Supporting Information

Nature of the E---E' Interactions (E, E' = O, S, Se, and Te) at Naphthalene 1,8-Positions with Fine Details of the Structures: Experimental and Theoretical Investigations

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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.

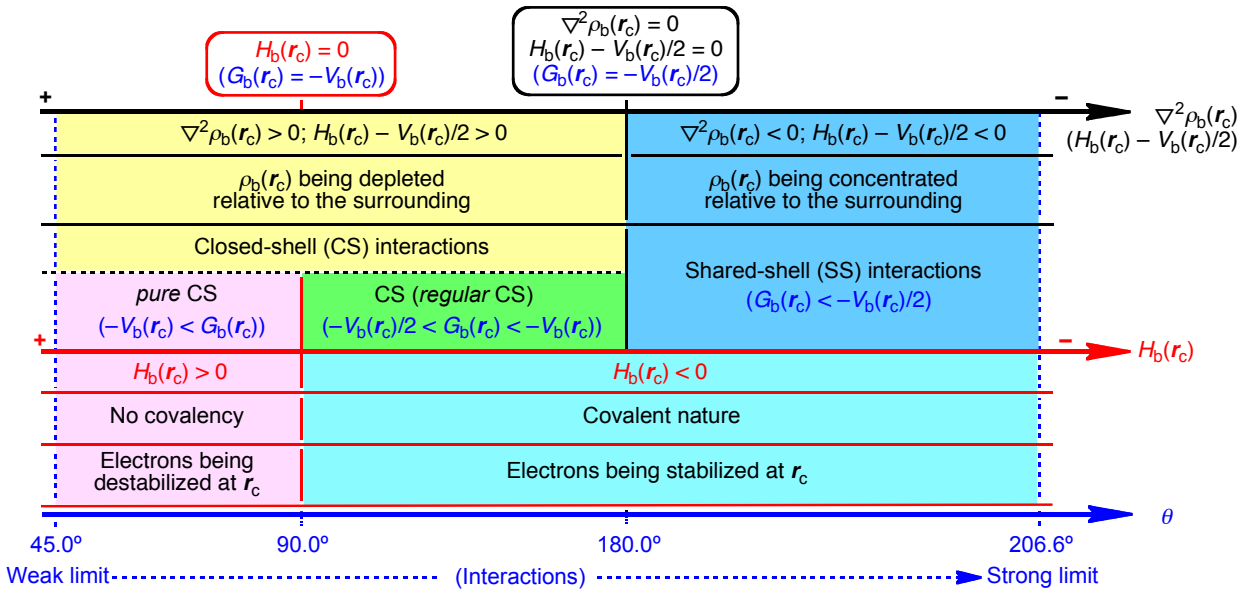
The sign of the Laplacian $\rho_b(\boldsymbol{r}_c)$ ($\nabla^2\rho_b(\boldsymbol{r}_c)$) indicates that $\rho_b(\boldsymbol{r}_c)$ is depleted or concentrated with respect to its surrounding, since $\nabla^2\rho_b(\boldsymbol{r}_c)$ is the second derivative of $\rho_b(\boldsymbol{r}_c)$. $\rho_b(\boldsymbol{r}_c)$ 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.

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

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

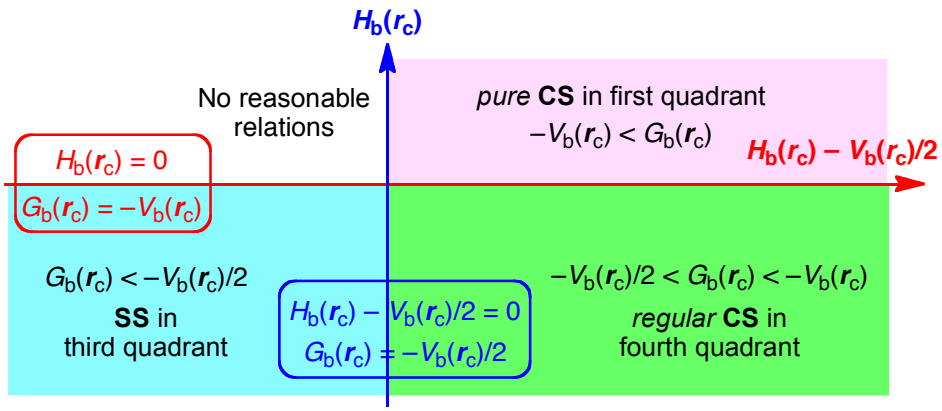
$$= G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2 \quad \text{(S2')}$$

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 quadrant. 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 of the $[(H_b(\boldsymbol{r}_c))^2 + (H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)^2]^{1/2}$ form in the plot, where $R = 0$ for the enough large interaction distance. 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.

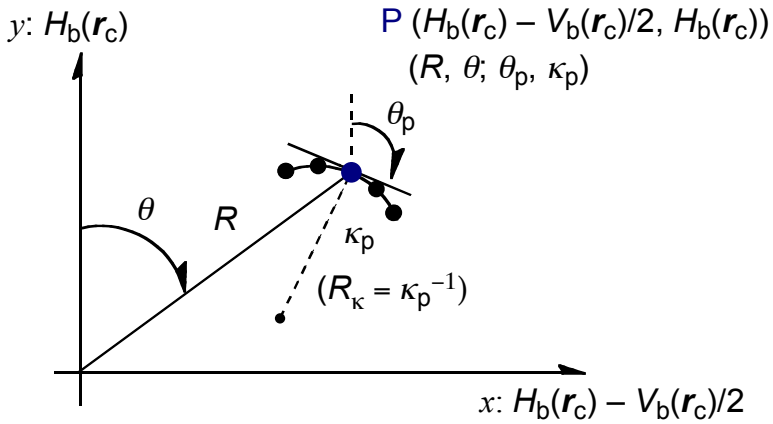


Figure S1. Polar (R, θ) coordinate representation of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, with ($\theta_p$, κ_p) parameters.

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

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

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

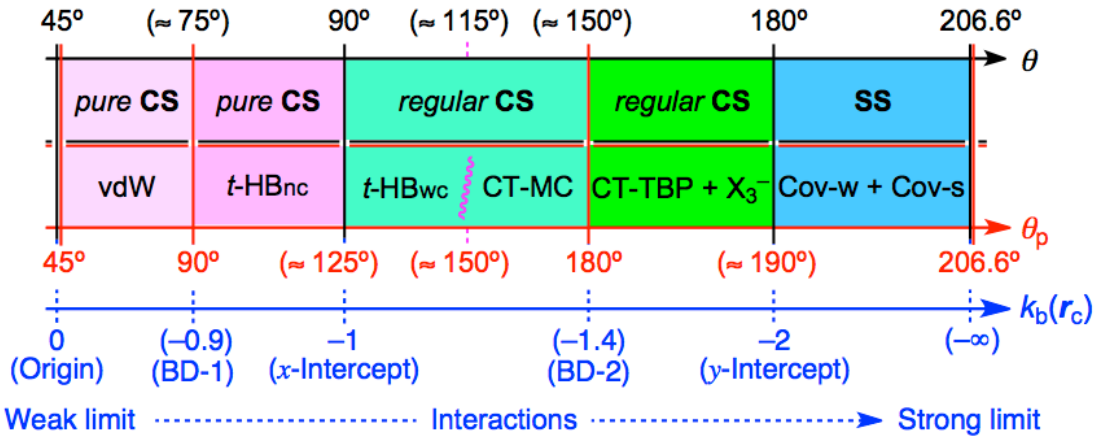
$$\kappa_p = |d^2y/dx^2| / [1 + (dy/dx)^2]^{3/2} \quad \text{(S6)}$$

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

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.

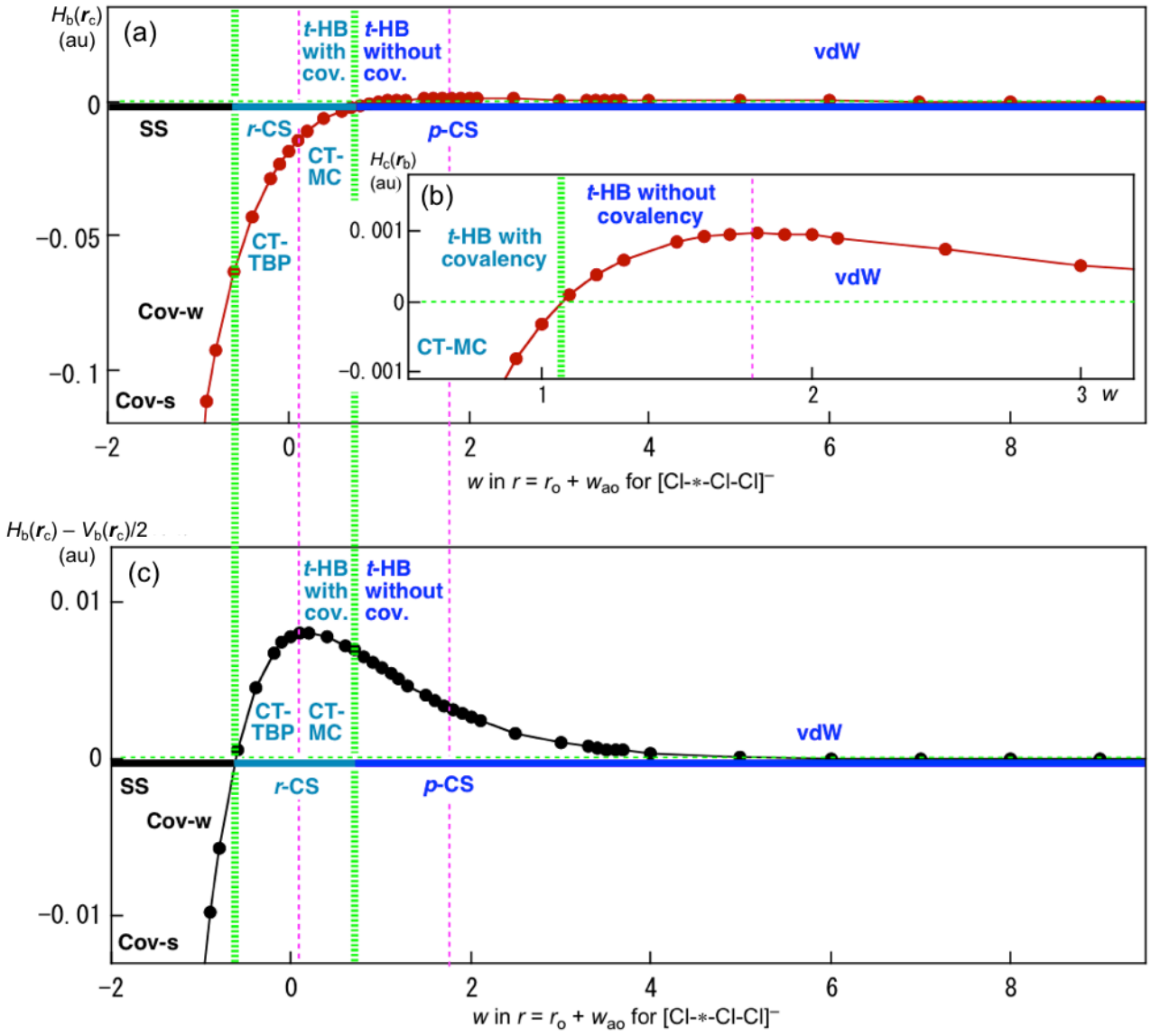


Figure S2. Plot of $H_b(\boldsymbol{r}_c)$ versus w in $r(^1\text{Cl-}^2\text{Cl}) = r_o(^1\text{Cl-}^2\text{Cl}) + wa_o$ for $^1\text{Cl-}^2\text{Cl-}^3\text{Cl}^-$ (a) with the magnified picture of (a) (b) and that of $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$ versus w (c). Typical hydrogen 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. Nonbonded E---E' distances, angles and torsional angles around E and E', observed in **1**–**3**.

