0.32667800	0.05781900	1.39092400
N	1.11907100	0.09343200	-0.83965300
N	-1.13487000	0.38365200	-0.36838300
H	1.31976900	-0.02391600	1.59504600
H	2.00767800	-0.26641800	-0.52833900
H	-1.37607700	-0.03049300	-1.25726600
H	-1.84879600	0.25537400	0.33427400
C	1.31292700	4.88267600	-0.68874000
C	0.16282600	5.51555200	-1.13773700
C	0.13340500	6.90155400	-1.10865500
C	2.33324800	6.99705200	-0.21193800
C	2.40319900	5.60862100	-0.22463600
H	-0.68182200	4.93919200	-1.49552500
H	3.29191800	5.09788300	0.12121700
Cl	1.38398600	3.14804300	-0.70701000
C	0.86312500	0.06876600	-2.27013400
H	1.81996200	0.11345000	-2.78687500
H	0.33999700	-0.83787200	-2.59279100
H	0.28100500	0.94412500	-2.56524900
C	1.19182700	7.66113300	-0.65607800
H	1.15760100	8.74364600	-0.63751000
C	3.47321500	7.83242400	0.27538400

O	3.44986400	9.03505100	0.30864900
O	4.51498900	7.09931500	0.66704600
H	5.21898100	7.69104400	0.97083000
N	-1.08563200	7.57935700	-1.58184000
H	-1.30944500	7.32335000	-2.54935100
H	-1.90023800	7.34424700	-1.00459600
H	-0.98192800	8.59797600	-1.55675800

Cation-Neutral-Br Me-gua TCM

C	-0.40292400	0.41314000	-0.36577100
N	-1.08857500	0.58692600	0.70673100
N	0.96360500	0.20814000	-0.42003200
N	-1.01708700	0.53871100	-1.59903600
H	-0.48594800	0.56123700	1.52573900
H	1.35774200	-0.14175000	0.44048500
H	-0.67918600	-0.05339300	-2.34375100
H	-2.02408100	0.54284200	-1.52294500
C	1.32607200	5.13774300	-0.44774100
C	0.08171000	5.75050600	-0.51223100
C	0.04215900	7.13460600	-0.58820400
C	2.41159700	7.27724200	-0.52362900
C	2.49616500	5.89131700	-0.45163100
H	-0.82639300	5.15910400	-0.50699400
H	3.46170300	5.40592100	-0.39790800
C	1.65582500	-0.18895900	-1.63778200
H	2.71935600	-0.26137800	-1.41788900
H	1.31736500	-1.15591400	-2.02641100
H	1.52487300	0.57362900	-2.40775300
C	1.17647600	7.91815400	-0.59569100
H	1.14024100	9.00001500	-0.65531700
C	3.63329400	8.14212600	-0.52938200
O	3.59266800	9.34172100	-0.58948500
O	4.76010200	7.43423200	-0.46061800
H	5.51412400	8.04206000	-0.46701500
N	-1.28117000	7.78389300	-0.68822400
H	-1.73024600	7.58679800	-1.58988600
H	-1.91682600	7.46204300	0.04879800
H	-1.20691200	8.80196100	-0.60170200
Br	1.40676700	3.25296600	-0.36311400

Cation-Neutral-Br Me-gua DCE

C	-0.38007600	0.26487200	-0.29802000
N	-1.01555200	0.35737000	0.81702000
N	0.99286800	0.23373500	-0.43373500
N	-1.07949100	0.30120300	-1.49035000
H	-0.36233700	0.42195000	1.59397800
H	1.48433100	-0.04848100	0.40118800
H	-0.71951700	-0.25366600	-2.25349400
H	-2.07393300	0.18886400	-1.35464400
C	1.23733600	5.16890200	-0.48771500
C	0.01929400	5.82851300	-0.57981900
C	0.03276700	7.21403500	-0.63848400
C	2.40469100	7.26465900	-0.51394400
C	2.43488300	5.87530200	-0.45433000

H	-0.91042700	5.27298400	-0.60588300
H	3.37954300	5.35315400	-0.38023900
C	1.66518200	-0.04638600	-1.69378300
H	2.73750300	0.05577600	-1.53682200
H	1.46564700	-1.05540500	-2.07043100
H	1.36660100	0.68508300	-2.44703600
C	1.19701600	7.95275600	-0.60824500
H	1.19959700	9.03569400	-0.65620300
C	3.65957000	8.07817700	-0.47861500
O	3.67205600	9.27993500	-0.52278900
O	4.75554000	7.32474700	-0.39324900
H	5.53291200	7.90220800	-0.37176700
N	-1.25869700	7.91622700	-0.75895400
H	-1.65612800	7.82066000	-1.70020700
H	-1.95036500	7.55494000	-0.09444900
H	-1.15877200	8.91821800	-0.57214300
Br	1.25045200	3.27961200	-0.40522600

Cation-Neutral-Br Me-gua Acetone

C	-0.16313000	0.15327200	-0.04600500
N	-0.42914500	0.11731300	1.21356100
N	1.10027300	0.22622700	-0.59207300
N	-1.19537200	0.22988000	-0.96195200
H	0.42867500	0.16180800	1.75827000
H	1.84027600	-0.05936400	0.03153000
H	-1.05965100	-0.22751000	-1.85192200
H	-2.09487300	0.03200300	-0.54789700
C	1.20837300	5.18248000	-0.57635800
C	0.02244900	5.85430600	-0.84056100
C	0.05395900	7.24106700	-0.86683700
C	2.38168700	7.26571200	-0.38660200
C	2.39208900	5.87549100	-0.34802800
H	-0.89702000	5.30936000	-1.01781800
H	3.31036800	5.34242600	-0.14078000
C	1.36890200	0.07372600	-2.01421100
H	2.43461600	0.22476200	-2.17591600
H	1.09799300	-0.91654700	-2.39570400
H	0.83354400	0.83822300	-2.58063200
C	1.20641600	7.96617700	-0.64737600
H	1.22095500	9.04914900	-0.67090800
C	3.62239200	8.06542700	-0.14789900
O	3.65414500	9.26759000	-0.18124300
O	4.68433000	7.30088000	0.10512500
H	5.45389500	7.87082000	0.25009300
N	-1.19963000	7.96219900	-1.15397700
H	-1.45103300	7.90315500	-2.14688700
H	-1.98696900	7.58761300	-0.61445800
H	-1.12314000	8.95669400	-0.92047600
Br	1.20712200	3.29129900	-0.52044700

