Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Nature of Intramolecular O-H---π Interactions, Elucidated with QTAIM Dual Functional Analysis and Theoretical Investigations

Satoko Hayashi,* Taro Nishide and Waro Nakanishi*

Faculty of Systems Engineering, Wakayama University, 930 Sakaedani, Wakayama 640-8510, Japan. Fax: +81 73 457 8253; Tel: +81 73 457 8252; E-mail: hayashi3@sys.wakayama-u.ac.jp and nakanisi@sys.wakayama-u.ac.jp.

Table of Contents **Pages**

Survey of QTAIM, closely related to QTAIM dual functional analysis (QTAIM-DFA)

The bond critical point (BCP; ∗) is an important concept in QTAIM. The BCP of $(\omega, \sigma) = (3, -1)$[S1] is a point along the bond path (BP) at the interatomic surface, where charge density $\rho(\boldsymbol{r})$ reaches a minimum. It is donated by $\rho_b(\boldsymbol{r}_c)$, so are other QTAIM functions, such as the total electron energy densities $H_b(\boldsymbol{r}_c)$, potential energy densities $V_b(\boldsymbol{r}_c)$, and kinetic energy densities $G_b(\boldsymbol{r}_c)$ at the BCPs. A chemical bond or interaction between A and B is denoted by A–B, which corresponds to the BP between A and B in QTAIM. We will use A-∗-B for BP, where the asterisk emphasizes the presence of a BCP in A–B.

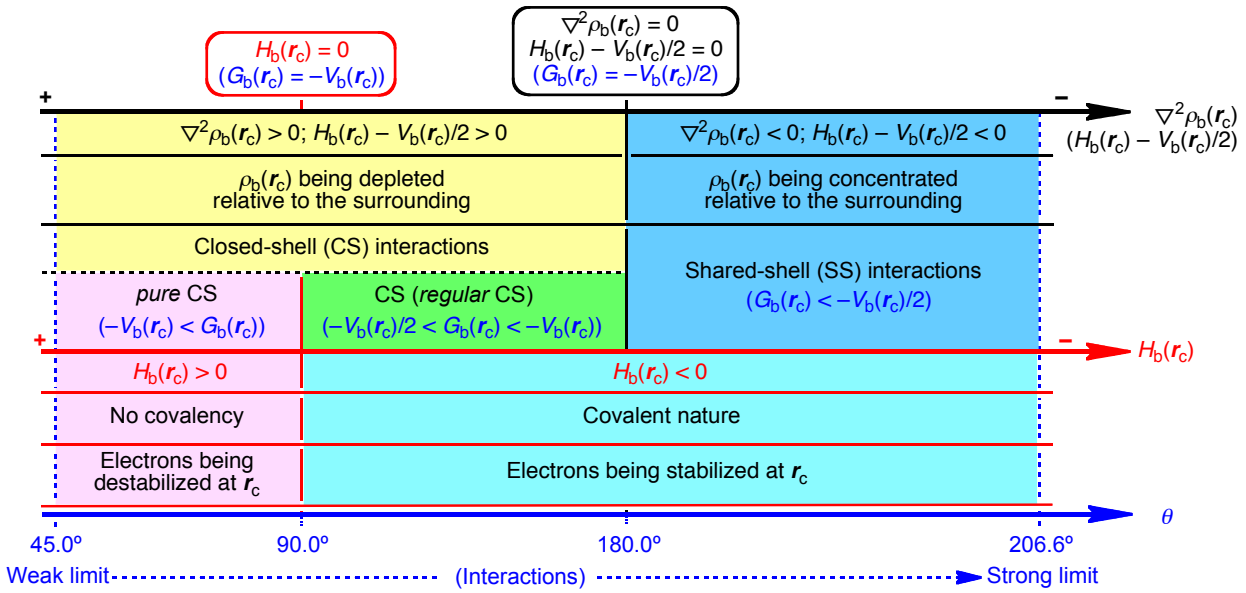
The sign of the Laplacian $\rho_b(\boldsymbol{r}_c)$ ($\nabla^2\rho_b(\boldsymbol{r}_c)$) indicates that $\rho_b(\boldsymbol{r}_c)$ is depleted or concentrated with respect to its surrounding, since $\nabla^2\rho_b(\boldsymbol{r}_c)$ is the second derivative of $\rho_b(\boldsymbol{r}_c)$. $\rho_b(\boldsymbol{r}_c)$ is locally depleted relative to the average distribution around $\boldsymbol{r}_c$ if $\nabla^2\rho_b(\boldsymbol{r}_c) > 0$, but it is concentrated when $\nabla^2\rho_b(\boldsymbol{r}_c) < 0$. Total electron energy densities at BCPs ($H_b(\boldsymbol{r}_c)$) must be a more appropriate measure for weak interactions on the energy basis.[S1–S8] $H_b(\boldsymbol{r}_c)$ are the sum of kinetic energy densities ($G_b(\boldsymbol{r}_c)$) and potential energy densities ($V_b(\boldsymbol{r}_c)$) at BCPs, as shown in Equation (2) (S1). Electrons at BCPs are stabilized when $H_b(\boldsymbol{r}_c) < 0$, therefore, interactions exhibit the covalent nature in this region, whereas they exhibit no covalency if $H_b(\boldsymbol{r}_c) > 0$, due to the destabilization of electrons at BCPs under the conditions.[S1] Equation (S2) represents the relation between $\nabla^2\rho_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c)$, together with $G_b(\boldsymbol{r}_c)$ and $V_b(\boldsymbol{r}_c)$, which is closely related to the virial theorem.

$$H_b(\boldsymbol{r}_c) = G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c) \quad \text{(S1)}$$

$$(\hbar^2/8m)\nabla^2\rho_b(\boldsymbol{r}_c) = H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 \quad \text{(S2)}$$

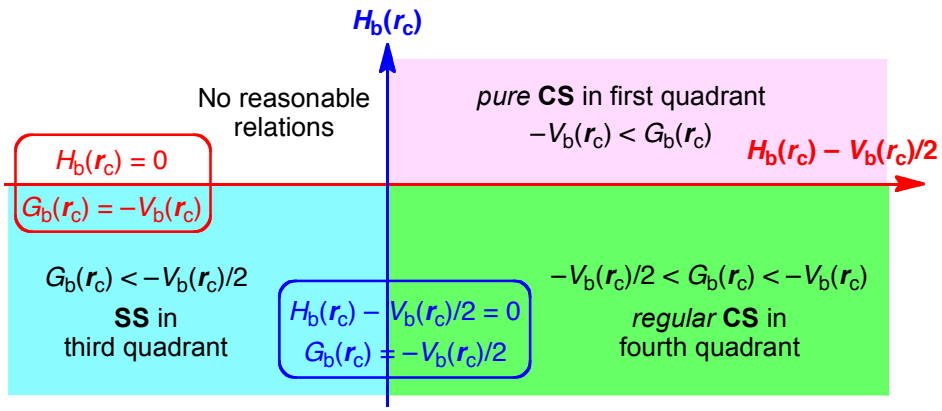
$$= G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2 \quad \text{(S2')}$$

Interactions are classified by the signs of $\nabla^2\rho_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c)$. Interactions in the region of $\nabla^2\rho_b(\boldsymbol{r}_c) < 0$ are called shared-shell (SS) interactions and they are closed-shell (CS) interactions for $\nabla^2\rho_b(\boldsymbol{r}_c) > 0$. $H_b(\boldsymbol{r}_c)$ must be negative when $\nabla^2\rho_b(\boldsymbol{r}_c) < 0$, since $H_b(\boldsymbol{r}_c)$ are larger than $(\hbar^2/8m)\nabla^2\rho_b(\boldsymbol{r}_c)$ by $V_b(\boldsymbol{r}_c)/2$ with negative $V_b(\boldsymbol{r}_c)$ at all BCPs (Equation (S2)). Consequently, $\nabla^2\rho_b(\boldsymbol{r}_c) < 0$ and $H_b(\boldsymbol{r}_c) < 0$ for the SS interactions. The CS interactions are especially called *pure* CS interactions for $H_b(\boldsymbol{r}_c) > 0$ and $\nabla^2\rho_b(\boldsymbol{r}_c) > 0$, since electrons at BCPs are depleted and destabilized under the conditions.[S1a] Electrons in the intermediate region between SS and *pure* CS, which belong to CS, are locally depleted but stabilized at BCPs, since $\nabla^2\rho_b(\boldsymbol{r}_c) > 0$ but $H_b(\boldsymbol{r}_c) < 0$.[S1a] We call the interactions in this region *regular* CS,[S4,S5] when it is necessary to distinguish from *pure* CS. The role of $\nabla^2\rho_b(\boldsymbol{r}_c)$ in the classification can be replaced by $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, since $(\hbar^2/8m)\nabla^2\rho_b(\boldsymbol{r}_c) = H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ (Equation (S2)). Scheme S1 summarizes the classification.



Scheme S1. Classification of interactions by the signs of $\nabla^2\rho_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c)$, together with $G_b(\boldsymbol{r}_c)$ and $V_b(\boldsymbol{r}_c)$.

We proposed QTAIM-DFA by plotting $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ (= $(\hbar^2/8m)\nabla^2\rho_b(\boldsymbol{r}_c)$),[S4a] after the proposal of $H_b(\boldsymbol{r}_c)$ versus $\nabla^2\rho_b(\boldsymbol{r}_c)$.[S4b] Both axes in the plot of the former are given in energy unit, therefore, distances on the (x, y) (= $(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2, H_b(\boldsymbol{r}_c))$ plane can be expressed in the energy unit, which provides an analytical development. QTAIM-DFA incorporates the classification of interactions by the signs of $\nabla^2\rho_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c)$. Scheme S2 summarizes the QTAIM-DFA treatment. Interactions of *pure* CS appear in the first quadrant, those of *regular* CS in the fourth quadrant and SS interactions do in the third one. No interactions appear in the second one.



Scheme S2. QTAIM-DFA: Plot of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ for Weak to Strong Interactions

In our treatment, data for perturbed structures around fully optimized structures are also employed for the plots, together with the fully optimized ones (see Figure S1).[S4–S8] We proposed the concept of the "dynamic nature of interaction" originated from the perturbed structures. The behavior of interactions at the fully optimized structures corresponds to "the static nature of interactions", whereas that containing perturbed structures exhibit the "dynamic nature of interaction" as explained below.

The method to generate the perturbed structures is discussed later. Plots of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ are analyzed employing the polar coordinate (R, θ) representation with (θ_p, κ_p) parameters.[S4a,S5–S8] Figure S1 explains the treatment. R in (R, θ) is defined by Equation (S3) and given in the energy unit. R corresponds to the energy for an interaction at BCP. The plots show a spiral stream, as a whole. θ in (R, θ) defined by Equation (S4), measured from the y-axis, controls the spiral stream of the plot. Each plot for an interaction shows a specific curve, which provides important information of the interaction (see Figure S1). The curve is expressed by θ_p and κ_p. While θ_p, defined by Equation (S5) and measured from the y-direction, corresponds to the tangent line of a plot, where θ_p is calculated employing data of the perturbed structures with a fully-optimized structure and κ_p is the curvature of the plot (Equation (S6)). While (R, θ) correspond to the static nature, (θ_p, κ_p) represent the dynamic nature of interactions. We call (R, θ) and (θ_p, κ_p) QTAIM-DFA parameters, whereas $\rho_b(\boldsymbol{r}_c)$, $\nabla^2\rho_b(\boldsymbol{r}_c)$, $G_b(\boldsymbol{r}_c)$, $V_b(\boldsymbol{r}_c)$, $H_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ belong to QTAIM functions. $k_b(\boldsymbol{r}_c)$, defined by Equation (S7), is an QTAIM function but it will be treated as if it were an QTAIM-DFA parameter, if suitable.

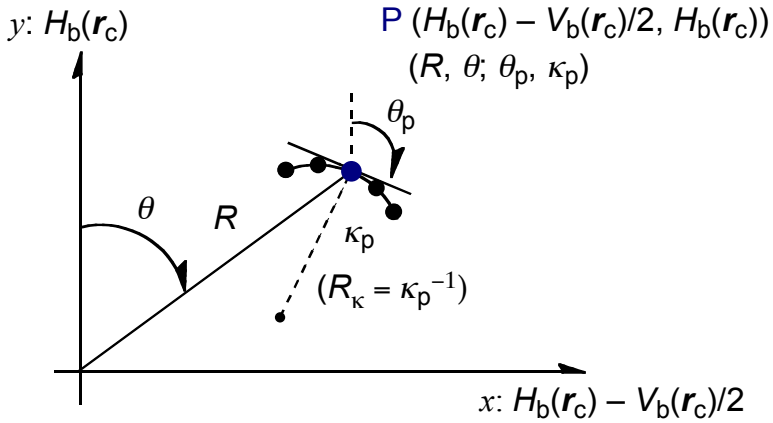


Figure S1. Polar (R, θ) coordinate representation of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, with ($\theta_p$, κ_p) parameters.

$$R = (x^2 + y^2)^{1/2} \quad \text{(S3)}$$

$$\theta = 90^o - \tan^{-1}(y/x) \quad \text{(S4)}$$

$$\theta_p = 90^o - \tan^{-1}(dy/dx) \quad \text{(S5)}$$

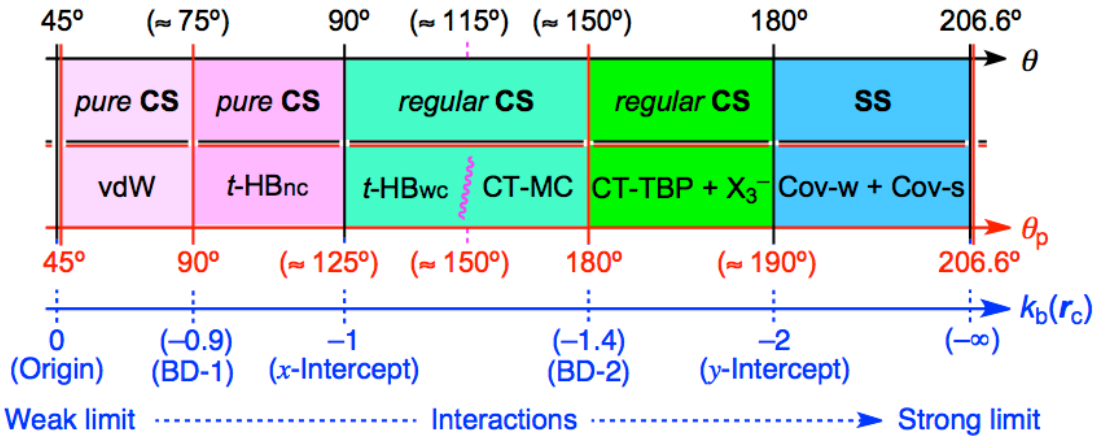
$$\kappa_p = |d^2y/dx^2| / [1 + (dy/dx)^2]^{3/2} \quad \text{(S6)}$$

$$k_b(\boldsymbol{r}_c) = V_b(\boldsymbol{r}_c)/G_b(\boldsymbol{r}_c) \quad \text{(S7)}$$

where $(x, y) = (H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2, H_b(\boldsymbol{r}_c))$

Criteria for classification of interactions: behavior of typical interactions elucidated by QTAIM-DFA

$H_b(\boldsymbol{r}_c)$ are plotted versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ for typical interactions in vdW (van der Waals interactions), HBs (hydrogen bonds), CT-MCs (molecular complexes through charge transfer), X_3^- (trihalide ions), CT-TBPs (trigonal bipyramidal adducts through charge-transfer), Cov-w (weak covalent bonds) and Cov-s (strong covalent bonds).[S4–S8] Rough criteria are obtained by applying QTAIM-DFA, after the analysis of the plots for the typical interactions according to Equations (S3)–(S7). Scheme S3 shows the rough criteria, which are accomplished by the θ and θ_p values, together with the values of $k_b(\boldsymbol{r}_c)$. The criteria will be employed to discuss the nature of interactions in question, as a reference.