Compd	**3a**	**3b**	**3c**	**3d**[k]	**3e**-A[k,l]	**3e**-B[k,l]	**3f**-A[k,l]	**3f**-B[k,l]
(Z, Z')	(O, S)	(O, Se)	(O, Te)	(S, Se)	(S, Te)	(S, Te)	(Se, Te)	(Se, Te)
Temp/K[a]	103(2)	103(2)	103(2)	103(2)	103(2)	103(2)	110(2)	110(2)
r/Å[b]	2.692(1)	2.723(2)	2.748(3)	3.030(1)	3.108(1)	3.076(1)	3.1920(3)	3.1526(3)
Δr/Å[c,d]	–0.63	–0.70	–0.83	–0.67	–0.75	–0.78	–0.77	–0.81
θ_1/°[e]	117.4(1)	118.2(2)	120.5(3)	103.2(2)	100.8(2)	103.7(2)	98.04(9)	100.49(9)
θ_2/°[f]	103.54(7)	101.4(1)	95.7(1)	99.6(1)	95.0(2)	95.5(1)	95.22(8)	95.77(8)
θ_3/°[g]	101.06(8)	98.6(2)	129.2(2)	90.2(1)	101.5(1)	95.4(1)	100.45(6)	95.05(6)
θ_4/°[h]	176.34(6)	176.4(1)	163.5(1)	164.6(1)	169.0(1)	169.9(1)	171.08(6)	171.95(6)
ϕ_1/°[i]	–107.4(2)	–105.9(3)	–176.8(3)	100.0(3)	–82.8(4)	–83.6(4)	82.4(2)	–83.7(2)
ϕ_2/°[j]	–176.0(1)	–174.7(2)	–177.4(3)	–152.7(3)	–161.6(3)	–165.3(3)	161.5(2)	–165.5(2)
Structure	**AB**	**AB**	**BB**	**AB**	**AB**	**AB**	**AB**	**AB**

Compd	**1g**-A[m]	**1g**-B[m]	**1h**-A[n]	**1h**-B[n]	**1i**-A[o]	**1i**-B[o]
(Z, Z')	(O, O)	(O, O)	(S, S)	(S, S)	(Se, Se)	(Se, Se)
Temp/K[a]	RT	RT	RT	RT	103	103
r/Å[b]	2.543	2.547	2.918	2.936	3.051(4)	3.064(4)
Δr/Å[c,d]	–0.50	–0.49	–0.68	–0.66	–0.75	–0.74
ϕ_1/°[i]	–179.85	–179.34	–143.2	–142.1	–154.1(3)	136.8(3)
ϕ_2/°[j]	–179.85	–179.34	–158.3	–153.0	–138.8(3)	148.0(3)
structure	**BB**	**BB**	**CC**	**CC**	**CC**	**CC**

Compd	**2g**-A[o]	**2g**-B[o]	**2h**[o]	**2i**-A[p]	**2i**-B[p]
(Z, Z')	(O, O)	(O, O)	(S, S)	(Se, Se)	(Se, Se)
Temp/K[a]	103	103	RT	RT	RT
r/Å[b]	2.590(3)	2.604(3)	3.047(2)	3.091(1)	3.048(1)
Δr/Å[c,d]	–0.45	–0.44	–0.55	–0.71	–0.75
ϕ_1/°[i]	174.5(3)	–174.8(3)	171.9(3)	122.4(7)	–133.0(7)
ϕ_2/°[j]	94.0(4)	–93.8(4)	69.5(4)	141.8(6)	–143.2(6)
structure	**AB**	**AB**	**AB**	**CC**	**CC**

Compd	**3g**[o]	**3h**[o,q]	**3h**[o,q]	**3i**[o]	**3j**[r]
(Z, Z')	(O, O)	(S, S)	(S, S)	(Se, Se)	(Te, Te)
Temp/K[a]	103 K	RT	RT	103 K	RT
r/Å[b]	2.616(9)	3.004	3.021(2)	3.135(2)	3.287
Δr/Å[c,d]	–0.42	–0.60	–0.58	–0.67	–0.83
ϕ_1/°[i]	169.28(13)	–159.99	–152.1(4)	–154.74(16)	–124.79
ϕ_2/°[j]	–82.92(19)	–95.25	101.7(4)	109.70(16)	–132.46
structure	**AB**	**AB**	**AB**	**AB**	**CC**

[a] Temperature for measurements. [b] r(E, E'). [c] r(E, E') – Σr_{vdW}(E/E'). [d] Ref. 16 in the text. [e] $\angle C_1EC_{11}$. [f] $\angle C_9E'C_{12}$. [g] $\angle E'EC_{11}$. [h] $\angle EE'C_{12}$. [i] $\angle C_{10}C_1EC_{11}$. [j] $\angle C_{10}C_9E'C_{12}$. [k] Reexamined data in this work. [l] Ref. 20 in the text. [m] Ref. 35 in the text. [n] Ref. 36 in the text. [o] Ref. 18 in the text. [p] Refs. 15c and 37 in the text. [q] Ref. 38 in the text. [r] Ref. 39 in the text.

Table S3. Torsional angles around E for optimized structures on **4** and **5** with MP2/BSS-A[a]

Species (E)	ϕ_1[b] (°)	ϕ_2[c] (°)	ΔE_{ES}[d,e] (kJ mol^{-1})	ΔE_{ZP}[d,e] (kJ mol^{-1})	Sym-metry
4A (O)	90.0[f]	-178.4	9.6	8.0	C_1
4A (S)	77.7	-177.3	-0.7	-0.9	C_1
4A (Se)	76.2	-177.0	-3.4	-3.6	C_1
4A (Te)	71.9	-176.5	-3.7	-3.5	C_1
5A (O)	73.9	-176.4	-1.4	-3.1	C_1
5A (S)	65.7	-179.6	-5.4	-6.2	C_1
5A (Se)	63.9	-178.8	-5.7	-6.1	C_1
5A (Te)	60.5	-177.8	-4.1	-4.1	C_1
4B (O)	-179.3	-178.0	0.0	0.0	C_1
4B (S)	-179.1	-178.4	0.0	0.0	C_1
4B (Se)	-178.9	-178.3	0.0	0.0	C_1
4B (Te)	-180.0[f]	-180.0[f]	0.0	0.0	C_1
5B (O)	-157.0	-179.1	0.0	0.0	C_1
5B (S)	-170.4	-177.1	0.0	0.0	C_1
5B (Se)	-167.0	-177.0	0.0	0.0	C_1
5B (Te)	-177.8	-178.3	0.0	0.0	C_1

[a] See text for BSS-A. [b] ϕ($C_{10}C_1EC_{Me}$ or $C_{10}C_1EC_{Ph}$). [c] ϕ($C_5C_{10}C_1E$). [d] ΔE_{ES} and ΔE_{ZP} correspond to those on the energy surface and corrected with the zero-point energies, respectively. [e] ΔE(***n***: E) = E(***n***A: E) – E(***n***B: E): ***n*** = 4 and 5. [f] Fixed.

Table S4. Torsional Angles around E for optimized structures on **1a**–**1f** and **2'b** with MP2/BSS-A.[a]

Species (type)	ϕ_1[b] (°)	ϕ_2[c] (°)	ΔE_{ES}[d,e] (kJ mol^{-1})	ΔE_{ZP}[d,e] (kJ mol^{-1})	Sym-metry
1a (**AA**)	83.7	65.7	3.2	-0.1	C_1
1a (**AB**)	-95.5	-179.5	1.0	-1.0	C_1
1a (**BB**)	179.1	-177.2	0.0	0.0	C_1
1a (**BA**)	174.9	70.8	7.1	6.5	C_1
1b (**AA**)	86.1	63.36	8.1	5.2	C_1
1b (**AB**)	-102.6	178.6	2.0	0.4	C_1
1b (**BB**)	-175.7	173.7	0.0	0.0	C_1
1b (**BA**)	173.8	70.5	11.1	10.5	C_1
1c (**AA**)	95.5	56.3	15.8	13.5	C_1
1c (**AB**)	-90.0	-171.3	5.5	4.1	C_1
1c (**BB**)	168.4	-170.5	0.0	0.0	C_1
1c (**BA**)	161.9	77.4	15.5	14.8	C_1
1d (**AA**)	60.6	55.7	-9.1	-7.1	C_1
1d (**AB**)	-70.4	-163.1	-15.3	-11.9	C_1
1d (**BB**)	180.0	180.0	0.0	0.0	C_1
1d (**BA**)	163.5	63.3	-8.5	-6.4	C_1
1e (**AA**)	62.7	47.3	-7.9	-5.0	C_1
1e (**AB**)	-74.9	-159.6	-23.3	-18.8	C_1
1e (**BB**)	180.0	180.0	0.0	0.0	C_s
1e (**BA**)	162.2	52.8	-2.6	0.5	C_1
1f (**AA**)	56.4	45.5	-10.9	-7.5	C_1
1f (**AB**)	-69.8	-154.3	-26.8	-21.9	C_1
1f (**BB**)	180.0	180.0	0.0	0.0	C_s
1f (**BA**)	-138.6	103.7	-12.4	-7.1	C_1
2'b (**AA**)	77.5	81.9	-3.2	-4.9	C_1
2'b (**AB**)	81.5	175.5	0.1	-0.5	C_1
2'b (**BB**)	179.5	-179.5	0.0	0.0	C_1

[a] See text for BSS-A. [b] ϕ($C_8C_1EC_{Me}$). [c] ϕ($C_1C_8E'C_{Me'}$). [d] ΔE_{ES} and ΔE_{ZP} correspond to those on the energy surface and corrected with the zero-point energies, respectively. [e] ΔE(***n***: **XX'**) = E(***n***: **XX'**) – E(***n***: **BB**): ***n*** = **1a**–**1f** and **2'b**.

Table S5. Lengths of bond paths (BPs: r_{BP}) and the corresponding straight-line distances (R_{SL}) for E-∗-E' interactions in **1a**–**1j** and **2'b** evaluated with MP2/BSS-A, together with the differences between them ($\Delta r_{BP} = r_{BP} - R_{SL}$)[a]

Species (type)	E-∗-E'	r_{BP}[b] (Å)	R_{SL}[c] (Å)	Δr_{BP}[d] (Å)
1a (**BB**)	O-∗-S	2.64153	2.62795	0.01358
1a (**AA**)	O-∗-S	2.96195	2.95247	0.00948
1a (**AB**)	O-∗-S	2.70495	2.69377	0.01118
1a (**BA**)	O-∗-S	2.87566	2.86291	0.01275
1b (**BB**)	O-∗-Se	2.66137	2.65626	0.00511
1b (**AA**)	O-∗-Se	3.01172	3.00651	0.00521
1b (**AB**)	O-∗-Se	2.70840	2.70517	0.00323
1b (**BA**)	O-∗-Se	2.92737	2.91943	0.00794
1c (**BB**)	O-∗-Te	2.72796	2.72410	0.00386
1c (**AA**)	O-∗-Te	3.08634	3.08020	0.00614
1c (**AB**)	O-∗-Te	2.80626	2.80420	0.00206
1c (**BA**)	O-∗-Te	3.01998	3.01051	0.00947
1d (**BB**)	S-∗-Se	2.95603	2.93905	0.01698
1d (**AA**)	S-∗-Se	3.27781	3.26455	0.01326
1d (**AB**)	S-∗-Se	3.01432	3.00654	0.00778
1d (**BA**)	S-∗-Te	3.10272	3.08713	0.01559
1e (**BB**)	S-∗-Te	3.07121	3.05660	0.01461
1e (**AA**)	S-∗-Te	3.37229	3.35937	0.01292
1e (**AB**)	S-∗-Te	3.06535	3.06047	0.00488
1e (**BA**)	S-∗-Te	3.26176	3.24398	0.01778
1f (**BB**)	Se-∗-Te	3.14252	3.13246	0.01006
1f (**AA**)	Se-∗-Te	3.45650	3.44676	0.00974
1f (**AB**)	Se-∗-Te	3.15972	3.15555	0.00417
1f (**BA**)	Se-∗-Te	3.27665	3.26623	0.01042
1g (**BB**)	O-∗-O	2.53244	2.52350	0.00894
1g (**AA**)	O-∗-O	2.74698	2.74484	0.00214
1g (**AB**)	O-∗-O	2.64343	2.63823	0.00520
1h (**BB**)	S-∗-S	2.91108	2.88580	0.02528
1h (**AA**)	S-∗-S	3.21554	3.19939	0.01615
1h (**AB**)	S-∗-S	3.00800	2.98954	0.01846
1h (**CC**)	S-∗-S	2.94729	2.91663	0.03066
1i (**BB**)	Se-∗-Se	3.00925	2.99860	0.01065
1i (**AA**)	Se-∗-Se	3.34888	3.33968	0.00920
1i (**AB**)	Se-∗-Se	3.10504	3.09855	0.00649
1i (**CC**)	Se-∗-Se	3.05914	3.04497	0.01417
1j (**BB**)	Te-∗-Te	3.29066	3.28086	0.00980
1j (**AA**)	Te-∗-Te	3.59016	3.57772	0.01244
1j (**AB**)	Te-∗-Te	3.34154	3.33604	0.00550
1j (**CC**)	Te-∗-Te	3.31352	3.30057	0.01295
2'b (**BB**)	O-∗-Se	2.65331	2.64871	0.00460
2'b (**AA**)	O-∗-Se	3.01423	3.00819	0.00604
2'b (**AB**)	O-∗-Se	2.72082	2.71760	0.00322

[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] $\Delta r_{BP} = r_{BP} - R_{SL}$.

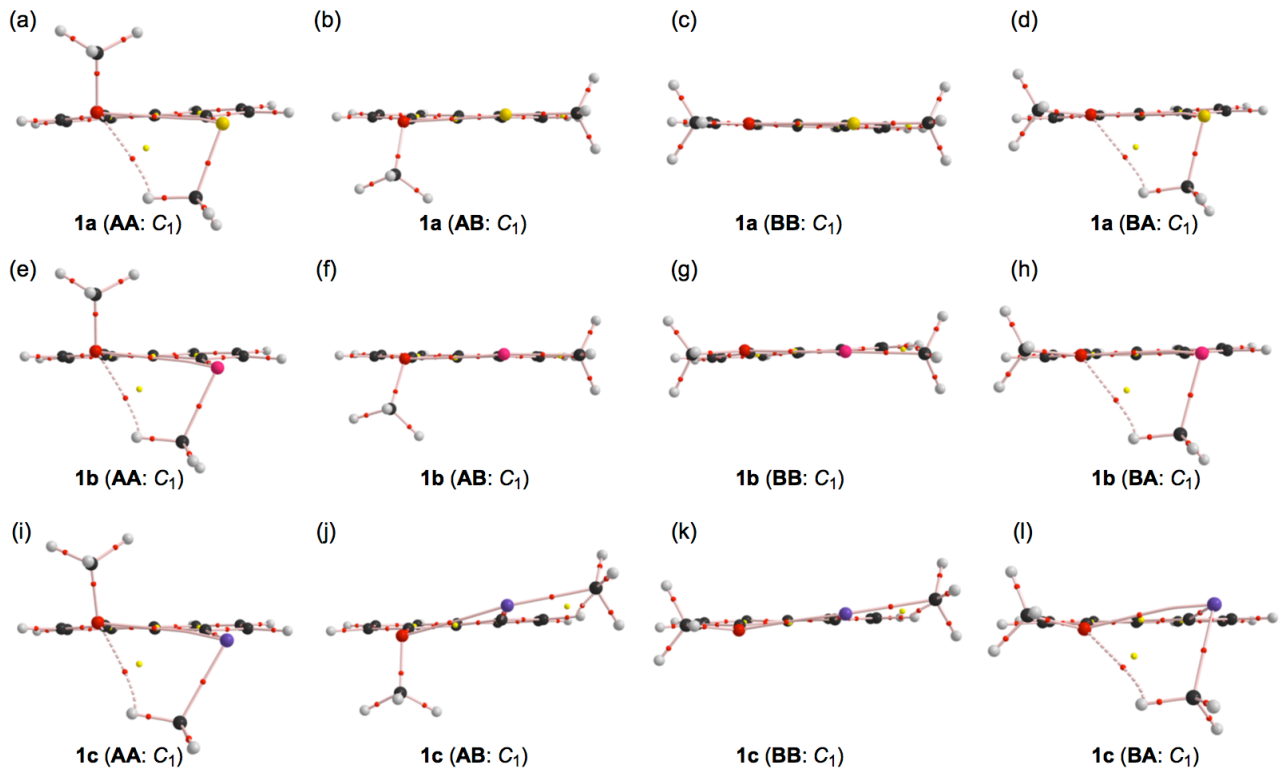


Figure S3. Molecular graphs, drawn on the optimized structures, for the conformers in **1a** (**AA**)–**1c** (**BA**), calculated with MP2/BSS-A.