Cation-Neutral-Br Me-gua DMSO

C	0.07105700	0.17745300	0.08193100
N	0.16899400	0.15587700	1.36661000
N	1.13175700	0.21147700	-0.79643800

N	-1.17439900	0.27999600	-0.50777800
H	1.14672200	0.17685400	1.64652100
H	2.01048200	-0.08700800	-0.40020600
H	-1.30665800	-0.18130800	-1.39626900
H	-1.92732700	0.10931300	0.14315100
C	1.26946200	5.18156300	-0.68658800
C	0.11512600	5.83854200	-1.08889100
C	0.11037100	7.22509900	-1.05290200
C	2.34349600	7.27851900	-0.23993800
C	2.38908500	5.88872300	-0.26212900
H	-0.75538000	5.28373400	-1.41719200
H	3.28414100	5.36596400	0.04753000
C	0.98722300	0.03632800	-2.23392900
H	1.96680200	0.16238300	-2.69135800
H	0.60288800	-0.95258100	-2.50580700
H	0.32653700	0.80391400	-2.64136900
C	1.19726000	7.96449600	-0.63615000
H	1.18358800	9.04741500	-0.60978600
C	3.51459200	8.09243700	0.20869300
O	3.50975900	9.29480900	0.25581400
O	4.56114700	7.34064300	0.54908500
H	5.28434900	7.91929900	0.83227000
N	-1.11488700	7.92460100	-1.47780300
H	-1.36815300	7.69123900	-2.44369500
H	-1.91545300	7.68447300	-0.88321100
H	-1.00123900	8.94157800	-1.43502000
Br	1.31115400	3.28980600	-0.71353400

Cation-Neutral-Br Me-gua Water

C	0.25954400	0.11319800	0.15375100
N	0.60723800	0.01601200	1.39102800
N	1.12637500	0.22169700	-0.91082400
N	-1.07827800	0.22448700	-0.17352100
H	1.62049400	0.03789300	1.47636400
H	2.07031300	-0.07521100	-0.71337200
H	-1.37798700	-0.18327800	-1.04730100
H	-1.68719400	-0.00231700	0.59939400
C	1.25477700	5.18518200	-0.70944900
C	0.15224300	5.85178900	-1.22493000
C	0.15644200	7.23831600	-1.19115400
C	2.29855400	7.27336400	-0.16162100
C	2.33259800	5.88298900	-0.17614900
H	-0.68468800	5.30540300	-1.64219100
H	3.18812100	5.35363700	0.22146300
C	0.70330100	0.12888400	-2.30029900
H	1.57157800	0.30538900	-2.93234400
H	0.28380000	-0.85077200	-2.55284500
H	-0.03291600	0.90429800	-2.52042200
C	1.20394200	7.96880200	-0.67060400
H	1.19798500	9.05205500	-0.65113000
C	3.43035000	8.07708900	0.39333100
O	3.44174000	9.28012600	0.41946600
O	4.42278600	7.31585200	0.85336000
H	5.12466000	7.88810700	1.19676800

N	-1.01347100	7.94730200	-1.73770900
H	-1.19850500	7.67842200	-2.70987600
H	-1.86269600	7.75162900	-1.19672400
H	-0.87643300	8.96216100	-1.72753100
Br	1.28781900	3.29313600	-0.74331700

Cation-Neutral-I Me-gua TCM

C	-0.38134600	0.24350800	-0.29988800
N	-1.01665800	0.32722100	0.81055800
N	0.99899800	0.36453900	-0.44211100
N	-1.07650200	0.14672900	-1.48882300
H	-0.37542000	0.49688200	1.58166200
H	1.49609900	0.12214100	0.40405100
H	-0.66104500	-0.40025600	-2.22832800
H	-2.05601300	-0.05325700	-1.34599600
C	1.18687700	5.50976000	-0.51964400
C	-0.01467300	6.20465900	-0.59432800
C	0.02791600	7.59085600	-0.63114400
C	2.39854000	7.59025100	-0.52328300
C	2.39608600	6.19916500	-0.48548500
H	-0.96015800	5.67544700	-0.62301100
H	3.33536500	5.66464600	-0.42707300
C	1.68653000	-0.01646700	-1.67196300
H	2.74961500	0.17752500	-1.53947800
H	1.55460200	-1.07366700	-1.92551100
H	1.33609500	0.60235200	-2.49972900
C	1.20618700	8.30569400	-0.59684400
H	1.23211100	9.38890200	-0.62644400
C	3.66952700	8.37905600	-0.48602800
O	3.70346700	9.58035000	-0.51036500
O	4.75165600	7.60319100	-0.42446200
H	5.53936500	8.16626900	-0.40216200
N	-1.24819700	8.32979400	-0.73854400
H	-1.58966600	8.35064300	-1.70576300
H	-1.98278200	7.90723300	-0.16195000
H	-1.14593700	9.30159300	-0.42984500
I	1.16032600	3.39087300	-0.45645900

Cation-Neutral-I Me-gua DCE

C	-0.21814800	0.19658000	-0.10463600
N	-0.54811500	0.25326900	1.13517100
N	1.07191800	0.36136600	-0.59330700
N	-1.19329500	0.08300500	-1.07420700
H	0.26782900	0.43693600	1.71417900
H	1.78029300	0.15144900	0.09639900
H	-0.96466800	-0.43332400	-1.91090400
H	-2.09655900	-0.15522600	-0.69089500
C	1.19297700	5.52513400	-0.60675400
C	0.00853300	6.22023300	-0.81689900
C	0.04933300	7.60736600	-0.81185900
C	2.38791300	7.60356000	-0.40225400
C	2.38579400	6.21196500	-0.39929900
H	-0.92618300	5.69593600	-0.97888200
H	3.31136500	5.67622700	-0.23379100

C	1.43602100	0.00696000	-1.96142600
H	2.49190400	0.23248700	-2.10003100
H	1.27397400	-1.05284500	-2.18393500
H	0.86996800	0.61705000	-2.66742900
C	1.21187800	8.32016800	-0.60912500
H	1.23546400	9.40353200	-0.60487600
C	3.64181300	8.38856000	-0.18469200
O	3.68225600	9.59074300	-0.19450000
O	4.70543400	7.61136800	0.01993300
H	5.48266800	8.17365700	0.15294000
N	-1.20766100	8.34338100	-1.05031200
H	-1.48677200	8.30236400	-2.03659200
H	-1.98210200	7.96570100	-0.49446700
H	-1.11634600	9.33332000	-0.80332200
I	1.17347600	3.40471000	-0.59261600

Cation-Neutral-I Me-gua Acetone

C	-0.28982700	0.17476200	-0.17892000
N	-0.77721100	0.11993400	1.00877800
N	1.05377000	0.33965400	-0.48835900
N	-1.12249900	0.07600600	-1.27238600
H	-0.03344700	0.12552000	1.70227600
H	1.65739200	0.14806800	0.29946200
H	-0.84085900	0.54014200	-2.12309500
H	-2.09806000	0.20007200	-1.04457100
C	1.19346100	5.50462300	-0.57189500
C	-0.00726000	6.18715200	-0.71700400
C	0.02167900	7.57433200	-0.74271100
C	2.38213200	7.59392800	-0.48490900
C	2.39203200	6.20246100	-0.45678500
H	-0.94675700	5.65487100	-0.80643200
H	3.33060600	5.67624900	-0.34264500
C	1.60177400	-0.08372800	-1.77614800
H	2.68594500	-0.00533200	-1.71977800
H	1.32919800	-1.11190300	-2.02749500
H	1.26921600	0.58093800	-2.57621800
C	1.18924200	8.29872200	-0.62910800
H	1.20292000	9.38219600	-0.64507200
C	3.64199800	8.38881900	-0.35934200
O	3.67381900	9.59161700	-0.37182300
O	4.72375300	7.62000800	-0.23227200
H	5.50412900	8.18807100	-0.15265600
N	-1.25587200	8.29197800	-0.90865400
H	-1.64455600	8.16358100	-1.84927600
H	-1.96160800	7.96982900	-0.23846000
H	-1.14238000	9.29951900	-0.76480400
I	1.18823400	3.38354400	-0.51808600