Scheme S3. Rough classification and characterization of interactions by θ and θ_p, together with $k_b(\boldsymbol{r}_c)$ (= $V_b(\boldsymbol{r}_c)/G_b(\boldsymbol{r}_c)$).

Characterization of interactions

The characterization of interactions is explained employing $[^1Cl\text{-}^2Cl\text{-}^3Cl]^-$. The wide range of the perturbed structures were generated by partially optimizing $r(^2Cl\text{-}^3Cl)$ in $[^1Cl\text{-}^2Cl\text{-}^3Cl]^-$, assuming the $C_{\infty v}$ symmetry, with $r(^1Cl\text{-}^2Cl)$ being fixed in the wide range. The partial optimization method is called POM.[S4b,S5] The QTAIM functions, such as $V_b(\boldsymbol{r}_c)$, $G_b(\boldsymbol{r}_c)$, $H_b(\boldsymbol{r}_c)$, $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ are calculated at BCPs for the wide varieties of the perturbed structures of $[^1Cl\text{-}^2Cl\text{-}^3Cl]^-$. $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ and $H_b(\boldsymbol{r}_c)$ are plotted versus the interaction distances $r(^1Cl\text{-}^2Cl)$ in the perturbed structures of $[^1Cl\text{-}^2Cl\text{-}^3Cl]^-$, in the wide range. Figure S2 shows the plots. Each plot is analyzed using a regression curve of the ninth function and the first derivative of each regression curve is obtained. As shown in Figure S2, the maximum value of $H_b(\boldsymbol{r}_c)$ ($d(H_b(\boldsymbol{r}_c))/dr = 0$) is defined as the borderline between vdW and t-HB interactions. Similarly, the maximum value of $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ ($d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/dr = 0$) does to the borderline between CT-MC and CT-TBP. However, it seems difficult to find a characteristic point

corresponding to the borderline between *t*-HB and CT-MC in nature. Therefore, the borderline is tentatively given by $\theta_p = 150^o$ based on the expectation form the experimental results, where θ_p is defined by $[90^o - \tan^{-1}[dH_b(\boldsymbol{r}_c)/d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)]]$ in the plot of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$. The proposed classification and characterization of interactions, by means of the QTAIM functions of $H_b(\boldsymbol{r}_c)$, $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, $G_b(\boldsymbol{r}_c)$, and/or $V_b(\boldsymbol{r}_c)$, are summarized in Table S1.

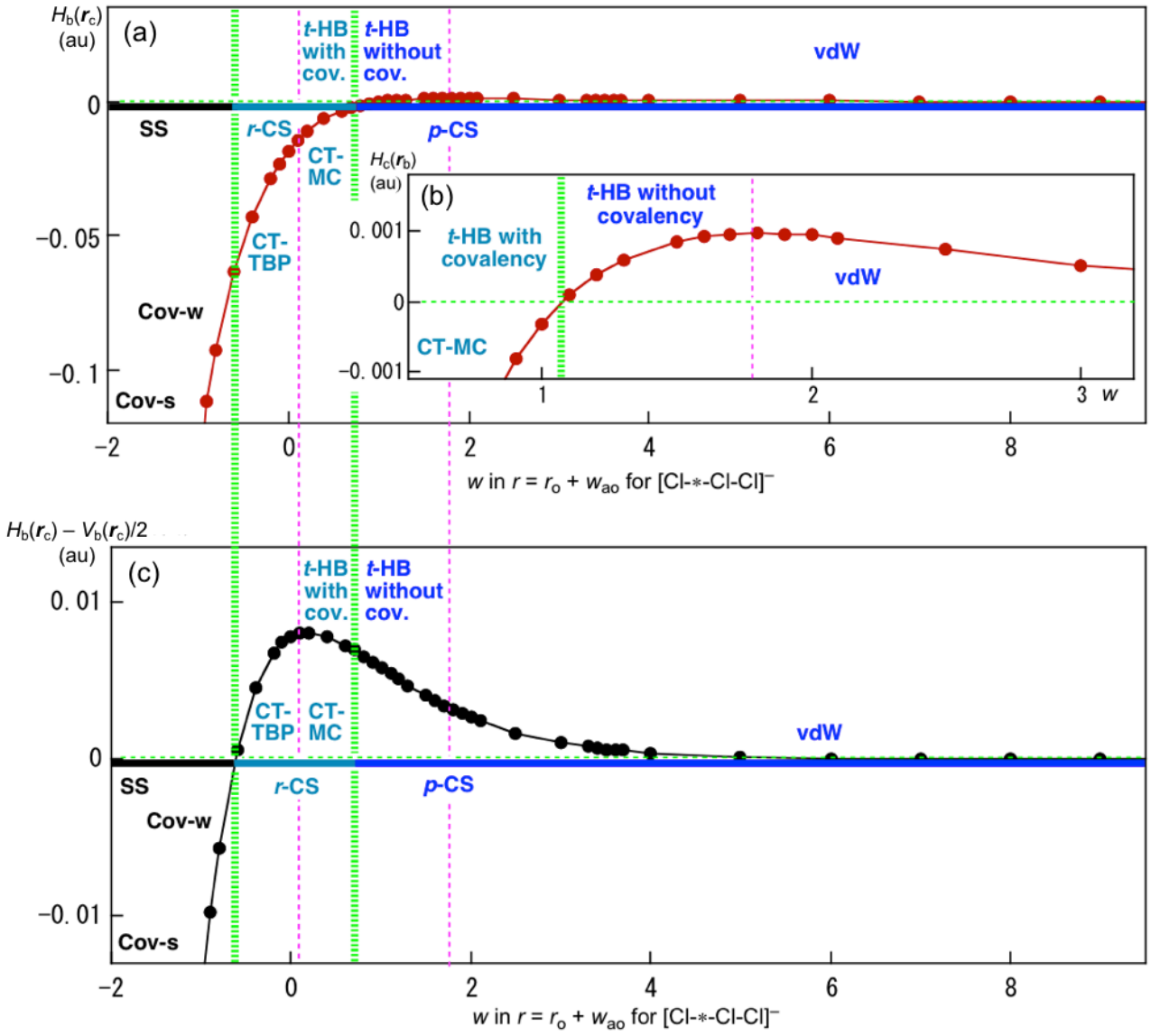


Figure S2. Plot of $H_b(\boldsymbol{r}_c)$ versus w in $r(^1\text{Cl-}^2\text{Cl}) = r_o(^1\text{Cl-}^2\text{Cl}) + wa_o$ for $^1\text{Cl-}^2\text{Cl-}^3\text{Cl}^-$ (a) with the magnified picture of (a) (b) and that of $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ versus w (c). Typical hydrogen bonds without covalency and typical hydrogen bonds with covalency are abbreviated as *t*-HB without cov. and *t*-HB with cov., respectively, whereas Cov-w and Cov-s stand for weak covalent bonds and strong covalent bonds, respectively.

Table S1. Proposed definitions for the classification and characterization of interactions by the signs $H_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ and their first derivatives, together with the tentatively proposed definitions by the characteristic points on the plots of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$. The tentatively proposed definitions are shown by italic. The requirements for the interactions are also shown.

ChP/Interaction	Requirements by $H_b(\boldsymbol{r}_c)$ and $V_b(\boldsymbol{r}_c)$	Requirements by $G_b(\boldsymbol{r}_c)$ and $V_b(\boldsymbol{r}_c)$
Origin	$H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 = 0$; $H_b(\boldsymbol{r}_c) = 0$	$G_b(\boldsymbol{r}_c) = 0$; $V_b(\boldsymbol{r}_c) = 0$
vdW	$H_b(\boldsymbol{r}_c) > 0$; $dH_b(\boldsymbol{r}_c)/d(-r) > 0$	$G_b(\boldsymbol{r}_c) > -V_b(\boldsymbol{r}_c)$; $dG_b(\boldsymbol{r}_c)/d(-r) > -dV_b(\boldsymbol{r}_c)/d(-r)$
Borderline (BD-1)	$H_b(\boldsymbol{r}_c) > 0$; $dH_b(\boldsymbol{r}_c)/d(-r) = 0$	$G_b(\boldsymbol{r}_c) > -V_b(\boldsymbol{r}_c)$; $dG_b(\boldsymbol{r}_c)/d(-r) = -dV_b(\boldsymbol{r}_c)/d(-r)$
t-HB$_{\text{with no covalency}}$	$H_b(\boldsymbol{r}_c) > 0$; $dH_b(\boldsymbol{r}_c)/d(-r) < 0$	$G_b(\boldsymbol{r}_c) > -V_b(\boldsymbol{r}_c)$; $dG_b(\boldsymbol{r}_c) < -dV_b(\boldsymbol{r}_c)$
Borderline (x-intercept)	$H_b(\boldsymbol{r}_c) = 0$ (θ_p[a)] = 125º)	$G_b(\boldsymbol{r}_c) = -V_b(\boldsymbol{r}_c)$ (θ_p[a)] = 125º)
t-HB$_{\text{with covalency}}$	$H_b(\boldsymbol{r}_c) < 0$; (125º <) θ_p[a)] < 150º	$G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$; (125º <) θ_p[b)] < 150º
Borderline (Tentative)	*θ_p[a)] = 150º*	*θ_p[b)] = 150º*
CT-MC	$d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/d(-r) > 0$; 150º < θ_p[a)] < 180º	$dG_b(\boldsymbol{r}_c) > dV_b(\boldsymbol{r}_c)/2$; 150º < θ_p[a)] < 180º
Borderline (BD-2)	$d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/d(-r) = 0$; ($H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 > 0$; $H_b(\boldsymbol{r}_c) < 0$)	$2dG_b(\boldsymbol{r}_c)/d(-r) = -dV_b(\boldsymbol{r}_c)/d(-r)$; ($-V_b(\boldsymbol{r}_c)/2 < G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$)
CT-TBP with X_3^-	$d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/d(-r) < 0$; ($H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 > 0$; $H_b(\boldsymbol{r}_c) < 0$)	$2dG_b(\boldsymbol{r}_c)/d(-r) < -dV_b(\boldsymbol{r}_c)/d(-r)$; ($-V_b(\boldsymbol{r}_c)/2 < G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$)
Borderline (y-intercept)	$H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 = 0$ ($H_b(\boldsymbol{r}_c) < 0$)	$G_b(\boldsymbol{r}_c) = -V_b(\boldsymbol{r}_c)/2$ ($G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$)
Cov-w	$H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 < 0$; *$R$[c)] < 0.15 au*	$G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)/2$; *$R$[c)] < 0.15 au*
Borderline (Tentative)	*R[c)] = 0.15 au*	*R[d)] = 0.15 au*
Cov-s	$H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 < 0$; *$R$[c)] > 0.15 au*	$G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)/2$; *$R$[d)] > 0.15 au*

a) $\theta_p = 90º - \tan^{-1}[dH_b(\boldsymbol{r}_c)/d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)]$, $\theta_p = 125º$ is tentatively given for $\theta = 90º$, where θ is defined by $90º - \tan^{-1}[H_b(\boldsymbol{r}_c)/(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)]$ with $H_b(\boldsymbol{r}_c) = 0$. b) $\theta_p = 90º - \tan^{-1}[d(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c))/d(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2)]$, $\theta_p = 125º$ is tentatively given for $\theta = 90º$, where θ is defined by $90º - \tan^{-1}[(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c))/(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2)]$ with $(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)) = 0$]. c) $R = [(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)^2 + (H_b(\boldsymbol{r}_c))^2]^{1/2}$. d) $R = [(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2)^2 + (G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c))^2]^{1/2}$.

Table S2. Selected structural parameters of *r*(O-H), *r*(H---C(π)), ∠OHC(π), and ∠HC(π)C(π) around the intramolecular OH-∗-C(π) interactions in **1**–**15**, together with the ΔE_{ES} and ΔE_{ZP} values, evaluated with MP2/BSS-A.[a] Each conformer is called **a**, **b**, ---, in the order of the increase of the *r*(H---C(π)) values.