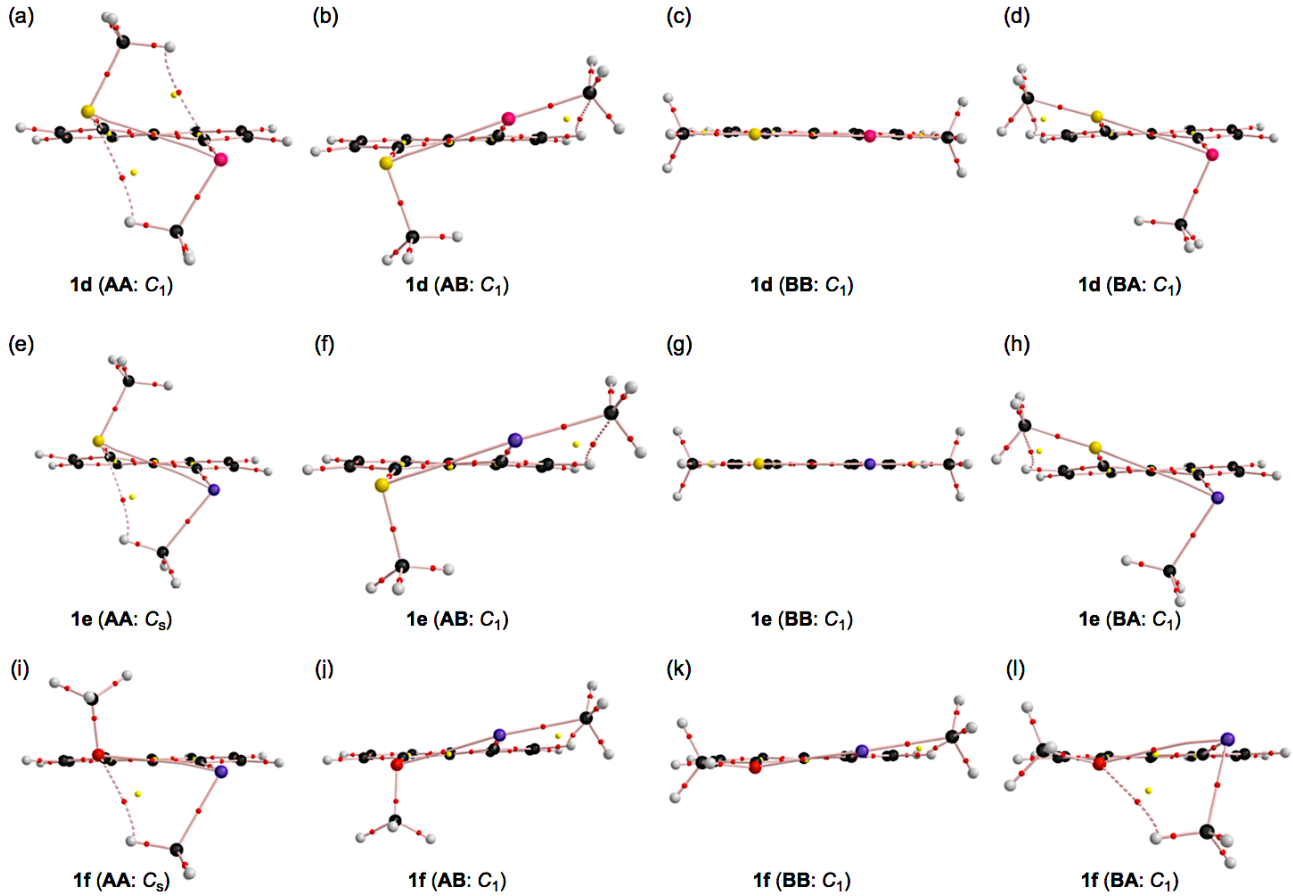


Figure S4. Molecular graphs, drawn on the optimized structures, for the conformers in **1d** (**AA**)–**1f** (**BA**), calculated with MP2/BSS-A.

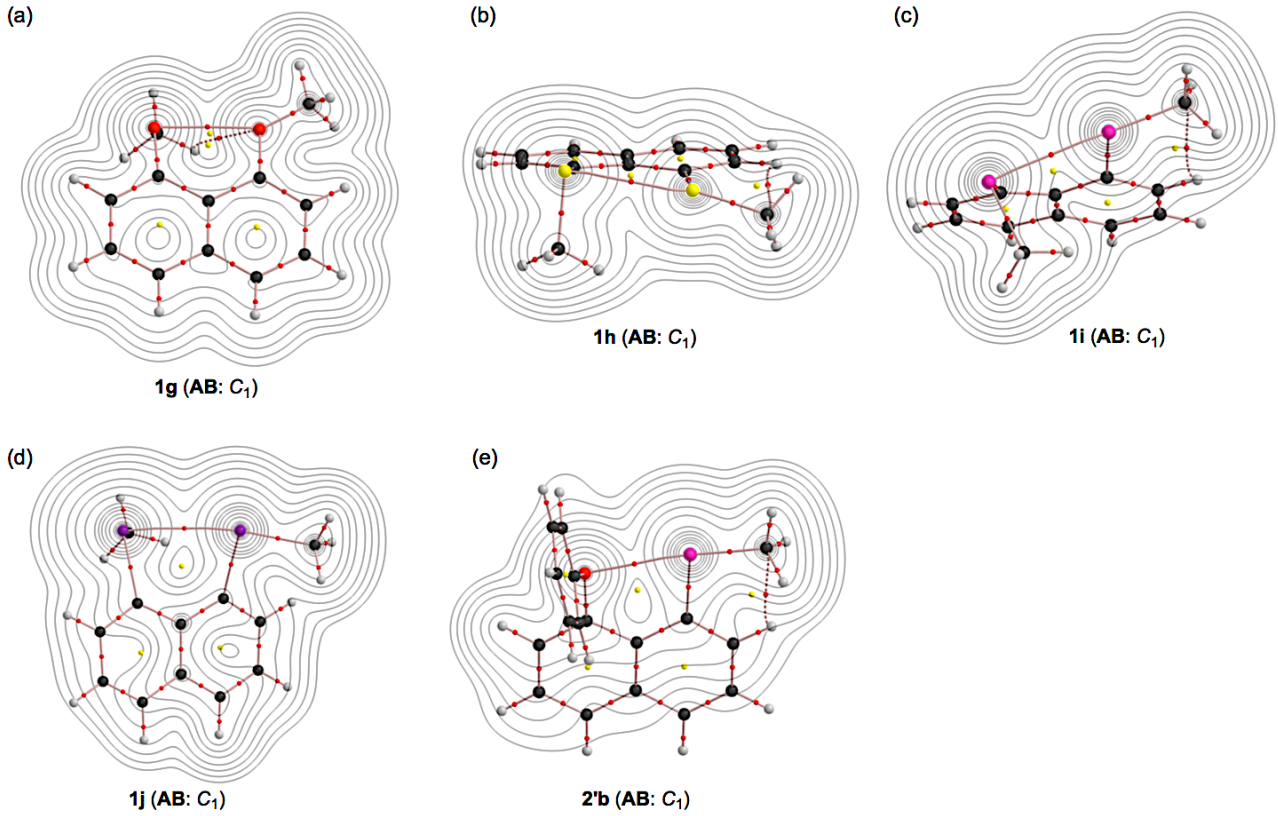


Figure S5. Molecular graphs, drawn on the optimized structures, for the conformers in **1g** (**AB**)–**1j** (**AB**) and **2'b** (**AB**), calculated with MP2/BSS-A.

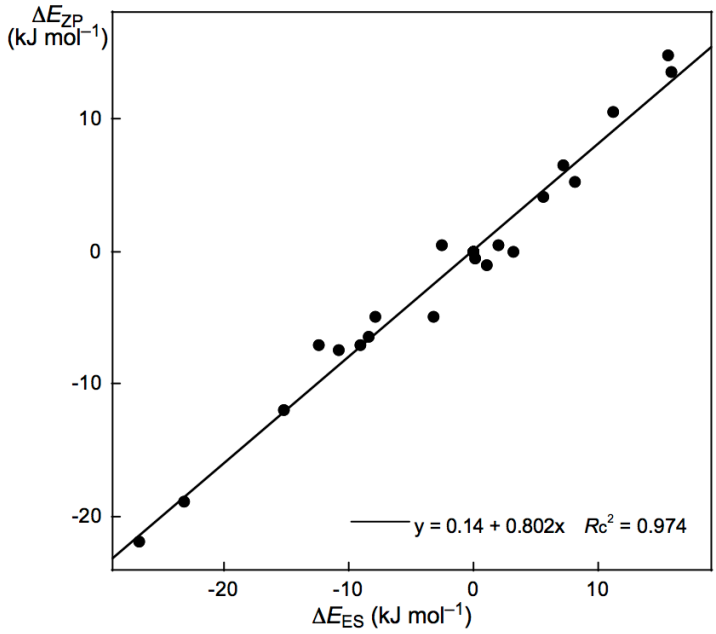


Figure S5. Plot of ΔE_{ZP} versus ΔE_{ES} for **1a**–**1j** and **2'b**, evaluated with MP2/BSS-A. Data are collected in Table S4 of the Supporting Information.

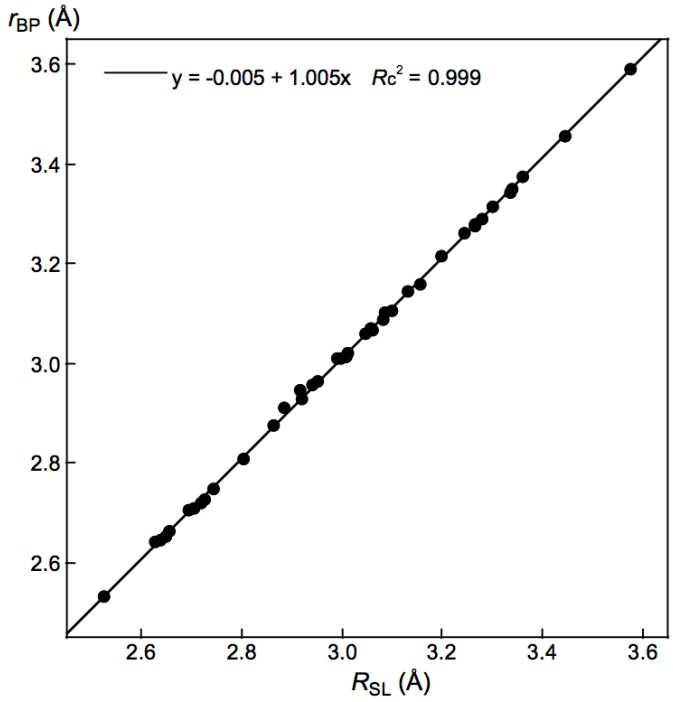


Figure S6. Plot of r_{BP} versus R_{SL} for **1a**–**1j** and **2'b** evaluated with MP2/BSS-A. Data are collected in Table S5 of the Supporting Information.