Cation-Neutral-I Me-gua DMSO

C	-0.03744800	0.13237100	0.02940300
N	-0.12064300	-0.03834100	1.30035900
N	1.13838600	0.31956100	-0.68323500
N	-1.18053700	0.15108900	-0.74231500
H	0.80530400	-0.11846400	1.71320200

H	1.96070200	0.07911200	-0.14659800
H	-1.16733600	0.72585600	-1.57276900
H	-2.02385000	0.25511100	-0.19661100
C	1.21100800	5.49809600	-0.64879000
C	0.03980000	6.17195900	-0.97149200
C	0.05598100	7.55989300	-0.96037000
C	2.34618100	7.59354200	-0.32838500
C	2.36762500	6.20197600	-0.32772600
H	-0.86546700	5.63189200	-1.22375000
H	3.28105400	5.67914300	-0.07666200
C	1.23412600	-0.02197400	-2.10244500
H	2.27908200	0.05950500	-2.39568800
H	0.88084600	-1.03508700	-2.31044500
H	0.66843600	0.68534800	-2.71218900
C	1.18289100	8.29018300	-0.64606700
H	1.18587800	9.37355300	-0.64066200
C	3.56060800	8.39677500	0.00945300
O	3.58086000	9.60009300	0.02036800
O	4.61699900	7.63570900	0.29614000
H	5.36933900	8.20955600	0.50292600
N	-1.18238500	8.27655700	-1.31571600
H	-1.36361100	8.24247700	-2.32472600
H	-2.00054200	7.87911000	-0.84350000
H	-1.13540600	9.26478500	-1.05070600
I	1.23308500	3.37624400	-0.63939400

Cation-Neutral-I Me-gua Water

C	-0.03428900	0.12877800	0.03050800
N	-0.11320300	-0.04361800	1.30175700
N	1.13883400	0.31751200	-0.68548500
N	-1.17998400	0.14743700	-0.73728700
H	0.81430600	-0.12282200	1.71126700
H	1.96345400	0.07722000	-0.15234300
H	-1.16956900	0.72232400	-1.56773800
H	-2.02149500	0.25195400	-0.18887300
C	1.20985700	5.49913700	-0.64757900
C	0.03962400	6.17327700	-0.97324400
C	0.05644500	7.56120300	-0.96278200
C	2.34539400	7.59395400	-0.32561900
C	2.36618400	6.20234700	-0.32433300
H	-0.86530900	5.63353700	-1.22731500
H	3.27875500	5.67905100	-0.07116900
C	1.22981500	-0.01951100	-2.10603200
H	2.27364200	0.06354100	-2.40268900
H	0.87644200	-1.03221200	-2.31591200
H	0.66150100	0.68929400	-2.71156900
C	1.18310800	8.29093800	-0.64613900
H	1.18636300	9.37427800	-0.64121700
C	3.55955800	8.39652000	0.01435200
O	3.58056000	9.59989900	0.02563400
O	4.61525600	7.63499500	0.30250900
H	5.36752800	8.20851300	0.51048800
N	-1.18041200	8.27839500	-1.32136100
H	-1.35835100	8.24559900	-2.33099800

H	-2.00020500	7.88052000	-0.85239000
H	-1.13428000	9.26630700	-1.05506000
I	1.23143500	3.37726600	-0.63776900

Cation-Cation-Cl Me-gua^{+} TCM

C	0.13756000	-0.21602600	0.09866900
N	0.38934700	-0.19151300	1.40784800
N	1.07873900	0.14522500	-0.76790200
N	-1.07054000	-0.56643400	-0.33717000
H	-0.27554900	-0.55570000	2.07181300
H	1.29229700	0.08601900	1.75922300
H	2.00383200	0.32277000	-0.40553900
H	-1.25607900	-0.69327100	-1.31942300
H	-1.79755900	-0.82999700	0.30977200
C	0.96314100	5.05629900	-0.68839000
C	-0.07335400	5.84471500	-1.16660100
C	0.11607800	7.21958900	-1.16878000
C	2.29325300	6.99696000	-0.24211700
C	2.14814600	5.61535500	-0.22397900
H	-0.99182100	5.39347000	-1.52355100
H	2.94460300	4.98388700	0.14666700
Cl	0.77656900	3.32866200	-0.67240000
C	0.89275900	0.15611900	-2.21531500
H	1.77763900	0.60319400	-2.65990100
H	0.77686900	-0.85563400	-2.60872900
H	0.02948400	0.76739800	-2.48375200
C	1.27353400	7.81754600	-0.71799800
H	1.41321200	8.89271800	-0.72261900
C	3.54128300	7.66659900	0.24531700
O	3.68597200	8.85838300	0.25391900
O	4.45756600	6.79396300	0.66139300
H	5.23937200	7.27953300	0.96426400
N	-0.96964400	8.07647500	-1.68444800
H	-1.12174500	7.93736600	-2.68975000
H	-1.85814500	7.89341900	-1.20679900
H	-0.75346500	9.06855600	-1.54681700

Cation-Cation-Cl Me-gua^{+} DCE

C	0.01725300	0.11130100	-0.00946100
N	0.08025000	0.16386100	1.32136500
N	1.12850500	-0.01746900	-0.72733700
N	-1.15901200	0.22700000	-0.62145600
H	-0.75869900	0.15654900	1.87987500
H	0.95986800	0.05943400	1.80189100
H	1.99604700	-0.16106400	-0.23113500
H	-1.24328900	0.12373300	-1.62005500
H	-2.00887500	0.33940400	-0.09142300
C	1.20603700	4.89578000	-0.66094100
C	0.04032400	5.56169100	-1.00983600
C	0.06075500	6.94847500	-0.98573100
C	2.33408700	6.97416800	-0.29019800
C	2.35749100	5.58440300	-0.30048700
H	-0.85038600	5.01083700	-1.28819000
H	3.25623400	5.04601200	-0.03082900

Cl	1.22564300	3.15749500	-0.66969400
C	1.14728500	-0.06584700	-2.18543800
H	2.18333100	-0.14295600	-2.50176100
H	0.60378300	-0.93694300	-2.55688400
H	0.72664100	0.85005700	-2.60548300
C	1.18033200	7.67410500	-0.63537900
H	1.18667300	8.75790400	-0.62169000
C	3.53881900	7.77530600	0.09345500
O	3.55268600	8.97683800	0.11927900
O	4.58373100	7.00845300	0.40134200
H	5.33089600	7.57639800	0.64129200
N	-1.16775100	7.66999100	-1.36541000
H	-1.32144000	7.65062100	-2.37980900
H	-1.99755300	7.26611200	-0.91935400
H	-1.12631700	8.65399200	-1.08361300