Species (symm)	*r*(O-H) (Å)	*r*(OH---C(π)) (Å)	∠OHC(π) (º)	∠HC(π)C(π) (º)	ΔE_{ES}[b] (kJ mol^{-1})	ΔE_{ZP}[c] (kJ mol^{-1})
1: $HOCH_2C{\equiv}CH$						
1a (C_1)	0.9604	2.5155	72.2	127.9	0.0	0.0
1b (C_s)	0.9604	3.1663	26.0	156.5	6.6	5.9
2: $HOCH_2CH_2C{\equiv}CH$						
2a (C_1)	0.9625	2.5009	104.6	100.1	0.0	0.0
2b (C_1)	0.9601	3.2663	63.3	127.8	10.3	9.3
2c (C_1)	0.9593	3.7298	27.6	121.7	9.4	8.2
2d (C_1)	0.9597	4.0049	65.8	157.4	6.0	5.3
2e (C_s)	0.9594	4.3819	37.1	147.9	5.1	4.2
3: $HOCH_2CH_2CH_2C{\equiv}CH$						
3a (C_1)	0.9624	2.2797	133.5	83.6	0.0	0.0
3b (C_1)	0.9609	2.4272	115.9	91.2	8.0	6.2
6: $HOCH_2CH_2CH_2CH{=}CH_2$						
6a (C_1)	0.9621	2.3020	129.2	83.5	0.0	0.0
6b (C_1)	0.9599	3.4771	53.3	119.3	13.8	12.0
9: $HOCH_2CH_2CH_2Ph$						
9a (C_1)	0.9623	2.3316	129.6	77.1	0.0	0.0
9b (C_1)	0.9610	2.6756	101.7	85.6	10.0	8.7
11: $HOCH_2C_6H_4C{\equiv}CH$						
11a (C_1)	0.9625	2.4507	123.3	88.1	0.0	0.0
11b (C_1)	0.9611	3.7307	53.9	117.0	6.4	5.6
12: $HOC_6H_4CH{=}CH_2$						
12a (C_1)	0.9655	2.4139	113.1	68.3	0.0	0.0
12b (C_s)	0.9620	3.8536	7.8	77.1	3.8	3.5
13: $HOC_6H_4CH_2CH{=}CH_2$						
13a (C_1)	0.9661	2.2783	137.7	76.4	0.0	0.0
13b (C_1)	0.9616	4.1427	20.7	81.9	7.8	6.7
15: $HOCH_2C_6H_4Ph$						
15a (C_1)	0.9633	2.3869	126.9	82.1	0.0	0.0
15b (C_1)	0.9615	4.1125	52.1	67.7	–0.2	0.1

[a] With the MP2/6-311++G(3df,3pd) (MP2/BSS-A) method of the Gaussian 09 program. [b] The energies on the energy surface from the components (ΔE_{ES}) [= E_{ES}(***x*m**) – E_{ES}(***x*a**): ***x*** = **1**–**15**]. [c] The energies with the zero-point energy collections from the components (ΔE_{ZP}) [= E_{ZP}(***x*m**) – E_{ZP}(***x*a**): ***x*** = **1**–**15**].

Table S3. Lengths of bond paths (BPs: r_{BP}) and the corresponding straight-line distances (R_{SL}), corresponding to the intramolecular non-covalent interactions around the OH group, evaluated with MP2/BSS-A, together with the differences between them ($\Delta r_{BP} = r_{BP} - R_{SL}$).[a]

Species (symm)	r_{BP}[b] (Å)	R_{SL}[c] (Å)	Δr_{BP}[d] (Å)
OH-∗-C(π)			
3a (C_1)	2.4248	2.2797	0.1452
6a (C_1)	2.4390	2.3020	0.1370
9a (C_1)	2.4786	2.3316	0.1470
11a (C_1)	2.5670	2.4507	0.1164
12a (C_1)	2.3970	2.2867	0.1103
13a (C_1)	2.5238	2.2782	0.2456
15a (C_1)	2.4569	2.3869	0.0699
O-∗-C(π)			
3b (C_1)	3.2709	2.9757	0.2951
6c (C_1)	2.9645	2.9580	0.0065
9b (C_1)	3.0586	3.0214	0.0372
14b (C_1)	3.0502	2.9122	0.1380
O-∗-H			
5e (C_1)	2.6129	2.4974	0.1155
5i (C_1)	2.6296	2.5373	0.0924
12b (C_1)	2.2717	2.2155	0.0562
15b (C_1)	2.3901	2.3578	0.0323
15c (C_1)	2.4920	2.4484	0.0436

[a] With the MP2/6-311++G(3df,3pd) for MP2/BSS-A method of the Gaussian 09 program. [b] The length of BPs. [c] Straight-line distances. [d] $\Delta r_{BP} = r_{BP} - R_{SL}$.

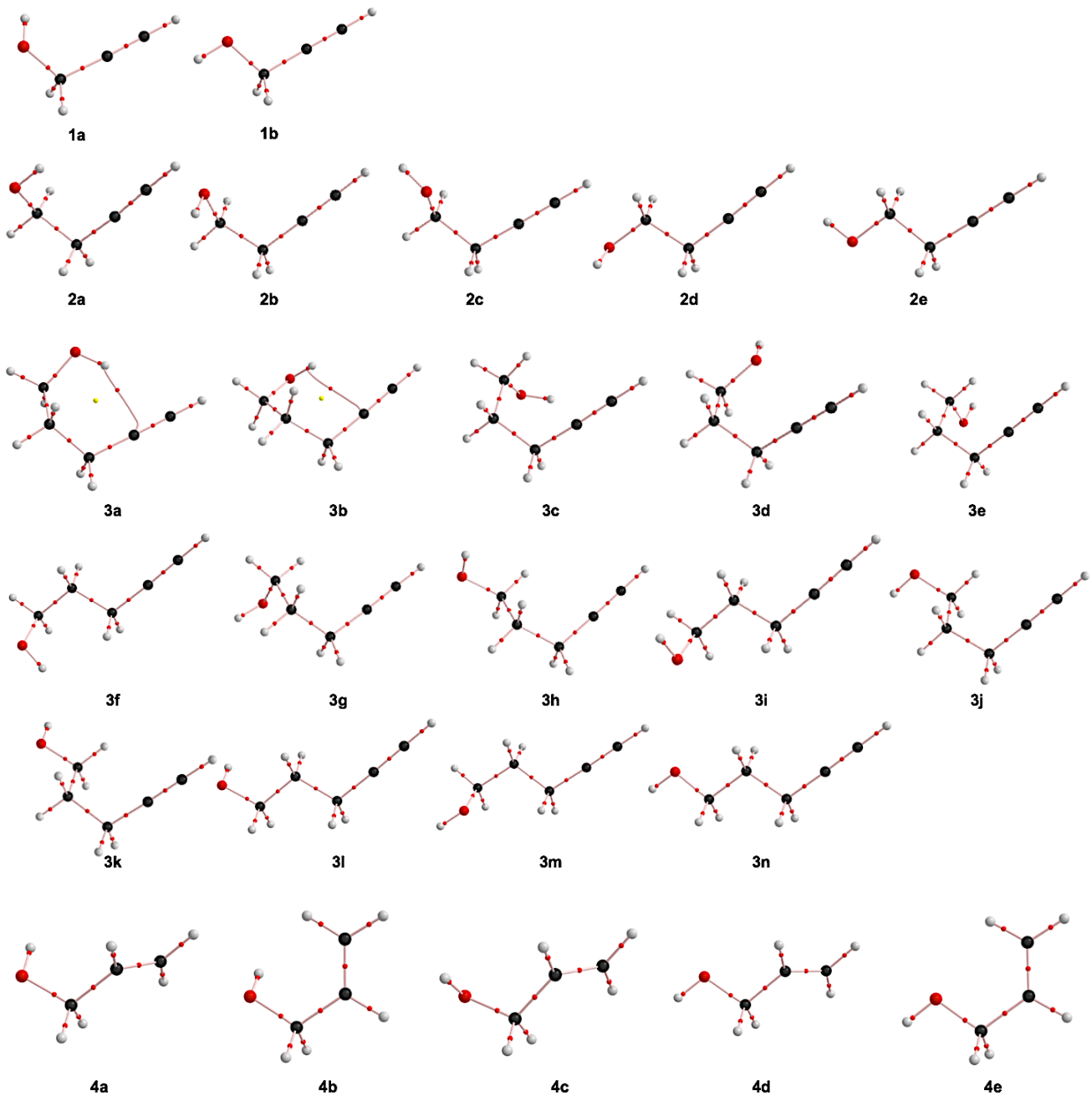


Figure S3. Molecular graphs, drawn on the optimized structures, for the conformers in **1**–**4**, calculated with MP2/BSS-A.

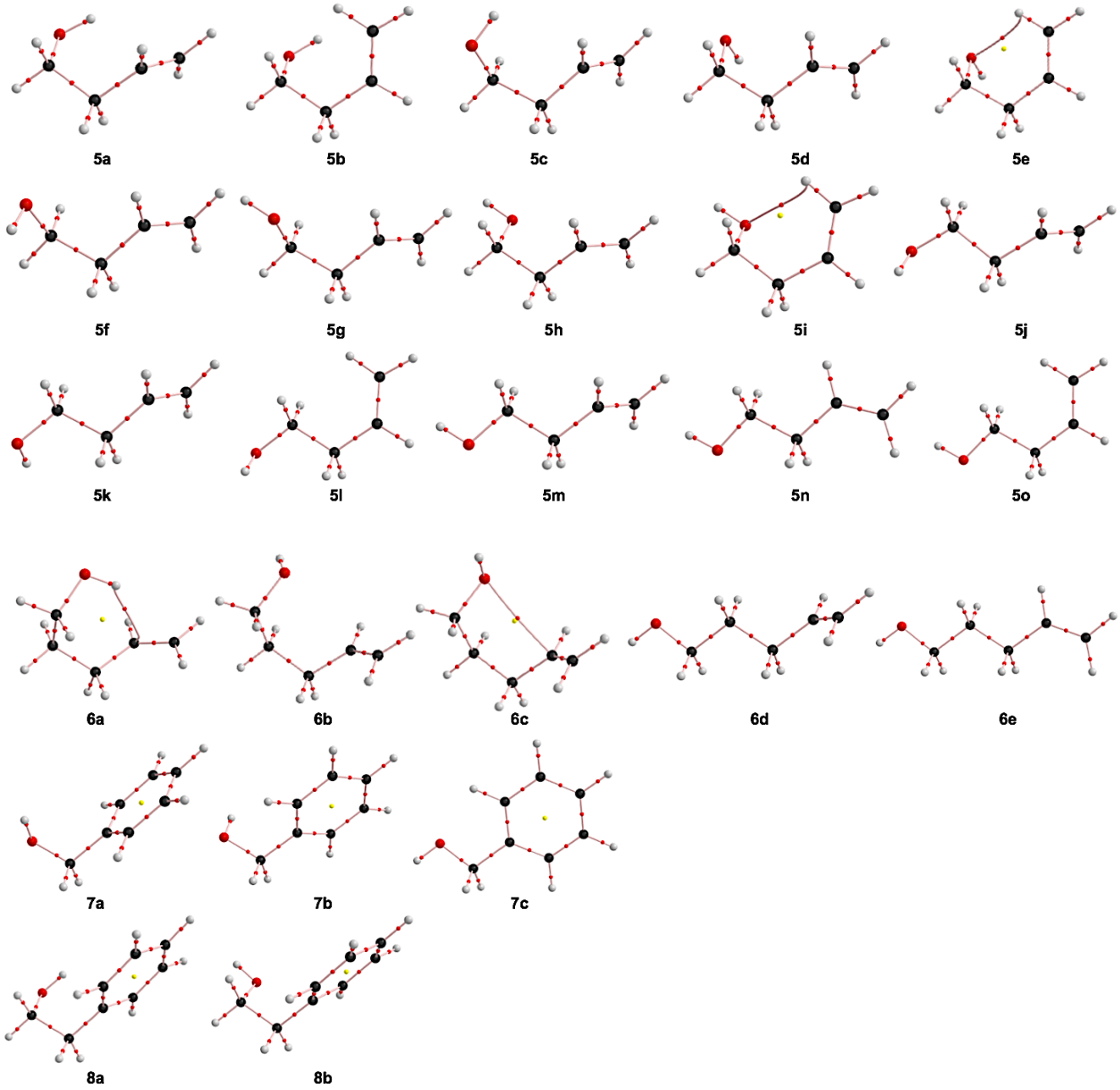


Figure S4. Molecular graphs, drawn on the optimized structures, for the conformers in **5**–**8**, calculated with MP2/BSS-A.

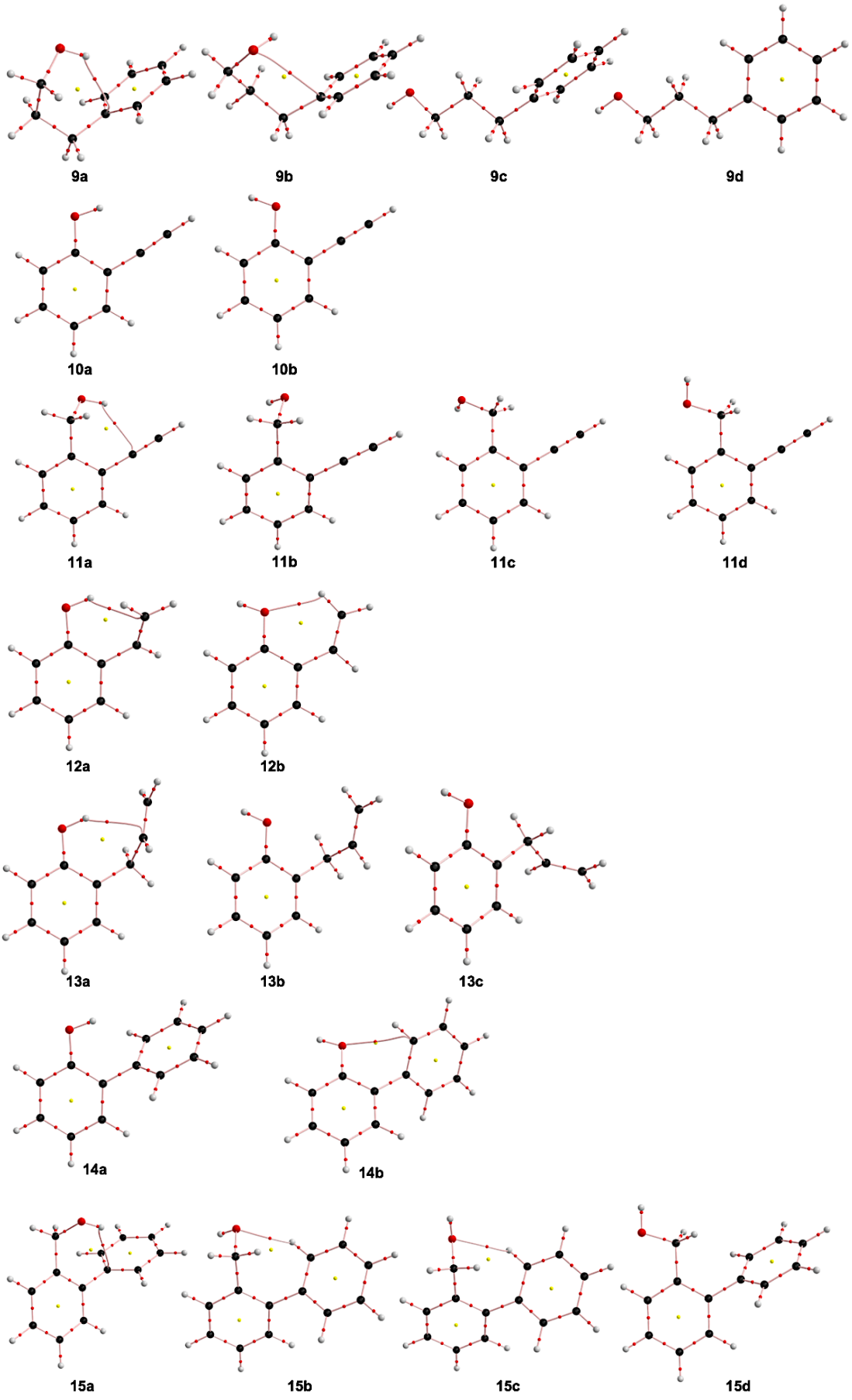


Figure S5. Molecular graphs, drawn on the optimized structures, for the conformers in **9**–**15**, calculated with MP2/BSS-A.