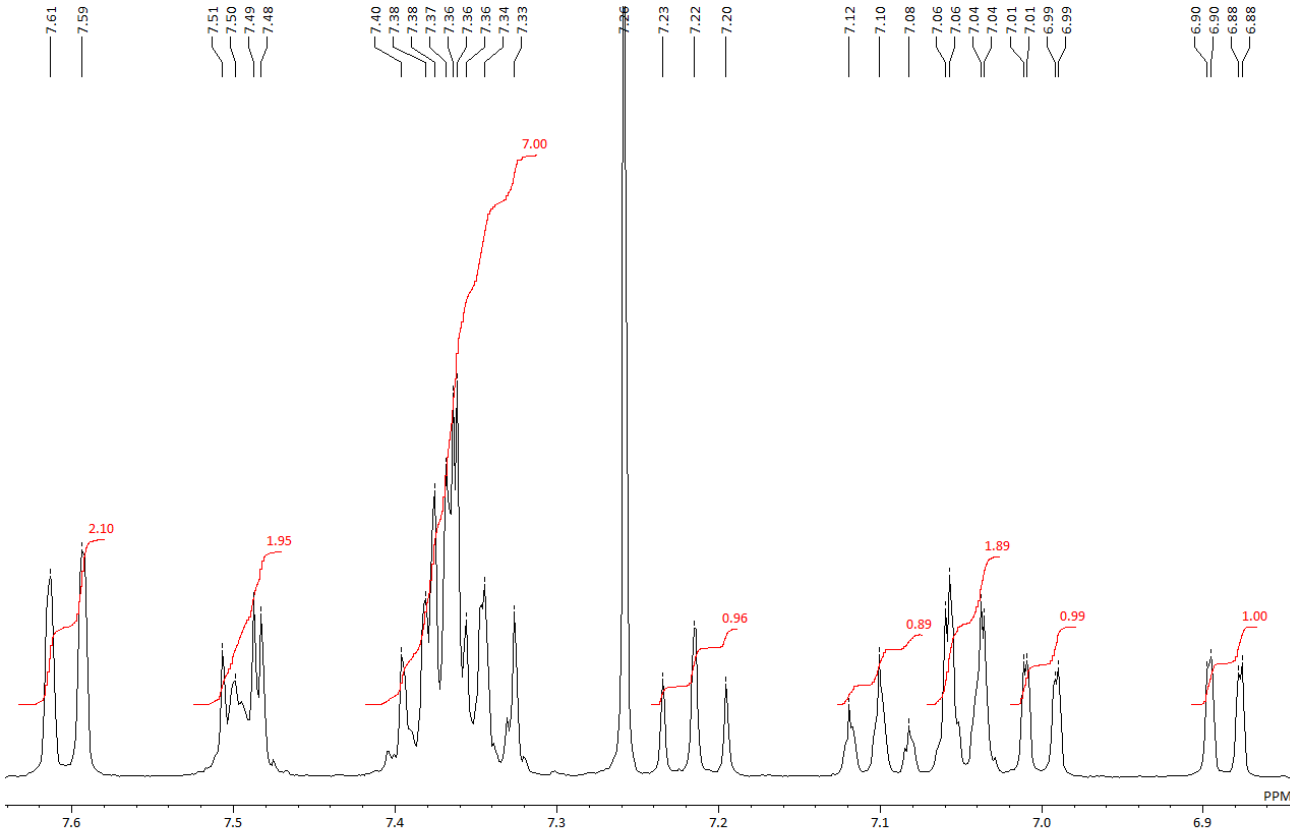


Figure S7. ^{1}H NMR spectrum of **3a** (O, S).

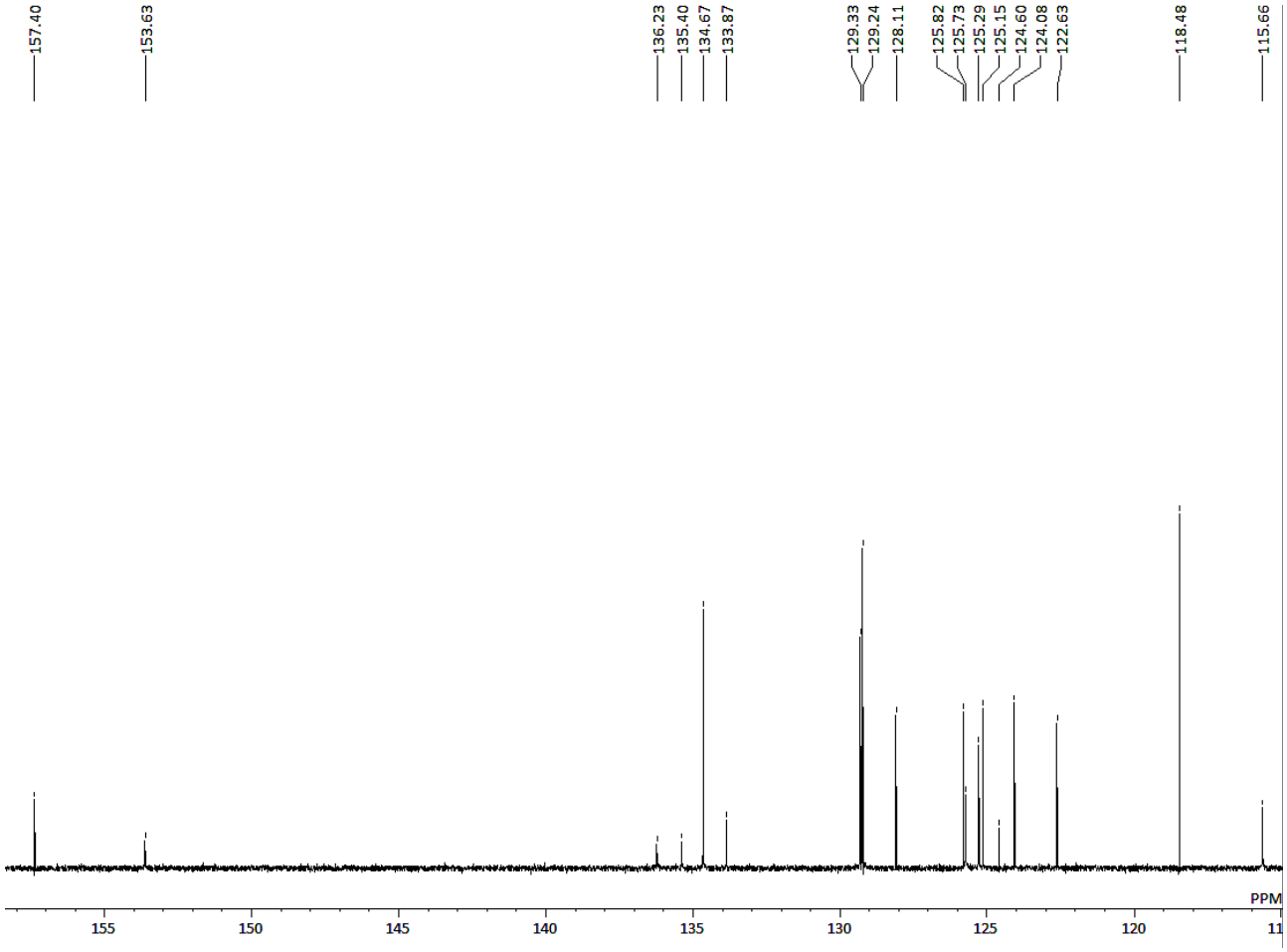


Figure S8. ^{13}C NMR spectrum of **3a** (O, S).

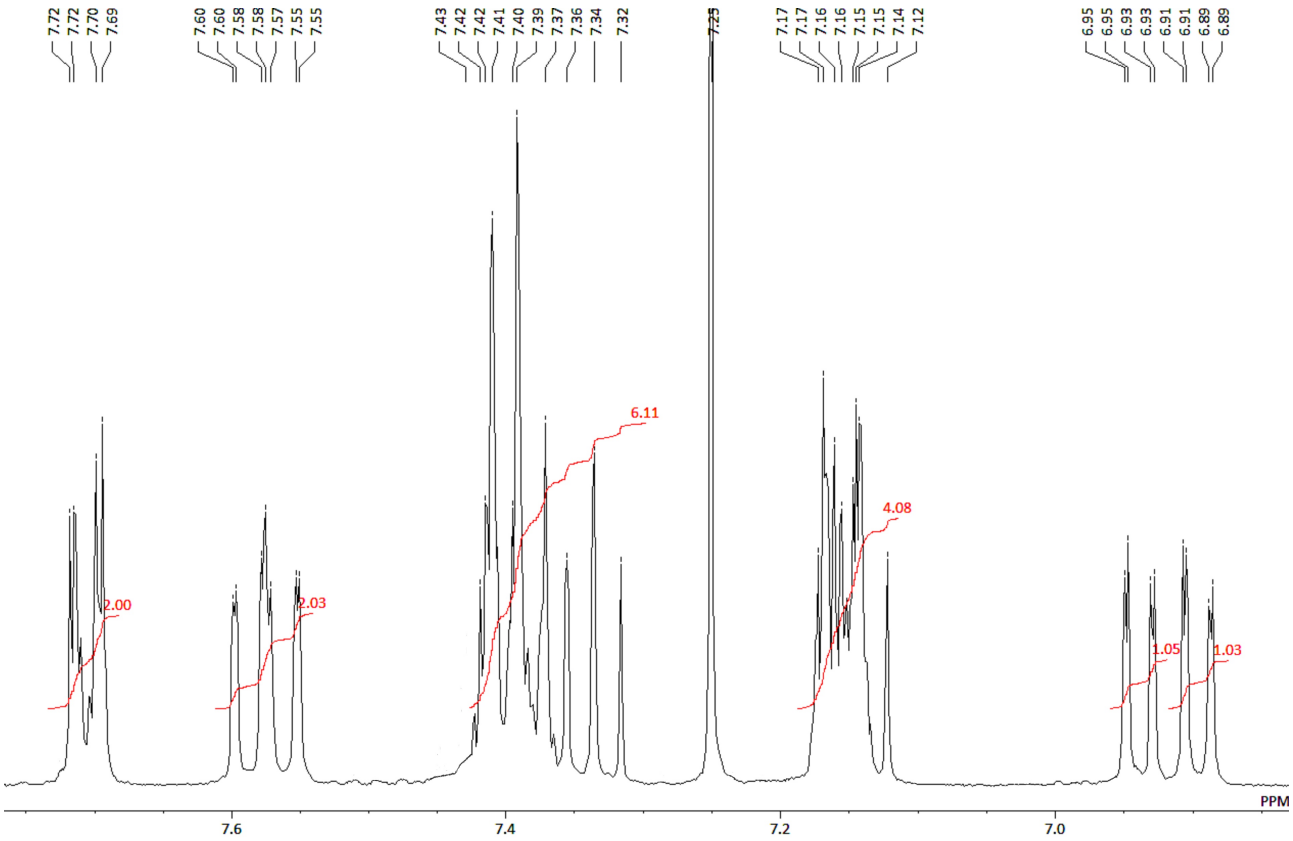


Figure S9. ^{1}H NMR spectrum of **3b** (O, Se).

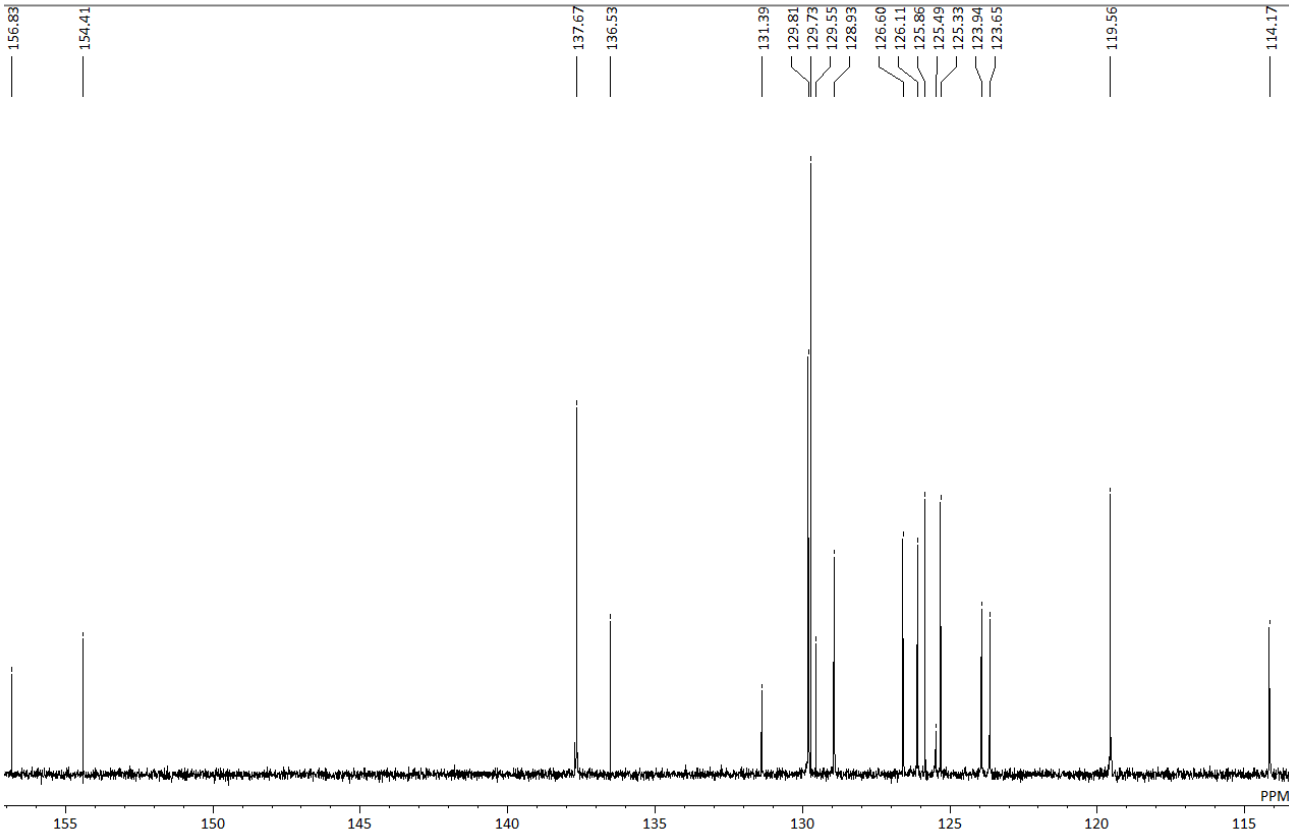


Figure S10. ^{13}C NMR spectrum of **3b** (O, Se).