Cation-Cation-Cl Me-gua^{+} Acetone

C	0.00197200	0.14488000	-0.01908500
N	0.06024600	0.20118700	1.31125900
N	1.11264700	-0.01925900	-0.73122700
N	-1.16831500	0.28716300	-0.63664700
H	-0.77966100	0.24757800	1.86609400
H	0.93710000	0.09961400	1.79716700
H	1.97404900	-0.18248000	-0.23041300
H	-1.25255400	0.17781300	-1.63453700
H	-2.01607000	0.42948500	-0.11048200
C	1.25169200	4.87573100	-0.66384100
C	0.07218400	5.52078000	-1.00564700
C	0.06557600	6.90775000	-0.97449300
C	2.34076300	6.97286900	-0.28482700
C	2.39109500	5.58387600	-0.30339100
H	-0.80819800	4.95379800	-1.28417500
H	3.30043500	5.06069600	-0.03984900
Cl	1.30486200	3.13846800	-0.68206100
C	1.13642500	-0.07508700	-2.18865700
H	2.17263400	-0.16799800	-2.50020000
H	0.58178100	-0.93963400	-2.55856100
H	0.73008900	0.84455000	-2.61440500
C	1.17247900	7.65191100	-0.62218600
H	1.15795200	8.73517000	-0.60139400
C	3.53133200	7.79385800	0.09786700
O	3.52414700	8.99590900	0.13215200
O	4.59330200	7.04608100	0.39495300
H	5.33006500	7.62766400	0.63417800
N	-1.17535900	7.60904000	-1.34892500
H	-1.33619100	7.58090100	-2.36182400
H	-1.99707600	7.19764300	-0.89487500
H	-1.14605200	8.59568500	-1.07506200

Cation-Cation-Cl Me-gua^{+} DMSO

C	-0.12511500	0.18853800	-0.09293600
N	-0.20926400	0.13944500	1.23615800
N	1.04113400	-0.02292400	-0.69495100
N	-1.20441300	0.47341300	-0.81814900

H	-1.08676100	0.28947000	1.70772200
H	0.61251300	0.00848300	1.80468900
H	1.82116600	-0.30622700	-0.12082000
H	-1.18815000	0.41194300	-1.82380900
H	-2.09729500	0.63007900	-0.37657100
C	1.38613400	4.82219900	-0.49789900
C	0.16114200	5.38769500	-0.81842400
C	0.08892000	6.77133000	-0.88707400
C	2.39179400	6.98778000	-0.33356600
C	2.50768600	5.60484100	-0.25447500
H	-0.70439500	4.76407500	-1.00766000
H	3.45411800	5.14364300	-0.00597900
Cl	1.51919300	3.09292500	-0.39732600
C	1.22997700	0.04055800	-2.13915300
H	2.29040600	-0.08412100	-2.34005200
H	0.68134900	-0.75568200	-2.64598700
H	0.91885500	1.01534100	-2.52005800
C	1.17572000	7.58761000	-0.65237500
H	1.10785300	8.66769500	-0.70658800
C	3.56039800	7.88504700	-0.07725900
O	3.50017400	9.08540200	-0.13015200
O	4.66958000	7.20784100	0.21654300
H	5.38986000	7.83597300	0.37460600
N	-1.20819400	7.38558400	-1.21941400
H	-1.55388700	7.07662400	-2.13427300
H	-1.92640300	7.15406200	-0.52437900
H	-1.14074500	8.40699900	-1.25348500

Cation-Cation-Cl Me-gua^{+} Water

C	-0.12799300	0.19840900	-0.09469600
N	-0.20926800	0.13707300	1.23421000
N	1.03402800	-0.02082500	-0.70219000
N	-1.20646800	0.50098800	-0.81380300
H	-1.08328800	0.29668000	1.70913500
H	0.61342500	-0.00114100	1.79966600
H	1.81321700	-0.31664700	-0.13315000
H	-1.19393500	0.45056400	-1.82008900
H	-2.09512100	0.66817300	-0.36771800
C	1.39731700	4.81272600	-0.47881500
C	0.17054700	5.36979000	-0.80723800
C	0.09233800	6.75242400	-0.88821400
C	2.39317200	6.98400300	-0.33167200
C	2.51490700	5.60229200	-0.23992000
H	-0.69138800	4.74009600	-0.99296800
H	3.46271200	5.14734400	0.01488100
Cl	1.53749500	3.08505900	-0.36243200
C	1.22082700	0.05998100	-2.14579700
H	2.27910600	-0.07617200	-2.35051700
H	0.66074700	-0.72187500	-2.66239300
H	0.92198300	1.04391500	-2.51280000
C	1.17509400	7.57551400	-0.65831400
H	1.10204600	8.65475900	-0.72235400
C	3.55736800	7.88828900	-0.08089100
O	3.49287600	9.08801400	-0.14521800

O	4.66861000	7.21844900	0.22208300
H	5.38582000	7.85104000	0.37633800
N	-1.20628600	7.35811000	-1.22934300
H	-1.54947200	7.03714600	-2.14110300
H	-1.92479600	7.13214400	-0.53270400
H	-1.14226700	8.37932200	-1.27507200

Cation-Cation-Br Me-gua^{+} TCM

C	0.04450700	-0.04571700	0.02368200
N	0.12267900	0.04808300	1.35039900
N	1.13604100	0.11195400	-0.72160800
N	-1.13223800	-0.25452700	-0.56205300
H	-0.67466600	-0.14425500	1.93619800
H	0.99585400	0.26378600	1.80540900
H	2.02716000	0.12741300	-0.24655900
H	-1.19321700	-0.45991000	-1.54674700
H	-1.97342900	-0.35323500	-0.01544200
C	1.05560100	5.27991200	-0.69058900
C	-0.05112300	6.03004900	-1.06312900
C	0.07206200	7.41241000	-1.03515000
C	2.32402100	7.27312400	-0.29016600
C	2.24623200	5.88562100	-0.30388800
H	-0.97734300	5.55261100	-1.36150600
H	3.10215000	5.28925400	-0.01701300
C	1.13650700	0.01413300	-2.17850900
H	2.12897600	0.28241100	-2.52951900
H	0.90667300	-1.00151200	-2.50878800
H	0.42225000	0.72132800	-2.60318700
C	1.23203500	8.05512200	-0.65879500
H	1.32055300	9.13538600	-0.63663900
C	3.57298200	7.99135500	0.12074600
O	3.66421000	9.18839100	0.14303600
O	4.55416000	7.15512600	0.45477200
H	5.33301600	7.67047100	0.71304800
N	-1.09783300	8.22384800	-1.42624300
H	-1.39544000	8.02103800	-2.38661500
H	-1.90043100	8.05644200	-0.80973400
H	-0.88741000	9.22571600	-1.38185600
Br	0.94808700	3.38981000	-0.70665200

Cation-Cation-Br Me-gua^{+} DCE

C	0.00446200	0.00598000	0.00570100
N	0.04857900	0.14552000	1.32967300
N	1.11721700	0.12580800	-0.71566600
N	-1.15903400	-0.21601600	-0.60011300
H	-0.77097800	-0.00634200	1.89618900
H	0.90628300	0.39084300	1.79852600
H	1.99586400	0.14892600	-0.21791700
H	-1.20254100	-0.45501800	-1.57799300
H	-2.01319500	-0.27790200	-0.06827300
C	1.12991300	5.25419400	-0.71249200
C	-0.00444900	5.97815800	-1.05053300
C	0.07532300	7.36183600	-0.99819100
C	2.34461200	7.27670600	-0.29631200