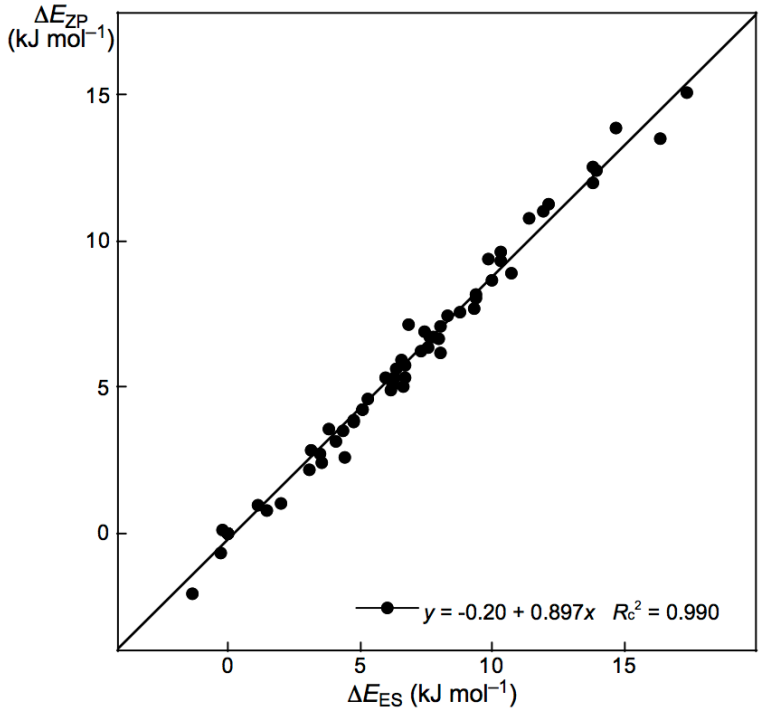


Figure S6. Plot of ΔE_{ZP} versus ΔE_{ES} for the conformers in **1**–**15**, evaluated with MP2/BSS-A. Data are collected in Table S2 of the Supporting Information.

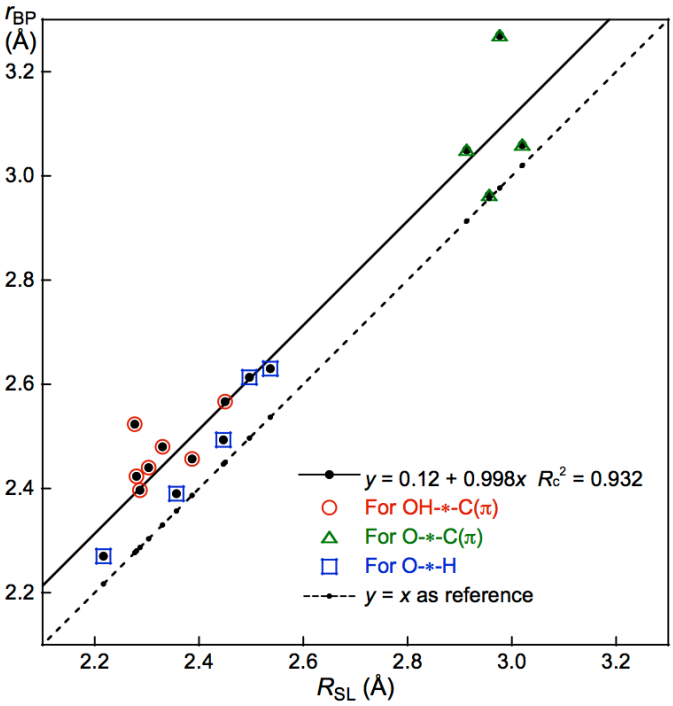


Figure S7. Plot of r_{BP} versus R_{SL} for the intramolecular OH-*-C(π) and O-*-X (X = C(π) and H (bonded to C(π))) in some conformers of **3a**, **6a**, **9a**, **11a**, **12a**, **13a**, **15a**, **3b**, **5e**, **5i**, **6c**, **9b**, **12b**, **14b**, **15b** and **15** evaluated with MP2/BSS-A. Data are collected in Table S3 of the Supporting Information.

References

S1 (a) *Atoms in Molecules. A Quantum Theory*: eds. R. F. W. Bader, Oxford University Press, Oxford, UK, 1990; (b) C. F. Matta, R. J. Boyd, *An Introduction to the Quantum Theory of Atoms in Molecules* in *The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design*: eds. C. F. Matta, R. J. Boyd, WILEY-VCH, Weinheim, Germany, 2007, Chapter 1.

S2 (a) R. F. W. Bader, T. S. Slee. D. Cremer, E. Kraka, *J. Am. Chem. Soc.* **1983**, *105*, 5061–5068; (b) R. F. W. Bader, *Chem. Rev.* **1991**, *91*, 893–926; (c) R. F. W. Bader, *J. Phys. Chem. A* **1998**, *102*, 7314–7323; (d) F. Biegler-König, R. F. W. Bader, T. H. Tang, *J. Comput. Chem.* **1982**, ***3***, 317–328; (e) R. F. W. Bader, *Acc. Chem. Res.* **1985**, *18*, 9–15; (f) T. H. Tang, R. F. W. Bader, P. MacDougall, *Inorg. Chem.* **1985**, *24*, 2047–2053; (g) F. Biegler-König, J. Schönbohm, D. Bayles, *J. Comput. Chem*. **2001**, *22*, 545–559; (h) F. Biegler-König, J. Schönbohm, *J. Comput. Chem.* **2002**, *23*, 1489–1494.

S3 W. Nakanishi, T. Nakamoto, S. Hayashi, T. Sasamori, N. Tokitoh, *Chem. Eur. J.* **2007**, *13*, 255–268.

S4 (a) W. Nakanishi, S. Hayashi, K. Narahara, *J. Phys. Chem. A* **2009**, *113*, 10050–10057; (*b*) W. Nakanishi, S. Hayashi, K. Narahara, *J. Phys. Chem. A* **2008**, *112*, 13593–13599.

S5 W. Nakanishi, S. Hayashi, *Curr. Org. Chem.* **2010**, *14*, 181–197.

S6 (a) W. Nakanishi, S. Hayashi, *J. Phys. Chem. A* **2010**, *114*, 7423–7430; (b) W. Nakanishi, S. Hayashi, K. Matsuiwa, M. Kitamoto, *Bull. Chem. Soc. Jpn* **2012**, *85*, 1293–1305.

S7 W. Nakanishi, S. Hayashi, *J. Phys. Chem. A* **2013**, *117*, 1795–1803.

S8 W. Nakanishi, S. Hayashi, *Int. J. Quantum Chem.* **2018**, *118*, e25590.

Optimized structures given by Cartesian coordinates

Optimized structures given by Cartesian coordinates for examined molecules, together with the total energies with the MP2/6-311++G(3df,3pd) method of the Gaussian 09 program. All positive frequencies were obtained for all species, except for **5n**, **6e**, and **7b** with one imaginary frequency.

Adduct **1a**
Symmetry C_1
energy MP2 = –191.503933 au
Standard orientation

6	0	-0.632082	0.590306	0.035513
1	0	-0.813225	1.143147	0.960373
1	0	-0.840704	1.258180	-0.797171
6	0	0.768658	0.166484	-0.005410
6	0	1.920604	-0.216989	-0.012340
1	0	2.929517	-0.547198	-0.030569
8	0	-1.540286	-0.491716	-0.098362
1	0	-1.296373	-1.159209	0.547683

Adduct **1b**
Symmetry C_s
energy MP2 = –191.501435 au
Standard orientation

6	0	-0.667836	-0.507976	0.000000
1	0	-1.305433	-0.579738	0.884684
1	0	-1.305433	-0.579738	-0.884684
6	0	0.000000	0.788554	0.000000
6	0	0.532068	1.878521	0.000000
1	0	1.008606	2.827061	0.000000
8	0	0.319507	-1.530937	0.000000
1	0	-0.139188	-2.374690	0.000000

Adduct **2a**
Symmetry C_1
energy MP2 = –230.734009 au
Standard orientation

1	0	-0.627391	-1.487064	-0.136163
8	0	-1.439291	-0.979579	-0.234771
6	0	-1.226273	0.275166	0.377889
1	0	-2.134150	0.851117	0.213252
1	0	-1.073161	0.167062	1.454963
6	0	-0.034192	1.013839	-0.231325
1	0	0.075209	1.988805	0.246383
1	0	-0.219649	1.176547	-1.293313
6	0	1.186466	0.233023	-0.059981
6	0	2.153133	-0.484594	0.105256
1	0	3.018665	-1.084429	0.242013

Adduct **2b**
Symmetry C_1
energy MP2 = –230.730070 au
Standard orientation

1	0	-1.708047	-0.865072	-1.054181

8	0	-1.506032	-0.965775	-0.121022
6	0	-1.200839	0.309100	0.408082
1	0	-2.051269	0.989917	0.312070
1	0	-1.007205	0.150299	1.466362
6	0	0.020382	0.951020	-0.248259
1	0	0.162526	1.946626	0.177456
1	0	-0.174482	1.089343	-1.314540
6	0	1.232341	0.160757	-0.068955
6	0	2.234573	-0.503518	0.098698
1	0	3.107995	-1.089065	0.243615

Adduct **2c**
Symmetry C_1
energy MP2 = –230.730446 au
Standard orientation

1	0	-2.170971	-1.350323	0.177149
8	0	-1.481771	-0.878285	-0.294496
6	0	-1.186961	0.314645	0.411908
1	0	-2.023859	1.016052	0.356866
1	0	-0.969562	0.107997	1.462298
6	0	0.029218	0.945480	-0.246717
1	0	0.181747	1.940190	0.174933
1	0	-0.178976	1.067229	-1.310464
6	0	1.236465	0.146966	-0.065965
6	0	2.238585	-0.515912	0.108165
1	0	3.111945	-1.101936	0.250838

Adduct **2d**
Symmetry C_1
energy MP2 = –230.731742 au
Standard orientation

1	0	2.491071	0.372233	0.747112
8	0	2.268150	-0.066219	-0.076968
6	0	0.924379	-0.506557	0.001974
1	0	0.763999	-1.144444	-0.863858
1	0	0.750438	-1.104610	0.899272
6	0	-0.060287	0.662811	-0.036053
1	0	0.121022	1.245426	-0.939261
1	0	0.122070	1.318762	0.817693
6	0	-1.438199	0.187820	-0.005189
6	0	-2.565294	-0.263554	0.024046
1	0	-3.557396	-0.640730	0.046119

Adduct **2e**
Symmetry C_s
energy MP2 = –230.732064 au
Standard orientation

1	0	-2.795531	-0.904535	0.000000
8	0	-2.220219	-0.136754	0.000000
6	0	-0.873246	-0.584793	0.000000
1	0	-0.654617	-1.184139	0.886660
1	0	-0.654617	-1.184139	-0.886660
6	0	0.000000	0.660293	0.000000

1	0	-0.241066	1.258720	0.878736
1	0	-0.241066	1.258720	-0.878736
6	0	1.414905	0.309308	0.000000
6	0	2.582003	-0.026013	0.000000
1	0	3.606673	-0.303363	0.000000

Adduct **3a**
Symmetry C_1
energy MP2 = –269.956612 au
Standard orientation

8	0	-1.082362	-1.459408	-0.128210
1	0	-0.127467	-1.469505	-0.009115
6	0	-1.555041	-0.194800	0.301201
1	0	-2.617455	-0.185276	0.065255
1	0	-1.456144	-0.089789	1.388211
6	0	-0.866634	0.975198	-0.388873
1	0	-0.807558	0.765112	-1.457323
1	0	-1.477907	1.870376	-0.258585
6	0	0.529731	1.279757	0.166508
1	0	0.443600	1.556428	1.219542
1	0	0.953179	2.140365	-0.353286
6	0	1.464163	0.161365	0.052931
6	0	2.233854	-0.775538	-0.039045
1	0	2.912209	-1.588333	-0.125352

Adduct **3b**
Symmetry C_1
energy MP2 = –269.953561 au
Standard orientation

6	0	0.785409	0.947912	0.473798
1	0	0.461180	0.768886	1.500878
1	0	1.366650	1.871626	0.477635
6	0	-0.452940	1.127821	-0.416239
1	0	-0.168887	1.040644	-1.466751
1	0	-0.864275	2.127866	-0.274262
6	0	-1.497595	0.154439	-0.109381
6	0	-2.351229	-0.651862	0.204988
1	0	-3.106546	-1.355066	0.455169
6	0	1.700350	-0.173259	0.008950
1	0	2.503267	-0.307100	0.739664
1	0	2.160380	0.102679	-0.940989
8	0	1.035173	-1.403243	-0.225954
1	0	0.262886	-1.453899	0.343597