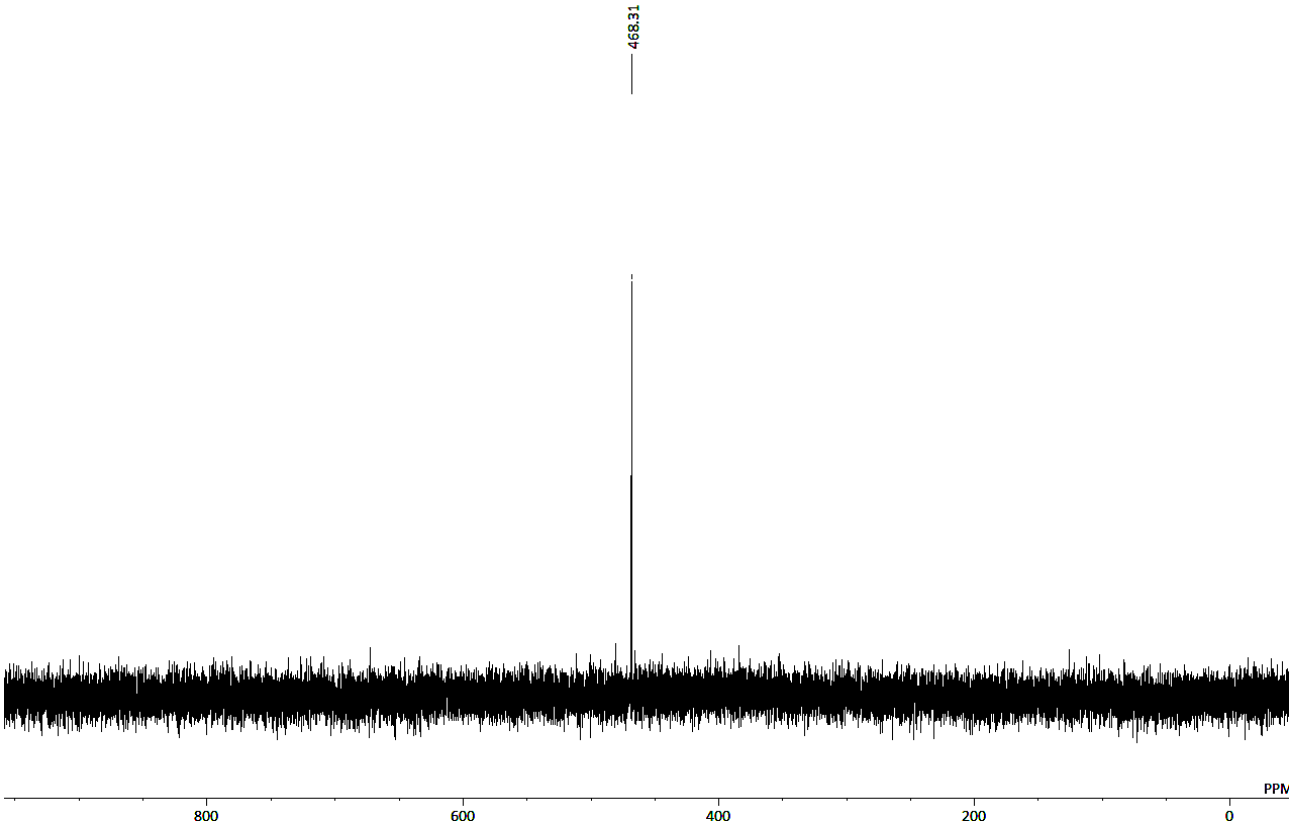


Figure S11. ^{77}Se NMR spectrum of **3b** (O, Se).

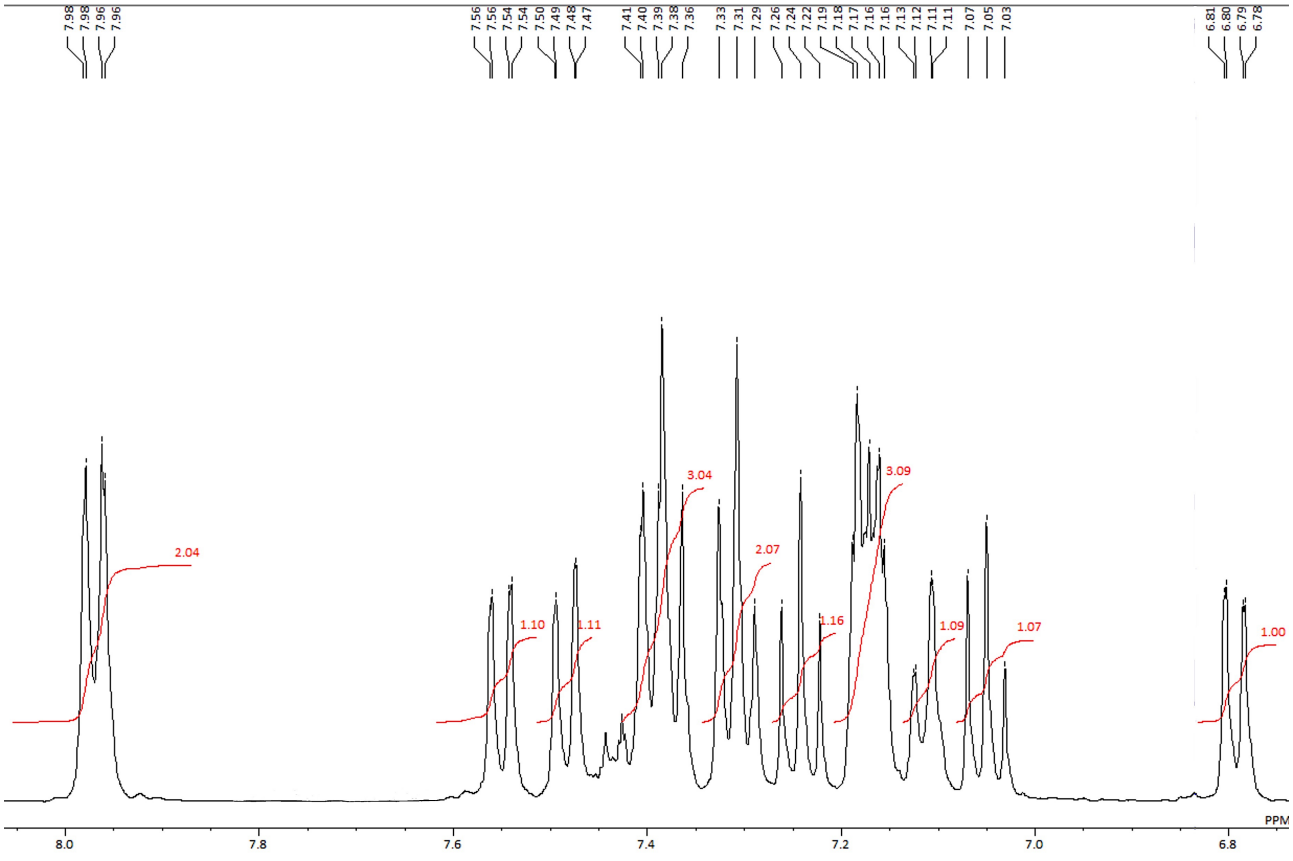


Figure S12. ^{1}H NMR spectrum of **3c** (O, Te).

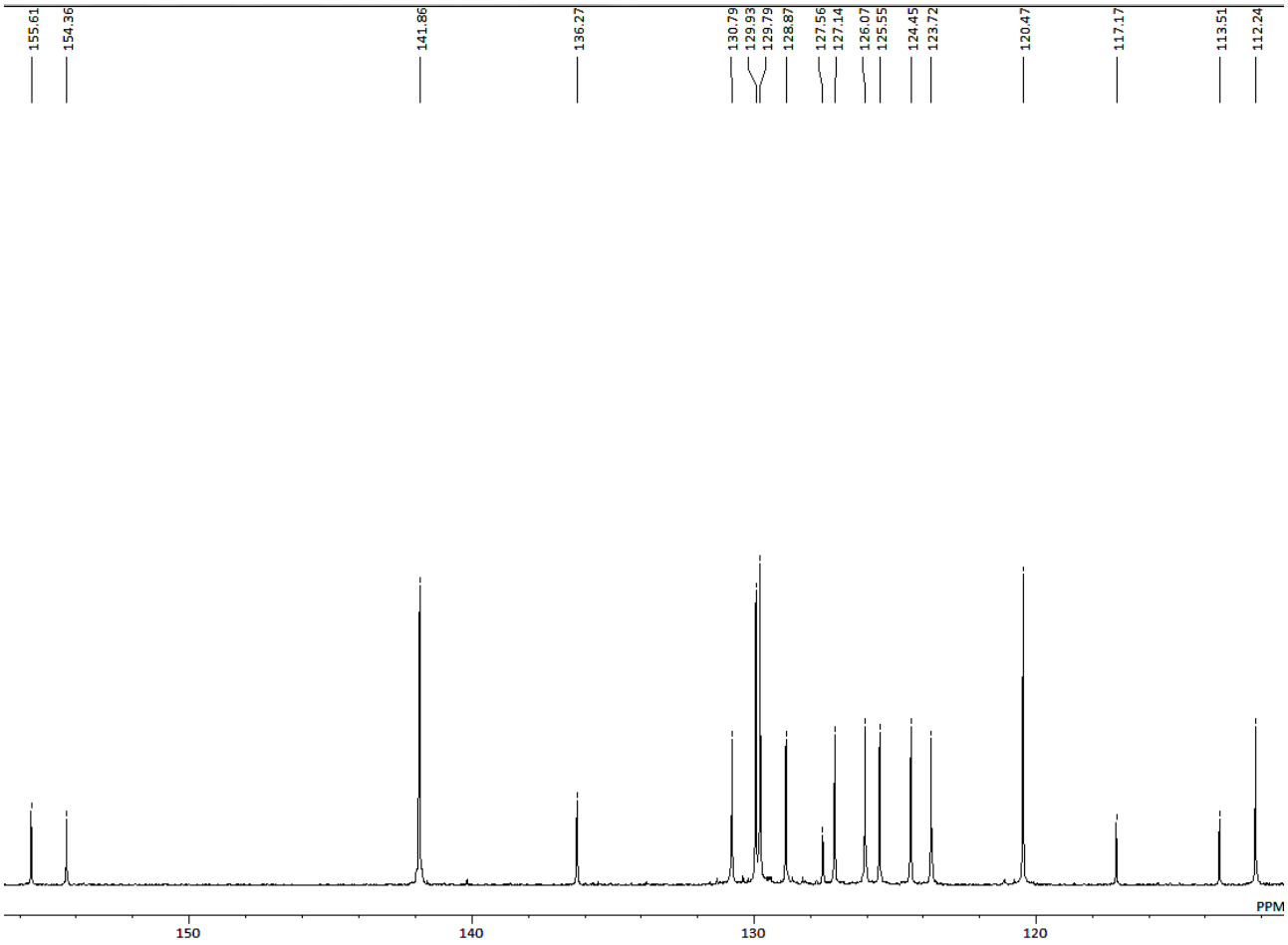


Figure S13. ^{13}C NMR spectrum of **3c** (O, Te).

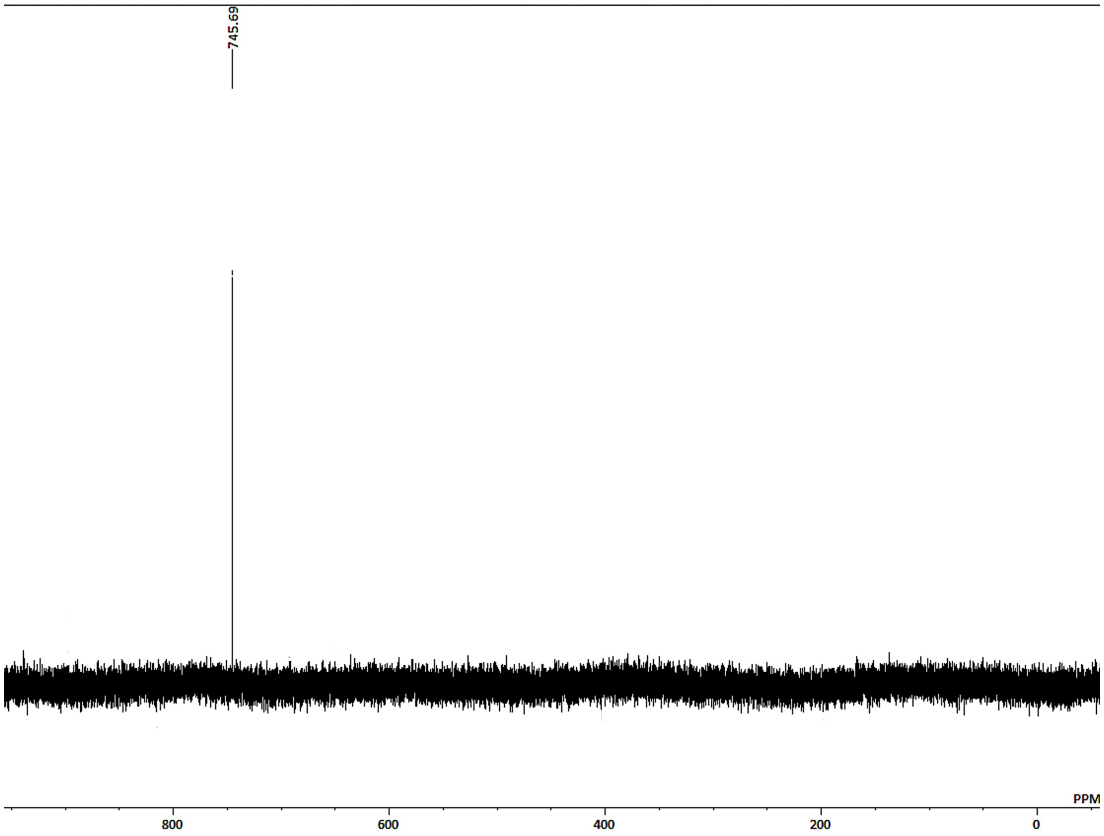


Figure S14. ^{125}Te NMR spectrum of **3c** (O, Te).