C	2.30863600	5.88718900	-0.33568200
H	-0.92075000	5.47941400	-1.34183100
H	3.18621900	5.31088700	-0.07479500
C	1.15114700	-0.01124400	-2.16869600
H	2.15565600	0.23349700	-2.50212900
H	0.91453900	-1.03160800	-2.47796800
H	0.45652300	0.69335500	-2.62915300
C	1.22234100	8.03185300	-0.62873600
H	1.27124900	9.11372300	-0.58926300
C	3.58062300	8.01907900	0.10542500
O	3.64474200	9.21847300	0.15229200
O	4.59131300	7.20382200	0.40305100
H	5.36070300	7.73511300	0.65678300
N	-1.12184400	8.14053200	-1.36379700
H	-1.32460600	8.07589900	-2.36742400
H	-1.95398500	7.81622700	-0.85953700
H	-1.00199800	9.13381000	-1.14300000
Br	1.07006400	3.36292500	-0.76123900

Cation-Cation-Br Me-gua^{+} Acetone

C	-0.01794400	0.14059000	-0.01868700
N	0.03693500	0.15453700	1.31209100
N	1.10088100	0.03631700	-0.73257100
N	-1.18932500	0.26538100	-0.63638500
H	-0.80350700	0.17873300	1.86765500
H	0.91868200	0.10043500	1.79692500
H	1.95767500	-0.16172600	-0.23576200
H	-1.26748600	0.17680000	-1.63686400
H	-2.04131600	0.38254500	-0.11074100
C	1.27113300	5.16040000	-0.62044100
C	0.08939700	5.79455300	-0.97642800
C	0.07733800	7.18217100	-0.97601200
C	2.35220400	7.27126300	-0.28853700
C	2.40779900	5.88186900	-0.27559100
H	-0.79102000	5.22250500	-1.24425800
H	3.32178100	5.37310100	-0.00021300
C	1.12369400	0.00212200	-2.19119000
H	2.16260500	-0.03610400	-2.50565800
H	0.60766800	-0.88038500	-2.57488800
H	0.67539000	0.90967100	-2.60052700
C	1.18136600	7.93808300	-0.64033500
H	1.16318200	9.02146200	-0.64293300
C	3.53939500	8.10578900	0.07514900
O	3.52627000	9.30825300	0.08429700
O	4.60573300	7.36984700	0.38573000
H	5.34014700	7.96028700	0.60996700
N	-1.16663600	7.87044800	-1.36525200
H	-1.32306500	7.82822100	-2.37833200
H	-1.98712800	7.45894300	-0.90917400
H	-1.14536600	8.86072500	-1.10392300
Br	1.33614400	3.26880100	-0.60020800

Cation-Cation-Br Me-gua^{+} DMSO

C	-0.12578600	0.18922700	-0.08729400

N	-0.21118800	0.14057100	1.24134800
N	1.05227300	0.02536000	-0.68498500
N	-1.21220800	0.42696800	-0.81711400
H	-1.09246700	0.27248300	1.71142600
H	0.61424700	0.04422700	1.81179300
H	1.83198700	-0.25843600	-0.11004300
H	-1.18796600	0.37391700	-1.82307100
H	-2.11047900	0.56406000	-0.37976900
C	1.38607300	5.12429100	-0.52293300
C	0.16100400	5.69486600	-0.83548500
C	0.08878300	7.07953700	-0.88840000
C	2.39201300	7.28915200	-0.33432400
C	2.50784200	5.90478500	-0.27064800
H	-0.70755700	5.07817200	-1.03250000
H	3.45672900	5.44538900	-0.02853600
C	1.23079400	0.03710200	-2.13246600
H	2.29447300	-0.05201900	-2.33524900
H	0.71022600	-0.79893900	-2.60373100
H	0.87996400	0.98305100	-2.54951200
C	1.17590800	7.89277200	-0.64536600
H	1.10836400	8.97342400	-0.68773500
C	3.56094400	8.18389500	-0.07031600
O	3.50010400	9.38472300	-0.11010800
O	4.67105700	7.50411000	0.21377900
H	5.39134000	8.13097500	0.37679100
N	-1.20870200	7.69748900	-1.21299900
H	-1.55739800	7.39480300	-2.12881100
H	-1.92512800	7.46188600	-0.51755100
H	-1.14054200	8.71906400	-1.24047400
Br	1.52792200	3.23873200	-0.43881300

Cation-Cation-Br Me-gua^{+} Water

C	-0.12666600	0.19651900	-0.09096900
N	-0.20889200	0.14374400	1.23770800
N	1.04859500	0.02696000	-0.69261900
N	-1.21378800	0.44356000	-0.81644700
H	-1.08904900	0.27517700	1.70998300
H	0.61682000	0.03768800	1.80591800
H	1.82797700	-0.26492900	-0.12131100
H	-1.19264000	0.39794300	-1.82277300
H	-2.10862700	0.59085700	-0.37546300
C	1.39608800	5.11781500	-0.51433000
C	0.16856300	5.68201500	-0.82886500
C	0.09010100	7.06615700	-0.88538300
C	2.39227400	7.28756400	-0.33093600
C	2.51426600	5.90383900	-0.26369100
H	-0.69681800	5.06046800	-1.02470200
H	3.46511300	5.44923000	-0.02023200
C	1.22444000	0.04915000	-2.14024600
H	2.28751400	-0.04180500	-2.34555900
H	0.70038300	-0.78146200	-2.61721800
H	0.87603800	0.99948400	-2.54937800
C	1.17355000	7.88483200	-0.64389100
H	1.10057200	8.96500900	-0.68925600

C	3.55731800	8.18778700	-0.06926900
O	3.49179100	9.38839300	-0.11195700
O	4.67042600	7.51351500	0.21640700
H	5.38791000	8.14390500	0.37817100
N	-1.20950600	7.67770200	-1.21261000
H	-1.55937700	7.36573100	-2.12481400
H	-1.92393600	7.44657500	-0.51361100
H	-1.14389500	8.69911200	-1.24942900
Br	1.54608100	3.23310500	-0.42632400

Cation-Cation-I Me-gua$^+$ TCM

C	-0.03726800	0.00765500	-0.00439700
N	0.01336500	0.10874900	1.32179900
N	1.07782700	0.14462500	-0.72564600
N	-1.20287100	-0.18523300	-0.61407400
H	-0.80572300	-0.04395200	1.88897100
H	0.87589100	0.32936100	1.79405600
H	1.95579600	0.08996200	-0.22739100
H	-1.24831300	-0.40559700	-1.59643000
H	-2.05755700	-0.25797600	-0.08374700
C	1.20965000	5.58626800	-0.66002500
C	0.05705600	6.27572900	-1.01130200
C	0.09892300	7.66274600	-0.99106000
C	2.36999300	7.65636000	-0.29709300
C	2.36955500	6.26503600	-0.30155500
H	-0.84890000	5.75058500	-1.29130600
H	3.26725700	5.72720300	-0.02675600
C	1.11060400	-0.00164500	-2.17985000
H	2.11665400	0.23471400	-2.51503100
H	0.86645400	-1.02165500	-2.48447100
H	0.42293500	0.70811800	-2.64258400
C	1.22847100	8.37390300	-0.64541200
H	1.25336800	9.45799800	-0.63751300
C	3.58650300	8.44276700	0.08525900
O	3.61416600	9.64310300	0.10536800
O	4.61921600	7.66159100	0.39794000
H	5.37471300	8.21916300	0.63631200
N	-1.12270500	8.40151200	-1.36980100
H	-1.27701800	8.38697400	-2.38437400
H	-1.95598700	8.00464300	-0.92365900
H	-1.06835400	9.38360900	-1.08296400
I	1.19739200	3.46931900	-0.66636000