Adduct **3c**
Symmetry C_1
energy MP2 = –269.956729 au
Standard orientation

6	0	0.695876	1.053074	0.392156
1	0	0.410108	1.469515	1.360058
1	0	1.447536	1.708594	-0.048574
6	0	-0.520931	1.021681	-0.539867
1	0	-0.190617	0.775313	-1.549635

1	0	-0.976480	2.010956	-0.589460
6	0	-1.520120	0.044875	-0.115809
6	0	-2.314210	-0.796986	0.256057
1	0	-3.024789	-1.519327	0.573841
6	0	1.292483	-0.327180	0.616316
1	0	0.605071	-0.935971	1.206835
1	0	2.225776	-0.239446	1.169329
8	0	1.612241	-0.981954	-0.604972
1	0	0.806882	-1.386789	-0.935730

Adduct **3d**
Symmetry C_1
energy MP2 = –269.951293 au
Standard orientation

6	0	0.742304	-0.964507	-0.464908
1	0	0.492366	-0.712125	-1.495613
1	0	1.260495	-1.925235	-0.475746
6	0	-0.543539	-1.111838	0.359798
1	0	-0.293808	-1.108044	1.423543
1	0	-0.991254	-2.084469	0.148626
6	0	-1.546637	-0.085932	0.092876
6	0	-2.410894	0.731345	-0.151785
1	0	-3.146468	1.466516	-0.362962
6	0	1.705551	0.063673	0.086864
1	0	2.628230	0.048350	-0.500638
1	0	1.957372	-0.193744	1.121406
8	0	1.090052	1.340875	0.025079
1	0	1.691945	1.985302	0.403681

Adduct **3e**
Symmetry C_1
energy MP2 = –269.957133 au
Standard orientation

6	0	0.566214	0.954632	0.511697
1	0	0.157252	1.220185	1.487365
1	0	1.296080	1.715606	0.232455
6	0	-0.555636	0.933934	-0.531729
1	0	-0.136391	0.659357	-1.499560
1	0	-0.983670	1.932031	-0.631278
6	0	-1.612143	-0.008456	-0.176657
6	0	-2.472266	-0.801072	0.153391
1	0	-3.233390	-1.488719	0.426838
6	0	1.269368	-0.379669	0.621620
1	0	0.547064	-1.157374	0.882804
1	0	2.031117	-0.333282	1.403974
8	0	1.866007	-0.650323	-0.643169
1	0	2.220666	-1.541438	-0.627176

Adduct **3f**
Symmetry C_1
energy MP2 = –269.954238 au
Standard orientation

6	0	0.339663	0.716663	-0.149482

1	0	-0.008842	1.664725	0.264399
1	0	0.246261	0.773611	-1.234045
6	0	-0.544188	-0.416041	0.377689
1	0	-0.423434	-0.500941	1.460801
1	0	-0.227502	-1.364705	-0.060154
6	0	-1.952748	-0.203032	0.066093
6	0	-3.116205	0.009646	-0.210077
1	0	-4.135381	0.185999	-0.448825
6	0	1.800085	0.525136	0.220089
1	0	1.910419	0.486192	1.308331
1	0	2.384405	1.368675	-0.141664
8	0	2.377311	-0.625675	-0.383256
1	0	2.075950	-1.402387	0.091335

Adduct **3g**
Symmetry C_1
energy MP2 = –269.956054 au
Standard orientation

6	0	0.549816	0.906437	0.554206
1	0	0.122901	1.118033	1.536354
1	0	1.275475	1.694087	0.336167
6	0	-0.554921	0.937411	-0.506454
1	0	-0.128032	0.674180	-1.474802
1	0	-0.961888	1.945655	-0.590604
6	0	-1.633973	0.008170	-0.186830
6	0	-2.512506	-0.775245	0.114495
1	0	-3.287129	-1.457342	0.362832
6	0	1.261392	-0.434221	0.600346
1	0	0.539271	-1.230937	0.770243
1	0	1.982221	-0.449087	1.421558
8	0	1.895689	-0.750412	-0.633267
1	0	2.632823	-0.146601	-0.750195

Adduct **3h**
Symmetry C_1
energy MP2 = –269.955065 au
Standard orientation

6	0	-0.515411	0.789175	-0.377971
1	0	-0.436183	0.491840	-1.425838
1	0	-1.123530	1.692942	-0.333951
6	0	0.884749	1.088986	0.166954
1	0	0.815989	1.367717	1.220833
1	0	1.308408	1.945820	-0.357916
6	0	1.789168	-0.049298	0.028248
6	0	2.519861	-1.010350	-0.108006
1	0	3.167120	-1.844507	-0.219662
6	0	-1.207797	-0.308704	0.409730
1	0	-1.326476	0.000430	1.447769
1	0	-0.600559	-1.216982	0.399163
8	0	-2.522291	-0.567415	-0.063327
1	0	-2.449858	-0.956797	-0.937519

Adduct **3i**

Symmetry C_1
energy MP2 = –269.955449 au
Standard orientation

6	0	0.345824	0.710689	-0.185519
1	0	0.026112	1.710557	0.113904
1	0	0.228177	0.649982	-1.270030
6	0	-0.547496	-0.337409	0.481026
1	0	-0.461369	-0.248143	1.566165
1	0	-0.192514	-1.333605	0.216927
6	0	-1.944971	-0.190759	0.091120
6	0	-3.098180	-0.036237	-0.258376
1	0	-4.109400	0.087632	-0.556326
6	0	1.806680	0.520315	0.181849
1	0	1.927679	0.546520	1.264271
1	0	2.408692	1.328778	-0.240695
8	0	2.310202	-0.746613	-0.221662
1	0	2.319866	-0.768418	-1.181519

Adduct **3j**
Symmetry C_1
energy MP2 = –269.954811 au
Standard orientation

6	0	-0.518166	0.786285	-0.369306
1	0	-0.448021	0.529462	-1.426239
1	0	-1.131939	1.686413	-0.284622
6	0	0.876341	1.090248	0.188011
1	0	0.802175	1.345783	1.247443
1	0	1.292850	1.961983	-0.317749
6	0	1.791286	-0.036658	0.029563
6	0	2.528703	-0.990411	-0.119706
1	0	3.179992	-1.819220	-0.246695
6	0	-1.189628	-0.354540	0.374004
1	0	-1.260192	-0.112574	1.439881
1	0	-0.594998	-1.260341	0.278047
8	0	-2.466807	-0.673869	-0.157819
1	0	-3.036630	0.089901	-0.042917

Adduct **3k**
Symmetry C_1
energy MP2 = –269.955276 au
Standard orientation

8	0	-2.488860	-0.494322	-0.196987
1	0	-2.905777	-1.259073	0.205164
6	0	-1.191178	-0.344213	0.366026
1	0	-1.257126	-0.117444	1.435373
1	0	-0.603843	-1.257315	0.245312
6	0	-0.514955	0.799603	-0.355958
1	0	-0.451185	0.560634	-1.417408
1	0	-1.130069	1.693798	-0.251757
6	0	0.883556	1.081297	0.199839
1	0	0.815810	1.329386	1.261345
1	0	1.305951	1.953342	-0.300344
6	0	1.790827	-0.050601	0.029577
6	0	2.525450	-1.005213	-0.128976

1	0	3.174914	-1.833990	-0.264837

Adduct **3l**
Symmetry C_1
energy MP2 = –269.954253 au
Standard orientation

6	0	-0.361356	-0.275825	-0.026233
1	0	-0.273110	-0.957730	0.822336
1	0	-0.289473	-0.873219	-0.934730
6	0	0.785722	0.736672	0.022686
1	0	0.700729	1.348119	0.923635
1	0	0.710204	1.416370	-0.828691
6	0	2.091193	0.086853	0.005204
6	0	3.160468	-0.488892	-0.009728
1	0	4.099932	-0.982862	-0.023911
6	0	-1.709567	0.420718	0.012674
1	0	-1.807642	1.092164	-0.839363
1	0	-1.791686	1.024991	0.922079
8	0	-2.797630	-0.483875	-0.091717
1	0	-2.766670	-1.073991	0.664767

Adduct **3m**
Symmetry C_1
energy MP2 = –269.955857 au
Standard orientation

6	0	0.339907	0.715812	-0.171466
1	0	0.000781	1.686788	0.191754
1	0	0.241657	0.715832	-1.257282
6	0	-0.538876	-0.389554	0.418945
1	0	-0.426806	-0.402052	1.505596
1	0	-0.195560	-1.356072	0.051332
6	0	-1.945013	-0.202852	0.080210
6	0	-3.106290	-0.011814	-0.221249
1	0	-4.123811	0.142459	-0.480932
6	0	1.795022	0.531176	0.197319
1	0	1.906259	0.530694	1.286427
1	0	2.387369	1.355486	-0.207496
8	0	2.224156	-0.711286	-0.348353
1	0	3.148360	-0.839463	-0.125127

Adduct **3n**
Symmetry C_s
energy MP2 = –269.954276 au
Standard orientation

6	0	0.000000	0.455158	0.000000
1	0	-0.550566	0.789625	0.878849
1	0	-0.550566	0.789625	-0.878849
6	0	0.099290	-1.071632	0.000000
1	0	0.657816	-1.405846	0.876991
1	0	0.657816	-1.405846	-0.876991
6	0	-1.214599	-1.704938	0.000000
6	0	-2.323803	-2.199505	0.000000
1	0	-3.290122	-2.638747	0.000000

6	0	1.372644	1.090361	0.000000
1	0	1.929840	0.770018	-0.886037
1	0	1.929840	0.770018	0.886037
8	0	1.194456	2.499839	0.000000
1	0	2.059105	2.915784	0.000000

Adduct **4a**
Symmetry C_1
energy MP2 = –192.744728 au
Standard orientation

1	0	1.380017	-0.670032	-1.073427
8	0	1.674472	-0.285400	-0.243824
6	0	0.603746	0.511251	0.254468
1	0	0.433003	1.384374	-0.381648
1	0	0.942012	0.862772	1.227674
6	0	-0.658874	-0.276849	0.386415
1	0	-0.620398	-1.144888	1.035207
6	0	-1.782141	0.022461	-0.269391
1	0	-2.677388	-0.572889	-0.161272
1	0	-1.829407	0.882680	-0.924894

Adduct **4b**
Symmetry C_1
energy MP2 = –192.744305 au
Standard orientation

1	0	-1.118006	-1.091454	0.754909
8	0	-1.346438	-0.638465	-0.060830
6	0	-0.731493	0.633855	-0.028754
1	0	-1.044279	1.136824	-0.944010
1	0	-1.110568	1.231393	0.806834
6	0	0.765478	0.593012	0.036704
1	0	1.255533	1.554248	0.152466
6	0	1.496655	-0.519715	-0.032107
1	0	2.574136	-0.480782	0.028517
1	0	1.030855	-1.485416	-0.167138

Adduct **4c**
Symmetry C_1
energy MP2 = –192.742341 au
Standard orientation

1	0	1.880202	-0.976269	-0.077002
8	0	1.655984	-0.108009	-0.419584
6	0	0.592256	0.419008	0.369392
1	0	0.422531	1.427704	-0.000996
1	0	0.899501	0.491071	1.416786
6	0	-0.662782	-0.386071	0.253761
1	0	-0.615519	-1.415814	0.595677
6	0	-1.806653	0.091234	-0.238103
1	0	-2.695316	-0.520250	-0.299419
1	0	-1.876197	1.112603	-0.588677

Adduct **4d**

Symmetry C_1
energy MP2 = –192.742790 au
Standard orientation

1	0	2.444121	0.150099	-0.206861
8	0	1.607699	-0.297518	-0.352493
6	0	0.585447	0.446610	0.305721
1	0	0.419514	1.408881	-0.185816
1	0	0.869266	0.635739	1.345408
6	0	-0.665611	-0.363369	0.268309
1	0	-0.598479	-1.363115	0.681754
6	0	-1.818455	0.083470	-0.230142
1	0	-2.710217	-0.526206	-0.219963
1	0	-1.894085	1.074478	-0.657906

Adduct **4e**
Symmetry C_s
energy MP2 = –192.743403 au
Standard orientation

1	0	1.921716	1.227500	0.000000
8	0	1.330913	0.472258	0.000000
6	0	0.000000	0.957117	0.000000
1	0	-0.188298	1.577731	0.882504
1	0	-0.188298	1.577731	-0.882504
6	0	-0.955308	-0.190265	0.000000
1	0	-2.004999	0.081747	0.000000
6	0	-0.594126	-1.472718	0.000000
1	0	-1.339128	-2.254734	0.000000
1	0	0.448311	-1.752849	0.000000

Adduct **5a**
Symmetry C_1
energy MP2 = –231.971273 au
Standard orientation

1	0	0.573415	-1.421230	0.264526
8	0	1.410186	-1.057536	-0.043898
6	0	1.357154	0.340898	0.167709
1	0	1.460386	0.577676	1.231972
1	0	2.214677	0.758143	-0.355832
6	0	0.063044	0.948359	-0.371789
1	0	-0.014679	0.718261	-1.434907
1	0	0.110147	2.033034	-0.256580
6	0	-1.113500	0.394148	0.364836
1	0	-1.257353	0.736162	1.385745
6	0	-1.938694	-0.534837	-0.127927
1	0	-2.751470	-0.936048	0.460840
1	0	-1.824633	-0.897124	-1.141560

Adduct **5b**
Symmetry C_1
energy MP2 = –231.968673 au
Standard orientation

1	0	0.693286	-1.251936	-0.714384
8	0	1.503714	-0.815769	-0.436473

6	0	1.140751	0.205258	0.479484
1	0	0.849942	-0.221038	1.444598
1	0	2.042025	0.792726	0.639718
6	0	0.035906	1.096186	-0.057908
1	0	0.362121	1.519207	-1.010053
1	0	-0.109270	1.940188	0.622814
6	0	-1.278804	0.396904	-0.256128
1	0	-2.012014	0.924078	-0.857537
6	0	-1.617341	-0.795860	0.243222
1	0	-2.595060	-1.215155	0.055051
1	0	-0.943821	-1.376856	0.859561