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Optimized structures given by Cartesian coordinates

Calculations were performed employing the Gaussian 09 program package. The basis sets of the (6211/311/21/2+1s1p), (63211/6111/31/2 + 1s1p1d1f), (743211/74111/721/2 + 1s1p1d1f), and (7433111/743111/7411/2 + 1s1p1d1f) types were employed for O, S, Se, and Te, respectively, implemented from Sapporo Basis Set Factory, with the 6-311G(d) basis set for C and H. The basis set system is called BSS-A, here. The Møller-Plesset second order energy correlation (MP2) level was applied to the calculations for **1a–1j** and **2'b**.

Adduct **1a** (**BB**)
Symmetry C_1
energy MP2 = –935.8832345 au
Standard orientation

6	0	0.38519	-0.31967	0.01800
6	0	1.14629	-1.54296	-0.01934
6	0	1.13141	0.90596	-0.00996
6	0	2.56685	-1.50437	0.02690
6	0	-1.05551	-0.40109	-0.01213
6	0	0.47909	-2.79490	-0.00773
6	0	2.51868	0.91260	0.03556
6	0	3.23852	-0.30270	0.02415
6	0	-1.65603	-1.66106	-0.02096
6	0	-0.89711	-2.84951	-0.03388
1	0	3.06491	1.84904	0.02283
1	0	4.32513	-0.27850	0.05704
1	0	3.11459	-2.44425	0.01255
1	0	-2.73510	-1.75229	-0.03900
1	0	-1.41216	-3.80757	-0.03438
1	0	1.07268	-3.70681	-0.01927
8	0	0.38404	2.04447	-0.02608
6	0	1.05278	3.29775	-0.03414
1	0	0.26177	4.04582	-0.05426
1	0	1.65965	3.42436	0.86832
1	0	1.68320	3.40124	-0.92335
16	0	-2.05566	1.06830	0.00678
6	0	-3.73434	0.40707	0.04278
1	0	-4.37350	1.29381	0.07266
1	0	-3.97491	-0.16539	-0.85663
1	0	-3.92285	-0.19073	0.93814

Adduct **1a** (**AA**)
Symmetry C_1
energy MP2 = –935.8820155 au
Standard orientation

6	0	0.43271	0.08046	-0.03964
6	0	1.78125	0.59616	0.05340
6	0	0.28086	-1.33894	0.08553
6	0	2.87417	-0.28297	0.27893
6	0	-0.63791	1.03305	-0.17131
6	0	2.02705	1.97832	-0.16292
6	0	1.36730	-2.16334	0.33565
6	0	2.66871	-1.63528	0.46249
6	0	-0.34216	2.38132	-0.36767
6	0	0.98611	2.85706	-0.38146
1	0	1.17909	-3.22969	0.43623
1	0	3.50715	-2.30017	0.65419
1	0	3.87568	0.13760	0.34500

1	0	-1.17212	3.07724	-0.46482
1	0	1.18003	3.91441	-0.54478
1	0	3.05348	2.33821	-0.11910
8	0	-0.94670	-1.94745	-0.06003
6	0	-1.27498	-2.19710	-1.43224
1	0	-2.27726	-2.62457	-1.43502
1	0	-1.27367	-1.26659	-2.00736
1	0	-0.55963	-2.90559	-1.86479
16	0	-2.36999	0.63869	-0.11662
6	0	-2.53588	0.07715	1.59832
1	0	-3.60459	-0.08691	1.76265
1	0	-1.99776	-0.85937	1.74683
1	0	-2.18023	0.85050	2.28265

Adduct **1a** (**AB**)
Symmetry C_1
energy MP2 = –935.8828581 au
Standard orientation

6	0	0.47897	0.19086	-0.05519
6	0	1.45943	1.24789	0.01413
6	0	0.97635	-1.13659	-0.22999
6	0	2.84426	0.93752	-0.04520
6	0	-0.91918	0.54300	-0.03407
6	0	1.04075	2.58810	0.22318
6	0	2.33324	-1.40359	-0.31434
6	0	3.27713	-0.35831	-0.24454
6	0	-1.27386	1.87628	0.16774
6	0	-0.30145	2.89327	0.28693
1	0	3.56172	1.75342	0.01793
1	0	2.64440	-2.43399	-0.46957
1	0	4.33918	-0.58123	-0.30978
1	0	1.79309	3.37141	0.29074
1	0	-2.31721	2.16657	0.20362
1	0	-0.62582	3.91920	0.44605
8	0	0.09460	-2.19455	-0.30256
6	0	-0.09126	-2.84298	0.96235
1	0	-0.84241	-3.61635	0.80313
1	0	0.84799	-3.29331	1.30071
1	0	-0.45075	-2.12815	1.70978
16	0	-2.15224	-0.70883	-0.27500
6	0	-3.69085	0.22895	-0.17710
1	0	-4.47533	-0.51698	-0.33089
1	0	-3.83442	0.69053	0.80315
1	0	-3.76247	0.98011	-0.96774

Adduct **1a** (**BA**)
Symmetry C_1
energy MP2 = –935.8805502 au
Standard orientation

6	0	-0.4607	-0.06955	-0.05958
6	0	-1.8840	-0.29668	0.04726
6	0	-0.0300	1.30373	-0.09151
6	0	-2.7788	0.78951	0.24705
6	0	0.3881	-1.22207	-0.22183
6	0	-2.4003	-1.61895	0.02170
6	0	-0.9324	2.34192	0.10950

6	0	-2.3133	2.08453	0.25179
6	0	-0.1776	-2.49769	-0.25832
6	0	-1.5687	-2.70315	-0.16379
1	0	-0.5930	3.37130	0.09787
1	0	-2.9971	2.91635	0.40267
1	0	-3.8424	0.58148	0.34092
1	0	0.4932	-3.34614	-0.36809
1	0	-1.9712	-3.71281	-0.19363
1	0	-3.4762	-1.75689	0.11260
8	0	1.3018	1.52268	-0.27214
6	0	1.7501	2.86319	-0.41898
1	0	2.8163	2.78691	-0.62765
1	0	1.2445	3.35827	-1.25442
1	0	1.5951	3.43887	0.50005
16	0	2.1609	-1.20579	-0.38888
6	0	2.6482	-0.73758	1.29233
1	0	3.7406	-0.78463	1.32319
1	0	2.3214	0.27906	1.51512
1	0	2.2366	-1.44387	2.01696

Adduct **1b** (**BB**)
Symmetry C_1
energy MP2 = –2938.2530693 au
Standard orientation

6	0	0.81885	0.30961	0.00484
6	0	1.85774	1.30775	-0.01377
6	0	1.23822	-1.06070	-0.02843
6	0	3.22269	0.91750	0.06765
6	0	-0.55401	0.73643	-0.04481
6	0	1.51322	2.68367	-0.01355
6	0	2.57682	-1.41485	0.05372
6	0	3.57449	-0.41392	0.07617
6	0	-0.83433	2.10176	-0.06906
6	0	0.19137	3.07036	-0.07502
1	0	2.87363	-2.45771	0.03845
1	0	4.61997	-0.70640	0.13745
1	0	3.98758	1.69122	0.07225
1	0	-1.85985	2.44954	-0.11114
1	0	-0.07446	4.12507	-0.08935
1	0	2.30977	3.42516	-0.01196
8	0	0.22651	-1.97065	-0.10078
6	0	0.54596	-3.35448	-0.04535
1	0	-0.41055	-3.87325	-0.08852
1	0	1.16496	-3.64821	-0.89915
1	0	1.06011	-3.59852	0.88973
34	0	-1.99848	-0.52380	0.00750
6	0	-3.50328	0.69819	0.11843
1	0	-4.37648	0.04625	0.20401
1	0	-3.44116	1.32831	1.00739
1	0	-3.60357	1.30504	-0.78299

Adduct **1b** (**AA**)
Symmetry C_1
energy MP2 = –2938.2499982 au
Standard orientation

6	0	0.802781	0.109647	-0.037294
6	0	2.073892	0.794884	0.062549

6	0	0.837878	-1.317859	0.080304
6	0	3.272278	0.062370	0.275756
6	0	-0.381470	0.915500	-0.155617
6	0	2.138423	2.198600	-0.142447
6	0	2.022218	-1.997525	0.319669
6	0	3.244896	-1.306679	0.447607
6	0	-0.264474	2.292264	-0.339241
6	0	0.991098	2.936757	-0.346829
1	0	1.973748	-3.079877	0.414051
1	0	4.163204	-1.858821	0.631091
1	0	4.210890	0.608862	0.344448
1	0	-1.174182	2.882138	-0.422539
1	0	1.045218	4.011943	-0.500062
1	0	3.109370	2.688525	-0.094360
8	0	-0.303577	-2.075123	-0.068634
6	0	-0.567364	-2.400693	-1.439011
1	0	-1.514871	-2.938440	-1.450242
1	0	-0.656282	-1.492214	-2.042493
1	0	0.234201	-3.034449	-1.834463
34	0	-2.184828	0.269904	-0.097710
6	0	-2.181793	-0.413219	1.722665
1	0	-3.213091	-0.698292	1.944653
1	0	-1.531278	-1.284361	1.785953
1	0	-1.864317	0.374944	2.406515

Adduct **1b** (**AB**)
Symmetry C_1
energy MP2 = –2938.2522937 au
Standard orientation

6	0	0.857782	0.211942	-0.034513
6	0	1.968853	1.132344	0.006139
6	0	1.172451	-1.169517	-0.203526
6	0	3.299592	0.639627	-0.054874
6	0	-0.479474	0.738516	0.000547
6	0	1.727239	2.517805	0.197122
6	0	2.479873	-1.618372	-0.289651
6	0	3.553958	-0.705594	-0.235852
6	0	-0.661028	2.107386	0.180842
6	0	0.435262	2.994356	0.263910
1	0	4.120380	1.352874	-0.009522
1	0	2.654509	-2.680780	-0.442273
1	0	4.576494	-1.068674	-0.302896
1	0	2.574102	3.199825	0.242189
1	0	-1.659193	2.528288	0.221683
1	0	0.247806	4.056358	0.406229
8	0	0.143011	-2.086169	-0.269833
6	0	-0.033608	-2.816115	0.952945
1	0	0.847328	-3.430686	1.163019
1	0	-0.212704	-2.125173	1.783114
1	0	-0.906946	-3.451254	0.806728
34	0	-1.988754	-0.422765	-0.188690
6	0	-3.424144	0.872809	-0.008684
1	0	-3.407684	1.360546	0.967545
1	0	-3.402116	1.609936	-0.813154
1	0	-4.338957	0.280987	-0.094953

Adduct **1b** (**BA**)
Symmetry C_1
energy MP2 = –2938.2488296 au
Standard orientation

6	0	-0.798236	-0.199792	-0.022995
6	0	-2.046120	-0.926652	0.041759
6	0	-0.894402	1.235361	-0.066306
6	0	-3.281665	-0.236676	0.175307
6	0	0.414927	-0.964469	-0.139130
6	0	-2.044752	-2.346058	0.049134
6	0	-2.119385	1.878454	0.064820
6	0	-3.318559	1.138925	0.156212
6	0	0.355421	-2.358897	-0.140076
6	0	-0.868622	-3.055177	-0.072190
1	0	-2.173416	2.960986	0.044309
1	0	-4.263941	1.667103	0.254203
1	0	-4.200454	-0.815823	0.237912
1	0	1.288358	-2.912642	-0.208109
1	0	-0.873941	-4.142588	-0.073664
1	0	-2.999604	-2.865210	0.110513
8	0	0.277682	1.918087	-0.178710
6	0	0.224477	3.326399	-0.360951
1	0	1.257467	3.633459	-0.519299
1	0	-0.377374	3.586950	-1.237573
1	0	-0.177249	3.828610	0.525831
34	0	2.200234	-0.275387	-0.303287
6	0	2.398965	0.416695	1.503421
1	0	3.432793	0.759066	1.595341
1	0	1.713777	1.250325	1.653793
1	0	2.211892	-0.380455	2.224133

Adduct **1c** (**BB**)
Symmetry C_1
energy MP2 = –7150.0697329 au
Standard orientation

6	0	-1.183603	0.296027	-0.016767
6	0	-2.318181	1.182375	-0.006690
6	0	-1.459038	-1.107591	-0.060622
6	0	-3.632070	0.650779	0.109146
6	0	0.139812	0.846550	-0.082059
6	0	-2.107321	2.584871	-0.009732
6	0	-2.747137	-1.604979	0.056456
6	0	-3.841446	-0.711241	0.121509
6	0	0.286605	2.233254	-0.110715
6	0	-0.829249	3.097567	-0.099746
1	0	-2.932834	-2.673400	0.031657
1	0	-4.848619	-1.111079	0.210773
1	0	-4.474463	1.338794	0.139486
1	0	1.274440	2.678182	-0.168391
1	0	-0.668719	4.173352	-0.119446
1	0	-2.970709	3.247215	0.012668
8	0	-0.355440	-1.899386	-0.199093
6	0	-0.487277	-3.303251	-0.004205
1	0	0.526188	-3.699474	-0.053734
1	0	-0.926162	-3.517100	0.975135
1	0	-1.096720	-3.749950	-0.795526
52	0	1.881079	-0.357215	0.001947
6	0	3.270430	1.260242	0.195986