Cation-Cation-I Me-gua$^+$ DCE

C	-0.04352300	0.02593500	-0.01470500
N	-0.01743900	0.14618100	1.31048900
N	1.08529400	0.14851900	-0.71696200
N	-1.19885800	-0.17150500	-0.64153400
H	-0.85146400	0.01516600	1.86094300
H	0.83633000	0.37084700	1.79666600
H	1.95384700	0.10079900	-0.20200100
H	-1.23081300	-0.40158200	-1.62210200
H	-2.06148400	-0.23245800	-0.12280400
C	1.20547100	5.57842600	-0.66213400

C	0.04903900	6.26917000	-0.99786700
C	0.08992300	7.65620200	-0.97260800
C	2.36943400	7.64656700	-0.30275800
C	2.36928000	6.25511600	-0.31352200
H	-0.85998000	5.74565600	-1.26995700
H	3.26934900	5.71519300	-0.05131600
C	1.14491200	-0.01263300	-2.16796300
H	2.15687300	0.22243200	-2.48596000
H	0.90810200	-1.03589500	-2.46701300
H	0.46446300	0.69047400	-2.65129800
C	1.22358700	8.36487700	-0.63474000
H	1.24558300	9.44843600	-0.62213400
C	3.59061400	8.42884100	0.06661200
O	3.62497100	9.63031300	0.08786100
O	4.62659900	7.64680300	0.36769900
H	5.38496100	8.20410900	0.59718100
N	-1.13273800	8.39614100	-1.33749400
H	-1.30018600	8.37722000	-2.34963400
H	-1.96256700	8.00487600	-0.88030900
H	-1.07292900	9.37975800	-1.05758900
I	1.19444300	3.46164800	-0.67614100

Cation-Cation-I Me-gua^{+} Acetone

C	-0.04496200	0.03642700	-0.01930000
N	-0.02864000	0.16227100	1.30557600
N	1.09061800	0.14784900	-0.71277900
N	-1.19611800	-0.15637300	-0.65473800
H	-0.86983200	0.04825900	1.84884400
H	0.82202400	0.38647300	1.79754300
H	1.95481400	0.09723500	-0.19092900
H	-1.22254000	-0.38430800	-1.63592600
H	-2.06425400	-0.20378600	-0.14394400
C	1.20296000	5.57333100	-0.66272800
C	0.04453200	6.26426600	-0.99144800
C	0.08453700	7.65131100	-0.96377300
C	2.36782600	7.64090100	-0.30469500
C	2.36830500	6.24934500	-0.31872500
H	-0.86549900	5.74094400	-1.26011500
H	3.26964300	5.70876400	-0.06247500
C	1.16176200	-0.01947900	-2.16222700
H	2.17730400	0.21114600	-2.47217700
H	0.92390100	-1.04312100	-2.45900000
H	0.48767800	0.68354400	-2.65455200
C	1.21983100	8.35915700	-0.62897300
H	1.24021100	9.44247000	-0.61323700
C	3.59091500	8.42146500	0.05879600
O	3.62766700	9.62345800	0.08258000
O	4.62926000	7.63923500	0.35198600
H	5.38878300	8.19655200	0.57745900
N	-1.13844800	8.39169300	-1.32281800
H	-1.31067700	8.37203000	-2.33402100
H	-1.96709800	8.00223400	-0.86206900
H	-1.07704300	9.37572800	-1.04500500
I	1.19363200	3.45661100	-0.68022500

Cation-Cation-I Me-gua$^+$ DMSO

C	-0.04510200	0.04465000	-0.02217200
N	-0.03445100	0.17396100	1.30248500
N	1.09497300	0.14477800	-0.71019200
N	-1.19403400	-0.14136400	-0.66330500
H	-0.88047200	0.07454900	1.84112900
H	0.81501500	0.39481800	1.79815200
H	1.95639000	0.08855900	-0.18443000
H	-1.21725500	-0.36564900	-1.64538000
H	-2.06617000	-0.17628200	-0.15844900
C	1.20310800	5.56920300	-0.66365900
C	0.04277700	6.25903400	-0.98803600
C	0.08075700	7.64617600	-0.95829000
C	2.36629500	7.63752400	-0.30557000
C	2.36868700	6.24596300	-0.32221900
H	-0.86726600	5.73491600	-1.25490700
H	3.27135800	5.70584100	-0.06979800
C	1.17211200	-0.02571400	-2.15871900
H	2.19096100	0.19700900	-2.46367600
H	0.92798300	-1.04794000	-2.45527100
H	0.50573000	0.68125800	-2.65585100
C	1.21617500	8.35460400	-0.62483200
H	1.23442700	9.43777300	-0.60630100
C	3.58961900	8.41832000	0.05480800
O	3.62624200	9.62063400	0.08109600
O	4.63037700	7.63703300	0.34231000
H	5.38997100	8.19507900	0.56567200
N	-1.14321100	8.38578600	-1.31342100
H	-1.31988200	8.36371400	-2.32372100
H	-1.97041900	7.99823400	-0.84849900
H	-1.08062800	9.37065100	-1.03897100
I	1.19703000	3.45251700	-0.68307800

Cation-Cation-I Me-gua$^+$ Water

C	-0.04521700	0.04804600	-0.02307600
N	-0.03662300	0.17658300	1.30170000
N	1.09668300	0.14312600	-0.70876400
N	-1.19348100	-0.13312900	-0.66672800
H	-0.88518100	0.08650500	1.83802000
H	0.81240100	0.39532100	1.79912700
H	1.95691400	0.08467100	-0.18135100
H	-1.21562500	-0.35415500	-1.64955100
H	-2.06709400	-0.16374800	-0.16419000
C	1.20351200	5.56724500	-0.66407500
C	0.04232800	6.25641200	-0.98673900
C	0.07927700	7.64362300	-0.95625600
C	2.36567500	7.63607300	-0.30603500
C	2.36907100	6.24453800	-0.32363600
H	-0.86761300	5.73179300	-1.25292800
H	3.27235100	5.70476700	-0.07267100
C	1.17636600	-0.02802000	-2.15696800
H	2.19632100	0.19257300	-2.45985000
H	0.93060000	-1.04973300	-2.45388000

H	0.51259800	0.68021900	-2.65578100
C	1.21460600	8.35250200	-0.62340700
H	1.23197700	9.43562300	-0.60388300
C	3.58894100	8.41726200	0.05310700
O	3.62513300	9.61969000	0.08050700
O	4.63081900	7.63655100	0.33820200
H	5.39034100	8.19502300	0.56071900
N	-1.14524900	8.38265400	-1.31001600
H	-1.32280400	8.36068500	-2.32013900
H	-1.97200100	7.99479900	-0.84456400
H	-1.08302000	9.36755400	-1.03566900
I	1.19908800	3.45057800	-0.68431800