Adduct **5c**
Symmetry C_1
energy MP2 = –231.968454 au
Standard orientation

1	0	1.311668	-1.464993	-0.197435
8	0	1.860106	-0.713031	0.036854
6	0	1.197342	0.462957	-0.403740
1	0	1.928668	1.263780	-0.314067
1	0	0.913028	0.375567	-1.455994
6	0	-0.038008	0.791510	0.430974
1	0	-0.466822	1.724966	0.060258
1	0	0.278888	0.949658	1.463102
6	0	-1.061649	-0.297471	0.368128
1	0	-0.840280	-1.213650	0.906598
6	0	-2.203741	-0.218463	-0.319653
1	0	-2.899557	-1.044664	-0.353887
1	0	-2.470117	0.682385	-0.857661

Adduct **5d**
Symmetry C_1
energy MP2 = –231.967736 au
Standard orientation

1	0	1.292104	-1.283503	-0.831281
8	0	1.537029	-1.003704	0.054081
6	0	1.374663	0.401989	0.132241
1	0	1.508938	0.651131	1.184047
1	0	2.154799	0.916263	-0.436207
6	0	0.004859	0.871996	-0.342895
1	0	-0.108139	0.657100	-1.409114
1	0	-0.027495	1.959686	-0.231735
6	0	-1.113210	0.242492	0.422658
1	0	-1.095631	0.375379	1.500378
6	0	-2.098895	-0.468793	-0.126674
1	0	-2.881107	-0.907096	0.476081
1	0	-2.144210	-0.625432	-1.196805

Adduct **5e**
Symmetry C_1
energy MP2 = –231.966734 au
Standard orientation

1	0	1.688839	-0.561857	-1.192003

8	0	1.477116	-0.866371	-0.306563
6	0	1.126014	0.267413	0.474304
1	0	0.842654	-0.126654	1.449101
1	0	1.994572	0.916067	0.616957
6	0	-0.016061	1.080065	-0.108866
1	0	0.261672	1.423175	-1.111729
1	0	-0.120537	1.990582	0.488784
6	0	-1.345913	0.388337	-0.170143
1	0	-2.175506	1.000266	-0.510161
6	0	-1.585202	-0.882478	0.160496
1	0	-2.587026	-1.283536	0.100430
1	0	-0.794627	-1.547098	0.476378

Adduct **5f**
Symmetry C_1
energy MP2 = –231.968102 au
Standard orientation

1	0	2.218194	-0.617715	0.833825
8	0	1.875366	-0.718351	-0.057221
6	0	1.200491	0.483242	-0.403522
1	0	1.867912	1.343753	-0.306056
1	0	0.936044	0.376670	-1.453933
6	0	-0.058591	0.704430	0.427970
1	0	-0.492790	1.671839	0.166065
1	0	0.232665	0.755832	1.481900
6	0	-1.066249	-0.381057	0.225381
1	0	-0.739634	-1.391762	0.442513
6	0	-2.304748	-0.175955	-0.228245
1	0	-2.992035	-0.996493	-0.376930
1	0	-2.658704	0.820729	-0.459124

Adduct **5g**
Symmetry C_1
energy MP2 = –231.968723 au
Standard orientation

1	0	2.581222	-0.886300	-0.438257
8	0	1.808806	-0.699691	0.099183
6	0	1.196552	0.488626	-0.388754
1	0	1.872345	1.341215	-0.280827
1	0	0.932915	0.382743	-1.444680
6	0	-0.060640	0.722024	0.430535
1	0	-0.496971	1.679839	0.141931
1	0	0.235076	0.790123	1.479731
6	0	-1.062556	-0.372989	0.247632
1	0	-0.747304	-1.369054	0.536033
6	0	-2.282637	-0.190633	-0.262342
1	0	-2.968560	-1.016021	-0.389400
1	0	-2.623481	0.792818	-0.560428

Adduct **5h**
Symmetry C_1
energy MP2 = –231.967692 au
Standard orientation

1	0	2.302010	-1.283809	0.248630
8	0	1.451281	-0.984557	-0.078876
6	0	1.348094	0.412896	0.152700
1	0	1.431025	0.636622	1.221028
1	0	2.141027	0.951650	-0.372804
6	0	-0.005102	0.867773	-0.363413
1	0	-0.086925	0.603513	-1.418548
1	0	-0.039159	1.957769	-0.288544
6	0	-1.138359	0.269821	0.406735
1	0	-1.173986	0.496160	1.468755
6	0	-2.078616	-0.515645	-0.119765
1	0	-2.874441	-0.924431	0.486210
1	0	-2.065895	-0.770093	-1.171262

Adduct **5i**
Symmetry C_1
energy MP2 = –231.966655 au
Standard orientation

1	0	2.223369	-1.213469	-0.105404
8	0	1.448015	-0.759341	-0.442137
6	0	1.113492	0.284078	0.466727
1	0	0.826062	-0.126099	1.439671
1	0	1.969382	0.947117	0.614687
6	0	-0.034785	1.078294	-0.115076
1	0	0.242994	1.400915	-1.121827
1	0	-0.149287	1.990705	0.476279
6	0	-1.356402	0.370325	-0.162588
1	0	-2.195313	0.973324	-0.495523
6	0	-1.579968	-0.902944	0.167783
1	0	-2.576656	-1.317187	0.113852
1	0	-0.778699	-1.559094	0.474273

Adduct **5j**
Symmetry C_1
energy MP2 = –231.968206 au
Standard orientation

1	0	-2.597545	-0.103653	0.745445
8	0	-2.333555	-0.216584	-0.170459
6	0	-1.055944	0.378514	-0.336380
1	0	-0.819181	0.280802	-1.393954
1	0	-1.088349	1.446473	-0.099165
6	0	0.024353	-0.305815	0.494507
1	0	0.074514	-1.357841	0.213331
1	0	-0.264950	-0.256585	1.548377
6	0	1.352499	0.353078	0.300421
1	0	1.453795	1.370310	0.666758
6	0	2.389485	-0.214758	-0.319104
1	0	3.322282	0.313464	-0.455389
1	0	2.325523	-1.226409	-0.698402

Adduct **5k**
Symmetry C_1
energy MP2 = –231.968366 au

Standard orientation

1	0	-2.375800	-1.062119	-0.211336
8	0	-2.355653	-0.117910	-0.040076
6	0	-1.056365	0.357052	-0.357132
1	0	-0.811300	0.165612	-1.405573
1	0	-1.097474	1.436152	-0.217332
6	0	0.024315	-0.242485	0.536926
1	0	0.077048	-1.320907	0.370212
1	0	-0.268673	-0.078730	1.575432
6	0	1.355405	0.379121	0.260316
1	0	1.466272	1.427598	0.520248
6	0	2.381732	-0.255769	-0.309955
1	0	3.316263	0.248830	-0.509106
1	0	2.308363	-1.300675	-0.582866

Adduct **5l**
Symmetry C_1
energy MP2 = –231.966932 au
Standard orientation

1	0	2.503213	0.337116	0.701232
8	0	2.260467	-0.163188	-0.081039
6	0	0.874203	-0.464114	0.002991
1	0	0.660136	-1.086602	-0.863505
1	0	0.658127	-1.051020	0.899810
6	0	0.016748	0.787215	-0.025571
1	0	0.275082	1.363666	-0.916852
1	0	0.280337	1.419790	0.828294
6	0	-1.460559	0.537940	-0.002042
1	0	-2.087938	1.423334	-0.003860
6	0	-2.054815	-0.658067	0.017075
1	0	-3.132336	-0.736922	0.029371
1	0	-1.493821	-1.581705	0.019112

Adduct **5m**
Symmetry C_1
energy MP2 = –231.968491 au
Standard orientation

1	0	-2.981736	0.227786	-0.504165
8	0	-2.290791	-0.250520	-0.041137
6	0	-1.056342	0.419270	-0.262195
1	0	-0.828240	0.479231	-1.329763
1	0	-1.089917	1.437249	0.137971
6	0	0.028677	-0.374345	0.442956
1	0	0.079381	-1.371874	0.006299
1	0	-0.262893	-0.483007	1.489315
6	0	1.353045	0.311096	0.337132
1	0	1.452714	1.265070	0.846447
6	0	2.391744	-0.160282	-0.355925
1	0	3.324084	0.383049	-0.413375
1	0	2.330191	-1.107782	-0.875442

Adduct **5n**
Symmetry C_s

energy MP2 = –231.964663 au

Standard orientation

1	0	-3.049527	-0.580667	0.000000
8	0	-2.343474	0.068866	0.000000
6	0	-1.100372	-0.617886	0.000000
1	0	-1.006669	-1.253294	0.885948
1	0	-1.006669	-1.253294	-0.885948
6	0	0.000000	0.420780	0.000000
1	0	-0.123571	1.057318	0.877013
1	0	-0.123571	1.057318	-0.877013
6	0	1.362714	-0.217784	0.000000
1	0	1.399830	-1.303492	0.000000
6	0	2.514545	0.455888	0.000000
1	0	3.464271	-0.059005	0.000000
1	0	2.532375	1.538201	0.000000

Adduct **5o**

Symmetry C_s

energy MP2 = –231.967341 au

Standard orientation

1	0	-2.804063	-0.751360	0.000000
8	0	-2.227810	0.015599	0.000000
6	0	-0.879231	-0.438756	0.000000
1	0	-0.675912	-1.045431	0.886550
1	0	-0.675912	-1.045431	-0.886550
6	0	0.000000	0.790224	0.000000
1	0	-0.253840	1.397220	0.872090
1	0	-0.253840	1.397220	-0.872090
6	0	1.470061	0.507510	0.000000
1	0	2.114785	1.380215	0.000000
6	0	2.041284	-0.699728	0.000000
1	0	3.117017	-0.800724	0.000000
1	0	1.461558	-1.612002	0.000000

Adduct **6a**

Symmetry C_1

energy MP2 = –271.193839 au

Standard orientation

8	0	1.182650	-1.409455	-0.282388
1	0	0.228009	-1.478472	-0.184701
6	0	1.590517	-0.226820	0.387839
1	0	1.356408	-0.287215	1.457035
1	0	2.674138	-0.195609	0.289931
6	0	0.981377	1.038671	-0.197593
1	0	1.531367	1.899356	0.190104
1	0	1.122188	1.023519	-1.280249
6	0	-0.502533	1.215718	0.141197
1	0	-0.833125	2.184621	-0.241368
1	0	-0.625924	1.239932	1.226784
6	0	-1.380933	0.148936	-0.433774
1	0	-1.393071	0.061509	-1.516602
6	0	-2.127654	-0.691952	0.290148
1	0	-2.139964	-0.635598	1.371253
1	0	-2.745867	-1.443721	-0.179980

Adduct **6b**
Symmetry C_1
energy MP2 = –271.188588 au
Standard orientation

8	0	1.329903	-1.340668	-0.208012
1	0	1.833386	-1.278057	-1.022843
6	0	1.527349	-0.131036	0.513155
1	0	1.062188	-0.294572	1.485091
1	0	2.594339	0.040857	0.679359
6	0	0.903602	1.078513	-0.168388
1	0	1.362244	1.985182	0.233438
1	0	1.155340	1.047781	-1.232433
6	0	-0.613673	1.176950	0.009575
1	0	-0.966581	2.054712	-0.538991
1	0	-0.839808	1.351034	1.064423
6	0	-1.362524	-0.030812	-0.456445
1	0	-1.194615	-0.346343	-1.481192
6	0	-2.208731	-0.726582	0.305412
1	0	-2.391383	-0.445633	1.334728
1	0	-2.730473	-1.591815	-0.077333

Adduct **6c**
Symmetry C_1
energy MP2 = –271.189747 au
Standard orientation

8	0	1.360751	-1.235923	-0.380210
1	0	1.478571	-2.051399	0.111338
6	0	1.504829	-0.140238	0.518623
1	0	0.983445	-0.342493	1.459541
1	0	2.562436	0.023736	0.741119
6	0	0.911030	1.084857	-0.148520
1	0	1.363728	1.981920	0.277372
1	0	1.190201	1.053526	-1.203407
6	0	-0.610564	1.184022	-0.001369
1	0	-0.955277	2.046140	-0.578850
1	0	-0.860344	1.382101	1.043953
6	0	-1.343327	-0.038954	-0.453041
1	0	-1.153675	-0.376948	-1.466185
6	0	-2.193973	-0.724622	0.314321
1	0	-2.396367	-0.418769	1.333038
1	0	-2.706693	-1.600827	-0.056322

Adduct **6d**
Symmetry C_1
energy MP2 = –271.191305 au
Standard orientation

8	0	-2.842367	-0.487789	-0.157113
1	0	-3.664395	-0.003331	-0.258002
6	0	-1.778090	0.449755	-0.051209
1	0	-1.730066	1.082238	-0.943027
1	0	-1.920027	1.098896	0.818444
6	0	-0.488681	-0.326563	0.095423

1	0	-0.562719	-0.965274	0.977347
1	0	-0.365977	-0.980348	-0.768907
6	0	0.719890	0.601004	0.218632
1	0	0.566342	1.272503	1.068447
1	0	0.804141	1.223900	-0.674644
6	0	1.988585	-0.165829	0.412694
1	0	2.056010	-0.769494	1.313149
6	0	3.006607	-0.175513	-0.450235
1	0	2.971837	0.410894	-1.359401
1	0	3.893927	-0.764796	-0.268339

Adduct **6e**
Symmetry C_s
energy MP2 = –271.187602 au
Standard orientation

8	0	-1.339348	2.632351	0.000000
1	0	-2.232762	2.982082	0.000000
6	0	-1.412549	1.211812	0.000000
1	0	-1.945459	0.852509	0.885821
1	0	-1.945459	0.852509	-0.885821
6	0	0.000000	0.674460	0.000000
1	0	0.521081	1.058533	-0.878589
1	0	0.521081	1.058533	0.878589
6	0	0.031335	-0.848342	0.000000
1	0	-0.503228	-1.224784	-0.875642
1	0	-0.503228	-1.224784	0.875642
6	0	1.436480	-1.392857	0.000000
1	0	2.241588	-0.664337	0.000000
6	0	1.746283	-2.690875	0.000000
1	0	0.977033	-3.452827	0.000000
1	0	2.774844	-3.021438	0.000000