1	0	4.248591	0.790923	0.331853
1	0	3.301361	1.877802	-0.702735
1	0	3.045890	1.867387	1.074410

Adduct **1c** (**AA**)
Symmetry C_1
energy MP2 = –7150.0637292 au
Standard orientation

6	0	1.14909	0.13221	0.00241
6	0	2.42231	0.81951	0.04409
6	0	1.20386	-1.29733	0.05205
6	0	3.62065	0.09774	0.29243
6	0	-0.04395	0.91793	-0.15228
6	0	2.46870	2.23196	-0.08711
6	0	2.38674	-1.97286	0.30716
6	0	3.60877	-1.27703	0.41354
6	0	0.06422	2.30375	-0.28714
6	0	1.31488	2.95836	-0.29691
1	0	2.34994	-3.05767	0.37595
1	0	4.52820	-1.82175	0.61298
1	0	4.55837	0.64786	0.34289
1	0	-0.84409	2.89566	-0.37279
1	0	1.35511	4.03973	-0.40504
1	0	3.43683	2.72853	-0.05073
8	0	0.05613	-2.04631	-0.09441
6	0	-0.13692	-2.48663	-1.44582
1	0	-1.10033	-2.99464	-1.46731
1	0	-0.15896	-1.63031	-2.12707
1	0	0.66405	-3.17427	-1.73724
52	0	-2.04148	0.20928	-0.09503
6	0	-1.93773	-0.69783	1.83597
1	0	-2.96084	-0.92764	2.14257
1	0	-1.34428	-1.60837	1.77411
1	0	-1.50002	0.01248	2.53830

Adduct **1c** (**AB**)
Symmetry C_1
energy MP2 = –7150.0676492 au
Standard orientation

6	0	1.19135	0.20525	0.01391
6	0	2.34687	1.06614	-0.02996
6	0	1.41406	-1.18926	-0.18042
6	0	3.63453	0.50699	-0.24851
6	0	-0.11261	0.78947	0.12967
6	0	2.18885	2.45283	0.22788
6	0	2.67474	-1.70524	-0.42347
6	0	3.79167	-0.84384	-0.49319
6	0	-0.21395	2.15589	0.38363
6	0	0.93083	2.98341	0.43135
1	0	4.49498	1.17313	-0.27233
1	0	2.77785	-2.77764	-0.57141
1	0	4.77949	-1.25594	-0.68361
1	0	3.06713	3.09568	0.21849
1	0	-1.18682	2.62130	0.50567
1	0	0.81048	4.04508	0.63582
8	0	0.35131	-2.06347	-0.03097
6	0	0.23605	-2.53348	1.32513
1	0	-0.66652	-3.14236	1.36233

1	0	1.11293	-3.13473	1.58501
1	0	0.14510	-1.68820	2.01426
52	0	-1.86412	-0.35207	-0.19377
6	0	-3.21581	1.30744	-0.14244
1	0	-4.19963	0.89316	-0.37837
1	0	-3.25678	1.76518	0.84682
1	0	-2.95402	2.04728	-0.90049

Adduct **1c** (**BA**)
Symmetry C_1
energy MP2 = –7150.063828 au
Standard orientation

6	0	-1.17557	-0.18621	0.01366
6	0	-2.43471	-0.89024	0.07972
6	0	-1.24369	1.24770	0.03392
6	0	-3.66337	-0.17898	0.00904
6	0	0.04016	-0.95464	0.01823
6	0	-2.45016	-2.30922	0.10866
6	0	-2.45774	1.91656	-0.04714
6	0	-3.67315	1.19749	-0.04135
6	0	-0.03889	-2.34956	0.07074
6	0	-1.27422	-3.02860	0.13914
1	0	-2.48508	3.00093	-0.03987
1	0	-4.61351	1.74026	-0.09925
1	0	-4.59553	-0.73915	0.03995
1	0	0.88321	-2.92530	0.07011
1	0	-1.29074	-4.11535	0.17653
1	0	-3.41162	-2.81878	0.14365
8	0	-0.05216	1.89958	0.11923
6	0	-0.00443	3.27416	-0.24348
1	0	1.05522	3.52416	-0.29055
1	0	-0.46619	3.43315	-1.22287
1	0	-0.49699	3.90127	0.50689
52	0	2.01438	-0.24589	-0.31615
6	0	2.34892	0.63709	1.60185
1	0	3.40226	0.92391	1.64991
1	0	1.71030	1.51113	1.71654
1	0	2.13909	-0.10006	2.37739

Adduct **1d** (**BB**)
Symmetry C_1
energy MP2 = –3260.8289424 au
Standard orientation

6	0	0.63950	0.64519	-0.00002
6	0	1.37183	1.89862	0.00000
6	0	1.43783	-0.56175	-0.00004
6	0	2.79151	1.91964	0.00000
6	0	0.80399	0.73616	-0.00001
6	0	0.69107	3.14329	0.00002
6	0	2.83125	-0.48539	-0.00004
6	0	3.51095	0.74746	-0.00002
6	0	1.41940	1.98875	0.00000
6	0	0.68378	3.18884	0.00002
1	0	3.42524	-1.39104	-0.00007
1	0	4.59837	0.76029	-0.00003
1	0	3.29642	2.88346	0.00001

1	0	2.49952	2.06410	0.00000
1	0	1.21065	4.14030	0.00003
1	0	1.27978	4.05838	0.00003
16	0	0.65990	-2.15264	-0.00008
6	0	2.03829	-3.31645	0.00004
1	0	1.56177	-4.30033	-0.00030
1	0	2.65152	-3.21919	-0.89934
1	0	2.65103	-3.21958	0.89980
34	0	1.95292	-0.80685	0.00000
6	0	3.70333	0.03604	0.00018
1	0	4.39993	-0.80643	0.00020
1	0	3.86167	0.63144	0.90103
1	0	3.86182	0.63153	-0.90059

Adduct **1d** (**AA**)
Symmetry C_1
energy MP2 = –3260.8324141 au
Standard orientation

6	0	-0.84416	0.15733	0.01462
6	0	-2.15486	0.77692	-0.02787
6	0	-0.80614	-1.27416	-0.13629
6	0	-3.29556	0.02295	-0.41164
6	0	0.27872	1.03601	0.20258
6	0	-2.31483	2.14500	0.31630
6	0	-1.95150	-1.97122	-0.52128
6	0	-3.18963	-1.32160	-0.70282
6	0	0.07203	2.37288	0.54307
6	0	-1.22298	2.92194	0.64443
1	0	-1.88290	-3.05224	-0.61912
1	0	-4.06270	-1.89362	-1.00729
1	0	-4.25948	0.52638	-0.46151
1	0	0.94049	3.01599	0.66582
1	0	-1.34787	3.96680	0.91822
1	0	-3.31579	2.57266	0.30238
16	0	0.60112	-2.29060	0.23045
6	0	0.80932	-1.93422	1.99294
1	0	1.58862	-2.61313	2.35070
1	0	1.13440	-0.90275	2.14680
1	0	-0.12167	-2.13296	2.52863
34	0	2.11498	0.58261	-0.10149
6	0	1.94931	0.00673	-1.94905
1	0	2.96692	-0.05963	-2.34198
1	0	1.46797	-0.97120	-1.99765
1	0	1.38636	0.75320	-2.51134

Adduct **1d** (**AB**)
Symmetry C_1
energy MP2 = –3260.8347631 au
Standard orientation

6	0	0.86497	0.32136	-0.04876
6	0	1.93414	1.29576	-0.00693
6	0	1.24757	-1.04481	-0.26462
6	0	3.26921	0.90439	-0.29407
6	0	0.48388	0.80100	0.10888
6	0	1.66514	2.64173	0.35423
6	0	2.56754	-1.38410	-0.55406
6	0	3.57948	-0.40363	-0.60696

6	0	0.69141	2.12331	0.50159
6	0	0.37406	3.04016	0.62540
1	0	4.04728	1.66553	-0.27229
1	0	2.80799	-2.43388	-0.70540
1	0	4.60261	-0.69011	-0.83769
1	0	1.69700	2.48634	0.68036
1	0	0.16361	4.06277	0.93045
1	0	2.48843	3.35242	0.39147
16	0	0.11315	-2.39152	-0.06311
6	0	0.05931	-2.35431	1.74398
1	0	0.90910	-2.52856	2.21863
1	0	0.48299	-1.40016	2.06615
1	0	0.74977	-3.16057	2.00698
34	0	2.01222	-0.28084	-0.32222
6	0	3.36328	1.12452	-0.41738
1	0	3.61491	1.52743	0.56511
1	0	3.05208	1.91889	-1.09863
1	0	4.24240	0.62047	-0.82795

Adduct **1d** (**BA**)
Symmetry C_1
energy MP2 = –3260.8321648 au
Standard orientation

6	0	-0.70155	-0.48804	-0.08208
6	0	-1.80286	-1.42212	0.03461
6	0	-1.01723	0.91860	0.01433
6	0	-3.10360	-0.97136	0.38144
6	0	0.60381	-1.05677	-0.27041
6	0	-1.59940	-2.80453	-0.21841
6	0	-2.30085	1.30498	0.40500
6	0	-3.33618	0.36802	0.60196
6	0	0.75686	-2.42114	-0.51390
6	0	-0.34740	-3.29708	-0.52269
1	0	-2.53556	2.35504	0.53355
1	0	-4.32198	0.71816	0.89932
1	0	-3.90624	-1.70059	0.47141
1	0	1.76243	-2.81429	-0.64262
1	0	-0.20031	-4.35551	-0.72350
1	0	-2.45495	-3.47415	-0.14964
16	0	0.15796	2.15763	-0.47682
6	0	-0.88176	3.63208	-0.63602
1	0	-0.22267	4.37614	-1.09204
1	0	-1.73044	3.45103	-1.30079
1	0	-1.22318	4.01660	0.32807
34	0	2.24297	-0.08605	-0.09076
6	0	2.05252	0.33408	1.80124
1	0	2.98808	0.80742	2.10941
1	0	1.22419	1.02985	1.94493
1	0	1.89810	-0.58626	2.36626

Adduct **1e** (**BB**)
Symmetry C_s
energy MP2 = –7472.6434694 au
Standard orientation

6	0	-1.21721	0.19635	0.00000
6	0	-2.47267	0.92554	0.00000

6	0	-1.32213	-1.24483	0.00000
6	0	-3.71840	0.24307	0.00000
6	0	0.00000	0.97561	0.00000
6	0	-2.49070	2.34330	0.00000
6	0	-2.56827	-1.87052	0.00000
6	0	-3.76734	-1.13169	0.00000
6	0	-0.08435	2.37094	0.00000
6	0	-1.31375	3.05650	0.00000
1	0	-2.63519	-2.95196	0.00000
1	0	-4.72035	-1.65548	0.00000
1	0	-4.63298	0.83264	0.00000
1	0	0.81766	2.97079	0.00000
1	0	-1.32066	4.14416	0.00000
1	0	-3.45245	2.85252	0.00000
16	0	0.14715	-2.22434	0.00000
6	0	-0.44636	-3.92762	0.00000
1	0	0.46259	-4.53459	0.00000
1	0	-1.02420	-4.15072	0.90018
1	0	-1.02420	-4.15072	-0.90018
52	0	1.99546	0.21011	0.00000
6	0	3.02162	2.08874	0.00000
1	0	4.08237	1.82195	0.00000
1	0	2.80335	2.66639	-0.89949
1	0	2.80335	2.66639	0.89949

Adduct **1e** (**AA**)
Symmetry C_1
energy MP2 = –7472.6464814 au
Standard orientation

6	0	-1.15148	0.20822	0.01254
6	0	-2.40400	0.93557	-0.06940
6	0	-1.23895	-1.22282	-0.11837
6	0	-3.58889	0.28153	-0.50078
6	0	0.04028	0.97867	0.24542
6	0	-2.45469	2.31694	0.25118
6	0	-2.42285	-1.82416	-0.54383
6	0	-3.59261	-1.07106	-0.77385
6	0	-0.06594	2.33595	0.56168
6	0	-1.31160	2.99435	0.62285
1	0	-2.44456	-2.90818	-0.62979
1	0	-4.49969	-1.56640	-1.11144
1	0	-4.50357	0.86576	-0.58617
1	0	0.84367	2.91377	0.71059
1	0	-1.35221	4.04953	0.88257
1	0	-3.41383	2.82967	0.20345
16	0	0.06461	-2.33902	0.32233
6	0	0.18362	-2.00466	2.09773
1	0	0.92455	-2.70621	2.49124
1	0	0.52759	-0.98310	2.27696
1	0	-0.78145	-2.17989	2.57839
52	0	2.04190	0.34855	-0.06841
6	0	1.73878	-0.46842	-2.01679
1	0	2.70307	-0.45911	-2.53011
1	0	1.35725	-1.48735	-1.94056
1	0	1.03687	0.17035	-2.55556

Adduct **1e** (**AB**)
Symmetry C_1
energy MP2 = –7472.6523368 au
Standard orientation

6	0	1.18810	0.33302	-0.05095
6	0	2.29908	1.25868	-0.01379
6	0	1.51329	-1.04696	-0.26559
6	0	3.60209	0.82026	-0.37289
6	0	-0.13455	0.84254	0.18482
6	0	2.08231	2.62014	0.32232
6	0	2.80392	-1.44226	-0.60659
6	0	3.85280	-0.50198	-0.68181
6	0	-0.28376	2.17794	0.56276
6	0	0.81788	3.05554	0.65907
1	0	4.41273	1.54710	-0.36869
1	0	2.99757	-2.50051	-0.76678
1	0	4.85323	-0.82495	-0.95911
1	0	2.93202	3.29983	0.34611
1	0	-1.26855	2.57125	0.79117
1	0	0.65043	4.08966	0.95207
16	0	0.31726	-2.32719	-0.01108
6	0	0.31186	-2.34755	1.80534
1	0	-0.43972	-3.08179	2.10791
1	0	1.29450	-2.64449	2.17899
1	0	0.03147	-1.36409	2.19001
52	0	-1.91336	-0.24481	-0.24456
6	0	-3.18244	1.49309	-0.30515
1	0	-4.13438	1.13479	-0.70771
1	0	-3.36005	1.91565	0.68511
1	0	-2.77402	2.24774	-0.98018