HOOC-phBr-NH_3^+ Vacuum G4MP2

C	-0.91414300	0.05349100	0.00000100
C	0.17728900	-0.81413300	0.00001000
C	1.47598100	-0.30822400	0.00000800
C	1.69925500	1.07177300	-0.00000700
C	0.59023600	1.89630300	-0.00002200
C	-0.71836800	1.43409500	-0.00001800
H	0.03992800	-1.88873100	0.00000900
H	2.71338900	1.45453900	-0.00000200
H	-1.56758000	2.10863300	-0.00003200
N	0.80554200	3.37575400	0.00000700
H	0.39289400	3.82018500	0.82823500
H	1.80690300	3.59456600	-0.00029600
C	2.60817800	-1.29385100	-0.00000200
O	2.44912400	-2.48350000	-0.00002900
O	3.80441400	-0.67872700	0.00002600
H	4.48766300	-1.36752900	0.00001300
H	0.39237600	3.82027000	-0.82791300
Br	-2.66980700	-0.63174600	0.00000400

HOOC-phBr-NH_3· Vacuum G4MP2

C	-0.90119700	0.04648400	-0.00045700
C	0.15011600	-0.82402000	0.00028800
C	1.50847700	-0.33449700	-0.00059700
C	1.69667000	1.07355100	-0.00047000
C	0.59656900	1.88317000	-0.00199700
C	-0.74990600	1.45904900	-0.00006800
H	-0.00084400	-1.89508600	0.00270100
H	2.70482900	1.47605500	0.00291400
H	-1.59116800	2.13657200	-0.01645100
N	0.81983900	3.35191800	0.00197000
H	0.39273000	3.79278900	0.82842500
H	1.82061300	3.55742700	0.00149200
C	2.60145500	-1.26430600	-0.00031800
O	2.52340700	-2.48524200	0.00058600
O	3.84165300	-0.64663600	-0.00062100
H	4.46626200	-1.38370100	0.00036700
H	0.39209000	3.79758800	-0.82112700
Br	-2.69305600	-0.63218900	0.00028200

[HOOC-ph-NH_3·]$^+$ Vacuum G4MP2

C	-0.99798200	1.92809400	-0.00001500
C	0.32717600	1.57457500	0.00018100
C	0.61793000	0.20230300	0.00007600
C	-0.42050200	-0.73570000	-0.00019200
C	-1.72771100	-0.28018400	-0.00039600
C	-2.07173700	1.07239300	-0.00028800
H	1.14279700	2.28974400	0.00023700
H	-0.17950700	-1.79287400	-0.00031300
H	-3.10008200	1.42132900	-0.00051600
N	-2.82925100	-1.29435500	0.00038800
H	-3.43078600	-1.20183300	-0.82613800
H	-2.44613300	-2.24517100	-0.00241900
C	2.06193800	-0.20898600	0.00004800
O	2.97050500	0.57503900	0.00021600
O	2.19962200	-1.54711800	-0.00021000
H	3.14974500	-1.74396100	-0.00020500
H	-3.42696600	-1.20509300	0.83010700

HOOC-phBr-NH_2 Vacuum G4MP2

C	-0.88410600	0.07644700	-0.00399300
C	0.18929700	-0.80028500	-0.00293600
C	1.47764200	-0.25656200	-0.00320300
C	1.67668400	1.12225000	-0.00541000
C	0.58117600	1.99584400	-0.00833800
C	-0.71356500	1.45452100	-0.00601400
H	0.05967600	-1.87334700	0.00017600
H	2.68491100	1.51812400	-0.00850200
H	-1.57683700	2.11024900	-0.00945200
N	0.76898900	3.37128200	-0.07054100
H	0.00273600	3.93375000	0.26729000
H	1.66166400	3.70301000	0.26230800
C	2.61896300	-1.21254100	0.00153000
O	2.51295700	-2.41493500	0.00309700
O	3.82422300	-0.59377000	0.00446100
H	4.48392600	-1.30259800	0.00565100
Br	-2.65922800	-0.62561600	0.00245800

[HOOC-phBr-NH_2·]$^-$ Vacuum G4MP2

C	-0.86783200	0.07983800	-0.00766800
C	0.17817800	-0.79805700	-0.00155600
C	1.51886400	-0.28284400	-0.00825500
C	1.67324500	1.14888500	-0.00589600
C	0.58113200	1.99076200	-0.01930500
C	-0.74097800	1.48338100	-0.01720200
H	0.03533500	-1.86999500	0.01454100
H	2.67488400	1.56605900	0.00908600
H	-1.60018000	2.13765400	-0.07623800
N	0.75237900	3.40745300	-0.08281700
H	0.06855400	3.87529700	0.50337100
H	1.67527800	3.66571500	0.24853700
C	2.60605200	-1.19647000	0.00014000
O	2.57107700	-2.43800800	0.01007100
O	3.87066200	-0.58012500	0.00145900
H	4.45652400	-1.34710900	0.00896300

Br	-2.68008400	-0.63679100	0.00393400

HOOC-ph-NH_2· Vacuum G4MP2

C	1.08597300	1.87475700	0.00392100
C	-0.25062700	1.57604300	0.00329600
C	-0.56062600	0.20359500	-0.00154000
C	0.44988600	-0.75874400	-0.00711200
C	1.80335900	-0.39121100	-0.00852100
C	2.12667800	0.98236700	-0.00066300
H	-1.04648600	2.30965000	0.00731600
H	0.18113700	-1.80823100	-0.01395300
H	3.16505700	1.30127900	-0.00119700
N	2.80384400	-1.35650900	-0.07404600
H	3.70507800	-1.06984200	0.27797500
H	2.54178000	-2.27113600	0.26290000
C	-2.00034000	-0.17191100	0.00145600
O	-2.91958200	0.61110200	0.00537300
O	-2.19802300	-1.51351900	-0.00032400
H	-3.15844700	-1.63619600	-0.00014900

$^-$OOC-phBr-NH_2 Vacuum G4MP2

C	-0.82316800	0.08344700	-0.00964600
C	0.22982500	-0.81174700	-0.00984300
C	1.53258300	-0.29853900	-0.01329100
C	1.72867400	1.07833000	-0.01865900
C	0.65261200	1.96976500	-0.01942200
C	-0.65292000	1.46386200	-0.01521700
H	0.10766600	-1.88728500	-0.00181000
H	2.75948600	1.42235100	-0.01547200
H	-1.50813700	2.13055100	-0.01999100
N	0.86867200	3.36751500	-0.07678900
H	0.16183700	3.89243100	0.42258300
H	1.78408600	3.61662200	0.27578800
C	2.75851400	-1.26934300	0.00431500
O	2.46353000	-2.48094200	0.00597400
O	3.86850000	-0.69754800	0.01674700
Br	-2.64567500	-0.58897200	0.00529200