Adduct **7a**
Symmetry C_1
energy MP2 = –346.076818 au
Standard orientation

6	0	0.458901	0.169805	-0.248589
6	0	-0.094492	-1.114282	-0.230458
6	0	-1.458897	-1.293089	-0.025656
6	0	-2.287237	-0.186259	0.162898
6	0	-1.746492	1.096673	0.148005
6	0	-0.377418	1.269648	-0.053245
1	0	0.554759	-1.969794	-0.371157
1	0	-1.877237	-2.291021	-0.015612
1	0	-3.348721	-0.324829	0.320811
1	0	-2.384619	1.957776	0.296525
1	0	0.046464	2.267268	-0.061511
6	0	1.939045	0.345067	-0.443499
1	0	2.184268	1.410385	-0.470565
1	0	2.255264	-0.096107	-1.387545
8	0	2.701275	-0.328097	0.553004
1	0	2.359163	-0.054281	1.408278

Adduct **7b**
Symmetry C_s
energy MP2 = –346.074811 au
Standard orientation

6	0	0.210914	0.504618	0.000000
6	0	0.209333	-0.202971	1.203198
6	0	0.209333	-1.595554	1.206851
6	0	0.209048	-2.292576	0.000000
6	0	0.209333	-1.595554	-1.206851
6	0	0.209333	-0.202971	-1.203198
1	0	0.206053	0.343083	2.139041
1	0	0.210457	-2.134209	2.145246
1	0	0.211203	-3.374704	0.000000
1	0	0.210457	-2.134209	-2.145246
1	0	0.206053	0.343083	-2.139041
6	0	0.164178	2.000992	0.000000
1	0	0.671973	2.388919	-0.887020
1	0	0.671973	2.388919	0.887020
8	0	-1.209123	2.391425	0.000000
1	0	-1.244022	3.351814	0.000000

Adduct **7c**
Symmetry C_1
energy MP2 = –346.075006 au
Standard orientation

6	0	0.438874	0.264092	0.071866
6	0	-0.499461	1.293661	-0.021706
6	0	-1.861719	1.010866	-0.075518
6	0	-2.297738	-0.312568	-0.046035
6	0	-1.365807	-1.344479	0.037749
6	0	-0.003053	-1.058604	0.099944
1	0	-0.161543	2.323265	-0.057557
1	0	-2.577811	1.818715	-0.149800
1	0	-3.355127	-0.536899	-0.094551
1	0	-1.698320	-2.374239	0.054072
1	0	0.724660	-1.855830	0.157795
6	0	1.900301	0.597911	0.180639
1	0	2.138537	0.832720	1.223059
1	0	2.111922	1.486124	-0.421003
8	0	2.669436	-0.510419	-0.262468
1	0	3.593812	-0.315777	-0.093899

Adduct **8a**
Symmetry C_1
energy MP2 = –385.304916 au
Standard orientation

1	0	-1.438471	-1.048081	-1.155307
8	0	-2.359168	-0.888385	-0.923774
6	0	-2.420572	0.378631	-0.294342
1	0	-2.152298	1.174422	-0.996823
1	0	-3.459970	0.517142	-0.002716
6	0	-1.512353	0.458563	0.932162
1	0	-1.827817	-0.297302	1.651969
1	0	-1.632487	1.440553	1.394178

6	0	-0.081111	0.237432	0.537145
6	0	0.682368	1.287218	0.014891
6	0	0.491631	-1.037104	0.597271
6	0	1.984123	1.073234	-0.430148
6	0	1.794314	-1.258468	0.150633
6	0	2.542157	-0.202926	-0.364928
1	0	0.251616	2.280883	-0.036204
1	0	-0.088489	-1.856992	1.004304
1	0	2.562056	1.899098	-0.823970
1	0	2.222123	-2.250835	0.208471
1	0	3.553738	-0.371288	-0.709824

Adduct **8b**
Symmetry C_1
energy MP2 = –385.302044 au
Standard orientation

1	0	2.954094	1.099458	-1.423134
8	0	2.453349	0.965475	-0.615721
6	0	2.409350	-0.427794	-0.338716
1	0	2.048079	-0.985926	-1.207411
1	0	3.403635	-0.798363	-0.073385
6	0	1.457162	-0.633218	0.828068
1	0	1.794762	-0.007517	1.655667
1	0	1.527066	-1.674303	1.148104
6	0	0.039548	-0.301750	0.460472
6	0	-0.814520	-1.293319	-0.030368
6	0	-0.437306	1.008724	0.547553
6	0	-2.115735	-0.988295	-0.424168
6	0	-1.737474	1.320020	0.156254
6	0	-2.579526	0.322277	-0.331325
1	0	-0.457458	-2.315108	-0.097901
1	0	0.221066	1.785165	0.915520
1	0	-2.764866	-1.770332	-0.796190
1	0	-2.091872	2.339903	0.231208
1	0	-3.590291	0.563353	-0.633334

Adduct **9a**
Symmetry C_1
energy MP2 = –424.527896 au
Standard orientation

8	0	1.397281	-1.473433	-0.991554
1	0	0.526665	-1.245418	-0.650992
6	0	2.364230	-0.862876	-0.151320
1	0	2.293768	-1.254126	0.870831
1	0	3.327047	-1.172420	-0.553821
6	0	2.283057	0.659226	-0.128195
1	0	3.247119	1.057658	0.197534
1	0	2.115644	1.005240	-1.150096
6	0	1.192458	1.208076	0.801178
1	0	1.187123	2.298342	0.742774
1	0	1.439821	0.942501	1.831296
6	0	-0.173506	0.676710	0.467797
6	0	-0.865298	1.149402	-0.652997
6	0	-0.751190	-0.350525	1.221410

6	0	-2.092627	0.604342	-1.018762
6	0	-1.979256	-0.903749	0.858112
6	0	-2.650489	-0.428779	-0.265930
1	0	-0.429936	1.944943	-1.246818
1	0	-0.229765	-0.722313	2.095995
1	0	-2.611127	0.981066	-1.890725
1	0	-2.407261	-1.701524	1.450954
1	0	-3.601618	-0.857447	-0.552259

Adduct **9b**
Symmetry C_1
energy MP2 = –424.524085 au
Standard orientation

8	0	1.715622	-1.426914	-0.785086
1	0	1.041738	-0.981929	-1.306074
6	0	2.714938	-0.480436	-0.438866
1	0	3.242968	-0.914956	0.410457
1	0	3.435857	-0.366246	-1.254526
6	0	2.167022	0.883729	-0.055742
1	0	3.013253	1.497875	0.261766
1	0	1.742778	1.370600	-0.938560
6	0	1.110271	0.840624	1.055058
1	0	1.031778	1.834700	1.500420
1	0	1.441083	0.161803	1.843893
6	0	-0.252420	0.425555	0.565551
6	0	-0.970512	1.264547	-0.293624
6	0	-0.825582	-0.793770	0.934031
6	0	-2.222995	0.894391	-0.779226
6	0	-2.079217	-1.169013	0.455966
6	0	-2.780479	-0.326942	-0.405073
1	0	-0.546669	2.220953	-0.580062
1	0	-0.273895	-1.460360	1.585063
1	0	-2.762915	1.558886	-1.441374
1	0	-2.504155	-2.119733	0.750566
1	0	-3.752952	-0.618388	-0.779330

Adduct **9c**
Symmetry C_s
energy MP2 = –424.524850 au
Standard orientation

6	0	0.694654	-0.434444	0.000000
6	0	0.693422	-1.149172	1.200730
6	0	0.693422	-2.542332	1.205008
6	0	0.692382	-3.242097	0.000000
6	0	0.693422	-2.542332	-1.205008
6	0	0.693422	-1.149172	-1.200730
1	0	0.695965	-0.606690	2.139531
1	0	0.697086	-3.078776	2.144954
1	0	0.694482	-4.324074	0.000000
1	0	0.697086	-3.078776	-2.144954
1	0	0.695965	-0.606690	-2.139531
6	0	0.625940	1.065661	0.000000
1	0	1.142443	1.457658	-0.879278
1	0	1.142443	1.457658	0.879278

6	0	-0.823108	1.554112	0.000000
1	0	-1.342527	1.167029	-0.878265
1	0	-1.342527	1.167029	0.878265
6	0	-0.907373	3.064043	0.000000
1	0	-0.403072	3.462825	-0.885837
1	0	-0.403072	3.462825	0.885837
8	0	-2.283140	3.424101	0.000000
1	0	-2.346259	4.381565	0.000000

Adduct **9d**
Symmetry C_1
energy MP2 = –424.522638 au
Standard orientation

8	0	4.160213	0.653233	0.000048
1	0	5.041083	0.272857	0.000061
6	0	3.212277	-0.407029	0.000044
1	0	3.337424	-1.037074	-0.885978
1	0	3.337404	-1.037063	0.886077
6	0	1.831342	0.210021	0.000025
1	0	1.738420	0.848490	0.879780
1	0	1.738439	0.848477	-0.879741
6	0	0.750175	-0.859331	0.000022
1	0	0.882263	-1.503880	0.873884
1	0	0.882285	-1.503896	-0.873826
6	0	-0.670221	-0.346203	-0.000003
6	0	-0.984797	1.014207	-0.000024
6	0	-1.723717	-1.267885	-0.000008
6	0	-2.313395	1.441646	-0.000048
6	0	-3.050257	-0.848966	-0.000033
6	0	-3.349492	0.513038	-0.000053
1	0	-0.194624	1.752792	-0.000020
1	0	-1.495660	-2.328127	0.000006
1	0	-2.534168	2.501188	-0.000065
1	0	-3.846806	-1.581643	-0.000039
1	0	-4.379250	0.845038	-0.000067

Adduct **10a**
Symmetry C_s
energy MP2 = –382.854242 au
Standard orientation

1	0	-2.352627	0.085042	0.000000
8	0	-1.959519	-0.798127	0.000000
6	0	-0.610629	-0.657237	0.000000
6	0	0.000000	0.609488	0.000000
6	0	1.398449	0.700632	0.000000
6	0	2.175946	-0.449415	0.000000
6	0	1.559050	-1.701302	0.000000
6	0	0.173183	-1.807736	0.000000
1	0	1.855215	1.681343	0.000000
1	0	3.254211	-0.371590	0.000000
1	0	2.159713	-2.601193	0.000000
1	0	-0.319404	-2.770481	0.000000
6	0	-0.837816	1.759977	0.000000
6	0	-1.630188	2.685990	0.000000

1	0	-2.288923	3.519524	0.000000

Adduct **10b**
Symmetry C_s
energy MP2 = –382.848655 au
Standard orientation

1	0	-2.345283	-1.511415	0.000000
8	0	-2.022175	-0.605514	0.000000
6	0	-0.661754	-0.627870	0.000000
6	0	0.000000	0.611093	0.000000
6	0	1.401366	0.628437	0.000000
6	0	2.132130	-0.553362	0.000000
6	0	1.463802	-1.775625	0.000000
6	0	0.072586	-1.811258	0.000000
1	0	1.901368	1.587888	0.000000
1	0	3.212731	-0.520737	0.000000
1	0	2.020000	-2.703536	0.000000
1	0	-0.449201	-2.761519	0.000000
6	0	-0.746104	1.823100	0.000000
6	0	-1.369171	2.868332	0.000000
1	0	-1.919346	3.776354	0.000000

Adduct **11a**
Symmetry C_1
energy MP2 = –422.069713 au
Standard orientation

1	0	2.338636	-0.631805	0.858635
8	0	2.010304	-1.526166	0.721688
6	0	1.182551	-1.490624	-0.432895
1	0	0.921571	-2.525088	-0.646437
1	0	1.737000	-1.093825	-1.288560
6	0	-0.070433	-0.683892	-0.226531
6	0	0.011317	0.713746	-0.074536
6	0	-1.148129	1.471761	0.132308
6	0	-2.388574	0.845246	0.184701
6	0	-2.479733	-0.537172	0.036072
6	0	-1.323541	-1.288937	-0.164273
1	0	-1.063808	2.544284	0.248314
1	0	-3.281103	1.435828	0.343096
1	0	-3.443356	-1.027015	0.080252
1	0	-1.390703	-2.364776	-0.273313
6	0	1.286790	1.353182	-0.120746
6	0	2.389252	1.871899	-0.152654
1	0	3.342327	2.340480	-0.184155

Adduct **11b**
Symmetry C_1
energy MP2 = –422.067294 au
Standard orientation

1	0	1.284843	-2.012130	1.377243
8	0	1.917014	-1.674134	0.737093
6	0	1.213553	-1.455711	-0.482078
1	0	0.951949	-2.406745	-0.954545

1	0	1.913729	-0.929969	-1.128159
6	0	-0.030227	-0.640898	-0.276937
6	0	0.046989	0.749059	-0.058065
6	0	-1.122895	1.481879	0.183884
6	0	-2.359062	0.844983	0.213143
6	0	-2.443467	-0.528566	-0.004055
6	0	-1.281052	-1.257378	-0.247394
1	0	-1.048396	2.549372	0.344310
1	0	-3.254677	1.422194	0.401376
1	0	-3.403775	-1.026522	0.012276
1	0	-1.340719	-2.325300	-0.424616
6	0	1.306664	1.416456	-0.093180
6	0	2.377020	1.995326	-0.130740
1	0	3.315802	2.491271	-0.152104

Adduct **11c**
Symmetry C_1
energy MP2 = –422.068069 au
Standard orientation

1	0	1.230109	2.707805	-1.008087
8	0	1.454718	2.560749	-0.085981
6	0	1.485521	1.162090	0.133834
1	0	1.903250	1.027965	1.131938
1	0	2.162353	0.664693	-0.565335
6	0	0.126740	0.507807	0.064698
6	0	0.028571	-0.894907	-0.003647
6	0	-1.229774	-1.509385	-0.058841
6	0	-2.386132	-0.737839	-0.044364
6	0	-2.293875	0.650278	0.029701
6	0	-1.043246	1.263115	0.085852
1	0	-1.283902	-2.588782	-0.113297
1	0	-3.353865	-1.219409	-0.089300
1	0	-3.191000	1.255014	0.047081
1	0	-0.963443	2.339734	0.154585
6	0	1.211235	-1.693304	-0.009196
6	0	2.226136	-2.366827	-0.008584
1	0	3.107698	-2.959187	-0.006446