$^-$OOC-ph-NH_2· Vacuum G4MP2

C	0.99164700	1.88769600	0.00743700
C	-0.33269000	1.53187200	0.00390100
C	-0.61125500	0.15182300	-0.01020400
C	0.43966000	-0.76318300	-0.02164200
C	1.77627900	-0.35431900	-0.01879100
C	2.06461600	1.02268000	-0.00333900
H	-1.17669400	2.21245000	0.01598600
H	0.16905500	-1.81527500	-0.02666500
H	3.09622800	1.36912800	-0.00459700
N	2.82861400	-1.30621000	-0.08261100
H	3.64396000	-1.00736800	0.43877600
H	2.52777200	-2.20777800	0.26750000
C	-2.09880000	-0.34389400	0.00261000
O	-2.95570500	0.56124300	0.01036000
O	-2.22396500	-1.58670900	0.00557100

HOOC-CH_2-NH_3^+ Vacuum G4MP2

N	1.79197800	0.03246800	-0.00002200
H	1.36826900	0.99994900	0.00005400
C	0.57663600	-0.85411900	0.00001900
C	-0.61547600	0.12971200	-0.00000400
H	0.58101600	-1.48710800	-0.88949200
H	0.58106300	-1.48688000	0.88969200
O	-0.38171800	1.31271200	0.00003100
H	2.37848400	-0.08812900	-0.82859700
O	-1.83376000	-0.36274800	-0.00004900
H	-1.87451300	-1.33012400	0.00017500
H	2.37869600	-0.08826300	0.82838500

[HOOC-CH_2-NH_3·]$^{2+}$ Vacuum G4MP2

N	-1.90024300	0.03452600	-0.00032700
H	-2.01682700	0.63115200	0.83478300
C	-0.61799600	-0.75646600	0.00046700
C	0.68942000	0.08114500	0.00009300
H	-0.59039100	-1.38318600	0.90306200
H	-0.59037000	-1.38472300	-0.90099500
O	0.50103000	1.32479300	0.00017800
H	-2.69668900	-0.62641700	-0.00020400
O	1.85180000	-0.40873100	-0.00029100
H	1.96089000	-1.38524500	-0.00055400
H	-2.01609600	0.63016800	-0.83626200

HOOC-CH_2-NH_2 Vacuum G4MP2

N	1.95659800	-0.04164100	0.00008400
C	0.68732000	-0.74040600	-0.00008100
C	-0.55655900	0.15779600	-0.00012000
H	0.63254600	-1.40046000	-0.87694500
H	0.63241000	-1.40050500	0.87673500
O	-0.51891500	1.35565800	-0.00009500
H	1.98823500	0.57889500	0.80452400
O	-1.74613100	-0.49561200	0.00027400
H	-1.60222300	-1.45038500	-0.00111500
H	1.98865900	0.57923600	-0.80401300

[HOOC-CH_2-NH_2·]$^+$ Vacuum G4MP2

N	1.94705900	0.04888900	-0.00063500
C	0.82248900	-0.71426200	0.00099400
C	-0.68888600	0.19376700	0.00005600
H	0.69962100	-1.29319500	-0.91817700
H	0.69998200	-1.28982400	0.92236800
O	-0.65615100	1.36824400	0.00019800
H	2.33481100	0.41575300	-0.86293200
O	-1.71764300	-0.60776500	-0.00062100
H	-1.51005100	-1.55505600	0.00018200
H	2.33495900	0.41923400	0.86009300

$^-$OOC-CH_2-NH_2 Vacuum G4MP2

N	-1.88283300	0.04156700	0.00346900
C	-0.65079100	-0.77239700	0.11475000

C	0.67673900	0.06748100	0.00087700
H	-0.63598900	-1.27747000	1.09335700
H	-0.63727200	-1.57271700	-0.63509800
O	0.51145400	1.31339700	0.04035900
H	-2.11039300	0.09126100	-0.98913300
O	1.72682300	-0.59866700	-0.08666000
H	-1.49842100	0.97961100	0.18323400

[CH_2NH_2· + CO_2] Vacuum G4MP2

N	-2.13669400	0.37437600	-0.17897400
C	-1.53873800	-0.81120000	0.24448800
C	1.40689200	0.13535800	-0.01193300
H	-1.32125200	-0.87841500	1.30538600
H	-1.85957800	-1.71601000	-0.25952700
O	0.97947500	1.20770300	0.14710200
H	-2.27157900	0.45012900	-1.17809000
O	1.88408600	-0.91222700	-0.17166700
H	-1.70814400	1.21490600	0.18623400

Methylguanidine Vacuum G4MP2

C	0.61814500	-0.07240300	-0.00238500
N	1.76004700	-0.65533800	0.02638900
N	-0.61811300	-0.69296700	-0.04276800
N	0.56403800	1.31997700	-0.08254600
H	1.65827000	-1.66609400	-0.05130500
H	-0.61355800	-1.65668800	0.24486000
H	-0.11101500	1.76528600	0.52376000
H	1.49092400	1.70540500	0.03606700
C	-1.89144200	-0.00501700	-0.00350100
H	-2.68482800	-0.70904800	-0.26703700
H	-2.13958400	0.42170600	0.98223000
H	-1.90222700	0.80225200	-0.74079200

[Methylguanidine·]$^+$ Vacuum G4MP2

C	0.55427100	-0.03891300	0.00002200
N	1.75461800	-0.70031800	-0.00006500
N	-0.62105700	-0.66230800	0.00004600
N	0.65084700	1.28720300	0.00000900
H	1.62914800	-1.71809100	0.00016000
H	-0.60631500	-1.67275800	0.00009100
H	-0.14471300	1.90698600	0.00015200
H	1.57879000	1.68876400	-0.00004200
C	-1.91931400	0.00798900	-0.00003500
H	-2.70232800	-0.74847700	-0.00026100
H	-2.02772300	0.62842600	0.89658900
H	-2.02746000	0.62865700	-0.89653400

Methylguanidinium$^+$ Vacuum G4MP2

C	-0.51410800	-0.00650200	-0.01322200
N	-0.52415100	1.32827400	-0.00766000
N	-1.67213100	-0.67568500	0.02232200
N	0.63952500	-0.66935200	-0.04368200
C	1.96177300	-0.04767100	0.03837300
H	0.31547600	1.85807700	-0.17066700

H	-1.37509100	1.84477900	0.14332900
H	-2.55422400	-0.20473500	-0.09409000
H	-1.69851900	-1.67131100	0.16939300
H	0.59994100	-1.66549900	-0.19391800
H	2.01576600	0.62351400	0.89992400
H	2.69872300	-0.83767000	0.17813700
H	2.20923800	0.49521900	-0.87987600

[Methylguanidinium·]$^{2+}$ Vacuum G4MP2

C	0.56832000	0.02750500	0.02652200
N	0.64323600	1.33745500	0.02382100
N	1.59665400	-0.79339700	-0.06006600
N	-0.70312300	-0.58795300	0.13171600
C	-1.97565700	-0.00847000	-0.11163000
H	-0.13941100	1.93823200	0.26020100
H	1.53324000	1.81508600	-0.10807600
H	2.55370800	-0.44390500	-0.09870700
H	1.49812600	-1.79840400	-0.18104500
H	-0.70004200	-1.57193700	0.42802300
H	-1.93112100	0.98990700	-0.54250700
H	-2.55919200	-0.70665700	-0.75317500
H	-2.56865300	-0.02926500	0.83763500