Adduct **11d**
Symmetry C_s
energy MP2 = –422.068026 au
Standard orientation

1	0	1.466380	3.374459	0.000000
8	0	0.701881	2.794984	0.000000
6	0	1.172854	1.457261	0.000000
1	0	1.789061	1.257445	0.882122
1	0	1.789061	1.257445	-0.882122
6	0	0.000000	0.518937	0.000000
6	0	0.234250	-0.868583	0.000000
6	0	-0.844230	-1.762624	0.000000
6	0	-2.148725	-1.281763	0.000000
6	0	-2.382103	0.091604	0.000000
6	0	-1.311757	0.984803	0.000000
1	0	-0.643940	-2.826011	0.000000

1	0	-2.977662	-1.976977	0.000000
1	0	-3.395970	0.469778	0.000000
1	0	-1.483231	2.051590	0.000000
6	0	1.573731	-1.358927	0.000000
6	0	2.725350	-1.756185	0.000000
1	0	3.725034	-2.114740	0.000000

Adduct **12a**
Symmetry C_1
energy MP2 = –384.088003 au
Standard orientation

1	0	1.735230	1.483169	-0.387448
8	0	0.874229	1.868862	-0.182480
6	0	-0.025300	0.852062	-0.074011
6	0	0.350734	-0.502419	-0.114400
6	0	-0.661049	-1.471037	-0.065981
6	0	-1.998034	-1.121521	0.072820
6	0	-2.346161	0.227514	0.139168
6	0	-1.366491	1.209020	0.054826
1	0	-0.376085	-2.515072	-0.122050
1	0	-2.758211	-1.888618	0.123565
1	0	-3.383086	0.518060	0.244692
1	0	-1.618340	2.260647	0.078133
6	0	1.751190	-0.926206	-0.240944
1	0	1.934496	-1.770717	-0.897828
6	0	2.796243	-0.382004	0.402637
1	0	2.670884	0.416678	1.122480
1	0	3.794492	-0.767497	0.253606

Adduct **12b**
Symmetry C_s
energy MP2 = –384.086551 au
Standard orientation

1	0	-1.960718	-1.863825	0.000000
8	0	-1.810161	-0.913699	0.000000
6	0	-0.462190	-0.694839	0.000000
6	0	0.000000	0.634144	0.000000
6	0	1.391500	0.823440	0.000000
6	0	2.292172	-0.233948	0.000000
6	0	1.806744	-1.538797	0.000000
6	0	0.434061	-1.762135	0.000000
1	0	1.761584	1.841768	0.000000
1	0	3.356249	-0.042642	0.000000
1	0	2.486207	-2.380632	0.000000
1	0	0.047122	-2.775411	0.000000
6	0	-0.848552	1.825785	0.000000
1	0	-0.285642	2.754227	0.000000
6	0	-2.188176	1.917453	0.000000
1	0	-2.829782	1.053224	0.000000
1	0	-2.647085	2.896272	0.000000

Adduct **13a**
Symmetry C_1

energy MP2 = –423.311489 au

Standard orientation

1	0	1.442590	1.409722	-0.116665
8	0	0.579287	1.800650	-0.304230
6	0	-0.380160	0.842656	-0.141753
6	0	-0.094426	-0.526503	-0.259169
6	0	-1.139617	-1.437394	-0.086820
6	0	-2.440234	-1.013118	0.169301
6	0	-2.706733	0.351803	0.260630
6	0	-1.680094	1.277399	0.109470
1	0	-0.923112	-2.496134	-0.172280
1	0	-3.234044	-1.737166	0.291578
1	0	-3.713018	0.698400	0.455701
1	0	-1.861746	2.340943	0.187395
6	0	1.305842	-0.990290	-0.567448
1	0	1.646216	-0.564086	-1.515439
1	0	1.292324	-2.075485	-0.684525
6	0	2.272234	-0.614660	0.518951
1	0	2.027003	-0.956605	1.519594
6	0	3.367983	0.128280	0.327399
1	0	4.023997	0.385479	1.146577
1	0	3.636728	0.480699	-0.661456

Adduct **13b**

Symmetry C_1

energy MP2 = –423.308534 au

Standard orientation

1	0	-0.109520	2.712738	0.210488
8	0	-0.508713	1.856179	0.388256
6	0	0.431700	0.885703	0.179628
6	0	0.036192	-0.438477	0.405207
6	0	0.978283	-1.448177	0.205640
6	0	2.278732	-1.165212	-0.206699
6	0	2.651399	0.158187	-0.424955
6	0	1.729823	1.183820	-0.229565
1	0	0.678828	-2.474828	0.383174
1	0	2.990885	-1.965827	-0.351900
1	0	3.656997	0.398374	-0.743814
1	0	2.016879	2.216461	-0.394524
6	0	-1.385407	-0.745379	0.790561
1	0	-1.757891	0.002288	1.490866
1	0	-1.411689	-1.717941	1.285961
6	0	-2.258927	-0.770207	-0.430531
1	0	-2.035526	-1.539559	-1.163524
6	0	-3.239507	0.102572	-0.669865
1	0	-3.826908	0.051854	-1.575791
1	0	-3.466080	0.890029	0.036483

Adduct **13c**

Symmetry C_1

energy MP2 = –423.308156 au

Standard orientation

1	0	1.799702	2.646024	-0.012479
8	0	0.928680	2.238946	-0.020072

6	0	1.082568	0.878335	-0.011473
6	0	-0.090005	0.112516	-0.001423
6	0	0.036819	-1.276790	-0.011014
6	0	1.286198	-1.895345	-0.020327
6	0	2.438385	-1.115487	-0.020878
6	0	2.336940	0.273719	-0.016847
1	0	-0.864265	-1.877197	-0.014804
1	0	1.356488	-2.974477	-0.026366
1	0	3.415719	-1.579560	-0.025757
1	0	3.229906	0.888938	-0.021211
6	0	-1.430472	0.807738	-0.007668
1	0	-1.642442	1.177824	-1.014244
1	0	-1.359233	1.689640	0.632518
6	0	-2.550662	-0.064336	0.458762
6	0	-3.582482	-0.436102	-0.302110
1	0	-2.498452	-0.411375	1.486369
1	0	-4.372284	-1.062845	0.087102
1	0	-3.658317	-0.114027	-1.332682

Adduct **14a**
Symmetry C_1
energy MP2 = –537.423633 au
Standard orientation

1	0	-0.110680	1.962662	-0.651049
8	0	0.846395	2.087245	-0.632813
6	0	1.423600	0.909806	-0.259942
6	0	2.815974	0.859679	-0.247619
6	0	3.466360	-0.320670	0.094322
6	0	2.733248	-1.461784	0.418153
6	0	1.343722	-1.405780	0.403968
6	0	0.667442	-0.225047	0.076768
1	0	3.367832	1.749949	-0.517792
1	0	4.548039	-0.348189	0.103156
1	0	3.237147	-2.380875	0.683906
1	0	0.757108	-2.278054	0.666936
6	0	-0.806842	-0.177076	0.060869
6	0	-1.537959	-1.077756	-0.723828
6	0	-2.929700	-1.040530	-0.736622
6	0	-3.611848	-0.095561	0.028425
6	0	-2.897062	0.806855	0.813363
6	0	-1.504329	0.765019	0.831341
1	0	-1.003440	-1.799889	-1.328896
1	0	-3.480651	-1.742817	-1.348466
1	0	-4.693228	-0.064374	0.014784
1	0	-3.420755	1.534902	1.418982
1	0	-0.948154	1.445792	1.465753

Adduct **14b**
Symmetry C_1
energy MP2 = –537.419883 au
Standard orientation

1	0	-1.492754	2.727817	-0.780299
8	0	-0.822167	2.079240	-0.545980
6	0	-1.449995	0.907500	-0.226580

6	0	-2.839965	0.804680	-0.210316
6	0	-3.453858	-0.405899	0.097490
6	0	-2.676718	-1.523172	0.390653
6	0	-1.289871	-1.412301	0.371849
6	0	-0.647215	-0.206586	0.066033
1	0	-3.440604	1.676522	-0.445443
1	0	-4.533868	-0.469295	0.108578
1	0	-3.143303	-2.466728	0.638109
1	0	-0.674017	-2.269636	0.615042
6	0	0.825310	-0.139651	0.038196
6	0	1.524780	0.880841	0.693668
6	0	2.916402	0.897739	0.691003
6	0	3.630958	-0.099142	0.028293
6	0	2.944822	-1.116347	-0.631809
6	0	1.552585	-1.135602	-0.625713
1	0	0.973437	1.654831	1.209788
1	0	3.443191	1.689184	1.208159
1	0	4.712882	-0.081619	0.024579
1	0	3.491021	-1.890049	-1.155621
1	0	1.017947	-1.917309	-1.151655

Adduct **15a**
Symmetry C_1
energy MP2 = –576.639639 au
Standard orientation

1	0	-0.728266	1.674565	-1.036023
8	0	-0.016884	2.323797	-1.016953
6	0	0.741257	2.083457	0.161261
1	0	0.107559	2.181183	1.046685
1	0	1.487748	2.874596	0.200040
6	0	1.434200	0.743979	0.149545
6	0	2.827615	0.671343	0.128879
6	0	3.487522	-0.554575	0.069145
6	0	2.747951	-1.732878	0.010495
6	0	1.356085	-1.676723	0.021987
6	0	0.691498	-0.449779	0.101217
1	0	3.400827	1.590899	0.149486
1	0	4.568939	-0.587545	0.056593
1	0	3.249460	-2.690291	-0.043554
1	0	0.770518	-2.587574	-0.017806
6	0	-0.788300	-0.420702	0.105781
6	0	-1.504212	-0.802554	-1.036219
6	0	-2.897282	-0.758765	-1.047470
6	0	-3.591310	-0.335424	0.084443
6	0	-2.888663	0.036705	1.229653
6	0	-1.496520	-0.005112	1.240036
1	0	-0.957656	-1.119565	-1.916423
1	0	-3.437403	-1.050054	-1.938881
1	0	-4.672527	-0.298165	0.075562
1	0	-3.423769	0.356087	2.114442
1	0	-0.949403	0.271657	2.132993

Adduct **15b**
Symmetry C_1

energy MP2 = –576.639726 au

Standard orientation

1	0	-1.663685	2.773110	-0.790225
8	0	-0.829069	2.797424	-0.313488
6	0	-0.944112	1.889772	0.785504
1	0	-1.624251	2.298149	1.537832
1	0	0.051273	1.828460	1.219289
6	0	-1.433479	0.536659	0.353780
6	0	-2.812945	0.305629	0.342738
6	0	-3.346133	-0.910158	-0.075112
6	0	-2.484955	-1.927070	-0.480576
6	0	-1.109615	-1.717415	-0.462230
6	0	-0.562446	-0.493124	-0.054176
1	0	-3.475597	1.093415	0.685226
1	0	-4.417053	-1.064201	-0.075413
1	0	-2.880606	-2.878925	-0.810197
1	0	-0.438147	-2.504043	-0.784443
6	0	0.907274	-0.346824	-0.036177
6	0	1.687938	-1.327622	0.590910
6	0	3.076643	-1.231484	0.604871
6	0	3.707143	-0.152011	-0.011502
6	0	2.940190	0.827912	-0.638831
6	0	1.550271	0.735069	-0.651867
1	0	1.196093	-2.158036	1.083343
1	0	3.663505	-1.993594	1.101045
1	0	4.786451	-0.075062	-0.001959
1	0	3.423003	1.667444	-1.122093
1	0	0.956914	1.497887	-1.138497

Adduct **15c**

Symmetry C_1

energy MP2 = –576.638455 au

Standard orientation

1	0	-0.580437	3.611005	-0.018124
8	0	-0.886075	2.753424	-0.327478
6	0	-0.912353	1.868714	0.796830
1	0	-1.579354	2.264386	1.567295
1	0	0.087190	1.758138	1.222860
6	0	-1.430763	0.540372	0.334063
6	0	-2.812932	0.340280	0.292900
6	0	-3.357334	-0.875075	-0.108991
6	0	-2.507924	-1.919760	-0.468452
6	0	-1.129828	-1.734930	-0.431120
6	0	-0.572383	-0.509655	-0.041373
1	0	-3.464844	1.154251	0.587697
1	0	-4.430779	-1.007679	-0.135822
1	0	-2.915848	-2.871842	-0.782251
1	0	-0.465454	-2.538170	-0.726119
6	0	0.897434	-0.368596	-0.030189
6	0	1.684346	-1.304820	0.652793
6	0	3.072975	-1.200904	0.653627
6	0	3.695113	-0.159689	-0.033179
6	0	2.920950	0.774335	-0.719687
6	0	1.531615	0.673082	-0.719498
1	0	1.197732	-2.105965	1.196352

1	0	3.666713	-1.927908	1.192530
1	0	4.774159	-0.078265	-0.034696
1	0	3.398913	1.580302	-1.261695
1	0	0.927106	1.394225	-1.254539

Adduct **15d**
Symmetry C_1
energy MP2 = –576.637102au
Standard orientation

1	0	1.592806	3.634951	-0.602307
8	0	1.929628	2.737764	-0.553958
6	0	0.868673	1.902698	-0.112017
1	0	0.034695	1.916362	-0.819764
1	0	0.487279	2.254534	0.851475
6	0	1.377084	0.491267	0.021258
6	0	2.747403	0.230640	0.046933
6	0	3.221155	-1.076788	0.137232
6	0	2.325678	-2.141617	0.193758
6	0	0.956660	-1.889955	0.167250
6	0	0.470677	-0.581085	0.088217
1	0	3.436472	1.060186	-0.023541
1	0	4.287422	-1.260903	0.155316
1	0	2.687734	-3.159290	0.259547
1	0	0.246671	-2.706981	0.217194
6	0	-0.989071	-0.347895	0.059561
6	0	-1.760416	-0.835044	-1.001868
6	0	-3.136942	-0.622493	-1.035545
6	0	-3.760772	0.077732	-0.004630
6	0	-3.003639	0.559616	1.062174
6	0	-1.627366	0.348063	1.092745
1	0	-1.269203	-1.371784	-1.804647
1	0	-3.719893	-1.000562	-1.865380
1	0	-4.829818	0.242974	-0.029769
1	0	-3.484702	1.092886	1.871942
1	0	-1.041242	0.704688	1.931180