Adduct **1e** (**BA**)
Symmetry C_1
energy MP2 = –7472.6444515 au
Standard orientation

6	0	-1.03388	-0.48997	-0.08396
6	0	-2.14920	-1.40615	0.04857
6	0	-1.33929	0.91931	0.00176
6	0	-3.42836	-0.94047	0.45328
6	0	0.26191	-1.07104	-0.30800
6	0	-1.97393	-2.79042	-0.21053
6	0	-2.60015	1.32552	0.44116
6	0	-3.63897	0.40171	0.67863
6	0	0.37962	-2.44029	-0.56237
6	0	-0.74061	-3.29556	-0.56589
1	0	-2.81800	2.38016	0.56414
1	0	-4.60743	0.76252	1.01727
1	0	-4.23785	-1.65937	0.56356
1	0	1.37038	-2.86383	-0.70920
1	0	-0.61351	-4.35466	-0.77699
1	0	-2.83833	-3.44687	-0.12659
16	0	-0.17737	2.13399	-0.56796
6	0	-1.21452	3.60793	-0.74947
1	0	-0.57098	4.32795	-1.26235
1	0	-2.08905	3.40012	-1.37136
1	0	-1.51554	4.03352	0.21059
52	0	2.12372	-0.09248	-0.04716
6	0	1.70581	0.53912	1.95371

1	0	2.64789	0.87428	2.39426
1	0	0.98940	1.36150	1.93497
1	0	1.31700	-0.30823	2.51983

Adduct **1f** (**BB**)
Symmetry C_s
energy MP2 = –9475.0096778 au
Standard orientation

6	0	-1.22715	0.48919	0.00000
6	0	-2.46835	1.24681	0.00000
6	0	-1.36515	-0.94805	0.00000
6	0	-3.72911	0.59408	0.00000
6	0	0.00000	1.25256	0.00000
6	0	-2.46045	2.66503	0.00000
6	0	-2.62615	-1.54218	0.00000
6	0	-3.80943	-0.77897	0.00000
6	0	-0.05614	2.64882	0.00000
6	0	-1.27198	3.35786	0.00000
1	0	-2.72069	-2.62140	0.00000
1	0	-4.77356	-1.28209	0.00000
1	0	-4.62955	1.20509	0.00000
1	0	0.85770	3.23065	0.00000
1	0	-1.25923	4.44543	0.00000
1	0	-3.41339	3.19055	0.00000
34	0	0.16204	-2.10142	0.00000
6	0	-0.67535	-3.85350	0.00000
1	0	0.16610	-4.55037	0.00000
1	0	-1.27078	-4.00396	0.90183
1	0	-1.27078	-4.00396	-0.90183
52	0	1.97820	0.45080	0.00000
6	0	3.04817	2.30398	0.00000
1	0	4.10222	2.01268	0.00000
1	0	2.84130	2.88500	-0.89989
1	0	2.84130	2.88500	0.89989

Adduct **1f** (**AA**)
Symmetry C_1
energy MP2 = –9475.0138284 au
Standard orientation

6	0	1.18564	0.41312	0.00535
6	0	2.46988	1.08943	0.04285
6	0	1.21311	-1.00780	0.22460
6	0	3.61969	0.42057	0.54009
6	0	0.03231	1.22213	-0.28359
6	0	2.58397	2.43935	-0.37906
6	0	2.36449	-1.62715	0.70860
6	0	3.56120	-0.90795	0.90821
6	0	0.19999	2.54537	-0.70053
6	0	1.47508	3.13722	-0.81206
1	0	2.35134	-2.70464	0.85625
1	0	4.44094	-1.41581	1.29603
1	0	4.55869	0.96901	0.59279
1	0	-0.68225	3.15326	-0.88940
1	0	1.56506	4.16653	-1.15108
1	0	3.56557	2.90991	-0.36339
34	0	-0.20257	-2.20664	-0.23471

6	0	-0.31530	-1.76187	-2.12235
1	0	-0.96708	-2.51270	-2.57580
1	0	-0.75127	-0.76912	-2.24948
1	0	0.67957	-1.81591	-2.56666
52	0	-1.98774	0.72033	0.12052
6	0	-1.66482	0.01418	2.10851
1	0	-2.60710	0.11872	2.65125
1	0	-1.35032	-1.03039	2.08982
1	0	-0.90470	0.64002	2.57922

Adduct **1f** (**AB**)
Symmetry C_1
energy MP2 = –9475.0198784 au
Standard orientation

6	0	1.11843	0.66427	-0.05804
6	0	2.15566	1.67332	-0.01647
6	0	1.54925	-0.67961	-0.30554
6	0	3.47705	1.35226	-0.42768
6	0	-0.23270	1.06940	0.21741
6	0	1.84599	3.00193	0.37476
6	0	2.85618	-0.96182	-0.69258
6	0	3.82251	0.06270	-0.77897
6	0	-0.47131	2.37339	0.65452
6	0	0.56368	3.32730	0.76351
1	0	4.22753	2.14105	-0.42239
1	0	3.13899	-1.99672	-0.87044
1	0	4.83609	-0.17229	-1.09461
1	0	2.64307	3.74259	0.40205
1	0	-1.47805	2.68090	0.91732
1	0	0.32804	4.33316	1.10406
34	0	0.40890	-2.17512	0.01269
6	0	0.42825	-2.03224	1.95682
1	0	-0.21685	-2.82779	2.33695
1	0	1.44749	-2.16469	2.32237
1	0	0.02739	-1.06025	2.24977
52	0	-1.94886	-0.09650	-0.26627
6	0	-3.27294	1.59935	-0.39208
1	0	-4.17909	1.21765	-0.87145
1	0	-3.53818	1.99815	0.58832
1	0	-2.83835	2.37852	-1.02151

Adduct **1f** (**BA**)
Symmetry C_1
energy MP2 = –9475.0144161 au
Standard orientation

6	0	1.06422	0.75333	-0.02791
6	0	2.18683	1.66177	0.08890
6	0	1.37486	-0.63306	-0.24735
6	0	3.50393	1.22553	-0.21593
6	0	-0.25013	1.31055	0.13113
6	0	1.97339	3.01967	0.44431
6	0	2.67366	-1.00943	-0.58309
6	0	3.74021	-0.08584	-0.56846
6	0	-0.40625	2.65373	0.48005
6	0	0.70383	3.49790	0.69371
1	0	2.88557	-2.04854	-0.81745

1	0	4.74183	-0.41683	-0.83306
1	0	4.32259	1.93900	-0.14251
1	0	-1.41078	3.06231	0.56308
1	0	0.54824	4.53666	0.97518
1	0	2.83868	3.67427	0.53504
34	0	0.11603	-2.05328	0.05122
6	0	1.36718	-3.30648	0.89218
1	0	0.73977	-4.02689	1.42336
1	0	1.97160	-3.83486	0.15421
1	0	2.00114	-2.77273	1.60244
52	0	-2.03041	0.34789	-0.49232
6	0	-2.69318	-0.28991	1.43817
1	0	-3.72517	-0.63413	1.33570
1	0	-2.05128	-1.10093	1.78501
1	0	-2.65717	0.55735	2.12400

Adduct **1g** (**BB**)
Symmetry C_1
energy MP2 = –613.2962322 au
Standard orientation

6	0	0.00000	-0.27520	-0.03342
6	0	0.00000	-1.71312	0.02358
6	0	1.27444	0.39127	0.00190
6	0	1.22772	-2.42826	0.00024
6	0	-1.27444	0.39127	0.00192
6	0	-1.22772	-2.42826	0.00025
6	0	2.45346	-0.34461	-0.02054
6	0	2.42859	-1.75636	0.00903
6	0	-2.45346	-0.34461	-0.02053
6	0	-2.42859	-1.75636	0.00904
1	0	1.20021	-3.51549	0.02533
1	0	-1.20021	-3.51549	0.02533
1	0	3.41352	0.15774	-0.00693
1	0	3.36760	-2.30474	-0.00529
1	0	-3.41352	0.15774	-0.00690
1	0	-3.36760	-2.30474	-0.00528
8	0	1.26175	1.75495	-0.00939
6	0	2.51179	2.42658	0.01448
1	0	3.08137	2.17845	0.91664
1	0	3.10868	2.19008	-0.87305
1	0	2.26710	3.48758	0.01716
8	0	-1.26175	1.75495	-0.00935
6	0	-2.51180	2.42658	0.01444
1	0	-3.10864	2.19005	-0.87311
1	0	-3.08141	2.17848	0.91659
1	0	-2.26711	3.48758	0.01710

Adduct **1g** (**AA**)
Symmetry C_1
energy MP2 = –613.2974524 au
Standard orientation

6	0	-0.24841	0.00182	-0.03039
6	0	-1.69084	-0.01588	0.01896
6	0	0.42028	-1.26163	-0.11262
6	0	-2.38788	-1.23620	-0.19052
6	0	0.40242	1.26688	0.13098

6	0	-2.40742	1.20054	0.17781
6	0	-0.29264	-2.43025	-0.32257
6	0	-1.70415	-2.42504	-0.34753
6	0	-0.33152	2.42799	0.30963
6	0	-1.74183	2.39529	0.36540
1	0	-3.47606	-1.22386	-0.18062
1	0	-3.49494	1.16640	0.19969
1	0	0.26925	-3.35644	-0.41680
1	0	-2.24532	-3.35365	-0.51123
1	0	0.21593	3.35995	0.42854
1	0	-2.29812	3.31912	0.50349
8	0	1.79546	-1.35462	-0.08104
6	0	2.32199	-1.31122	1.25170
1	0	2.05844	-0.37248	1.74354
1	0	1.94518	-2.16230	1.82959
1	0	3.40511	-1.38075	1.15220
8	0	1.77513	1.38524	0.08303
6	0	2.28726	1.34417	-1.25497
1	0	2.05918	0.38763	-1.72956
1	0	1.86568	2.16927	-1.83962
1	0	3.36736	1.46333	-1.17044

Adduct **1g** (**AB**)
Symmetry C_1
energy MP2 = –613.2961814 au
Standard orientation

6	0	-0.25120	0.14213	-0.04278
6	0	-1.17431	1.24696	0.03174
6	0	1.15237	0.45148	-0.07012
6	0	-0.68731	2.56960	0.21701
6	0	-0.80614	-1.16503	-0.23396
6	0	-2.57347	1.00562	0.00323
6	0	1.59109	1.75642	0.11136
6	0	0.66630	2.81941	0.22878
6	0	-2.17871	-1.35472	-0.28278
6	0	-3.07105	-0.26706	-0.18906
1	0	-1.40209	3.38614	0.29377
1	0	2.65031	1.98664	0.10552
1	0	1.03760	3.83235	0.36502
1	0	-3.24865	1.85570	0.07930
1	0	-2.54068	-2.36867	-0.43511
1	0	-4.14365	-0.44052	-0.22869
8	0	2.00686	-0.60341	-0.21455
6	0	3.39241	-0.31687	-0.34369
1	0	3.79422	0.13429	0.56997
1	0	3.58006	0.34573	-1.19485
1	0	3.87081	-1.27965	-0.51603
8	0	-0.01834	-2.28778	-0.36181
6	0	0.42081	-2.80205	0.89662
1	0	1.02272	-2.06499	1.43411
1	0	-0.44227	-3.09370	1.50641
1	0	1.02857	-3.67916	0.67339

Adduct **1h** (**BB**)
Symmetry C_{2v}
energy MP2 = –1258.4606397 au

Standard orientation

6	0	0.00000	0.00000	0.59845
6	0	0.00000	0.00000	2.04919
6	0	0.00000	1.29661	-0.04785
6	0	0.00000	1.21512	2.78281
6	0	0.00000	-1.29661	-0.04785
6	0	0.00000	-1.21512	2.78281
6	0	0.00000	2.45982	0.72469
6	0	0.00000	2.42647	2.13177
6	0	0.00000	-2.45982	0.72469
6	0	0.00000	-2.42647	2.13177
1	0	0.00000	3.43030	0.24466
1	0	0.00000	3.35998	2.68970
1	0	0.00000	1.16603	3.86974
1	0	0.00000	-3.43030	0.24466
1	0	0.00000	-3.35998	2.68970
1	0	0.00000	-1.16603	3.86974
16	0	0.00000	1.44290	-1.81721
6	0	0.00000	3.22486	-2.10274
1	0	0.00000	3.32164	-3.19186
1	0	0.89930	3.70288	-1.70599
1	0	0.89930	3.70288	-1.70599
16	0	0.00000	-1.44290	-1.81721
6	0	0.00000	-3.22486	-2.10274
1	0	0.00000	-3.32164	-3.19186
1	0	0.89930	-3.70288	-1.70599
1	0	0.89930	-3.70288	-1.70599

Adduct **1h** (**AA**)
Symmetry C_2
energy MP2 = –1258.4643572 au
Standard orientation

6	0	0.00000	0.00000	0.55681
6	0	0.00000	0.00000	2.00635
6	0	0.00000	1.28739	-0.08840
6	0	-0.19865	1.20802	2.72616
6	0	0.00000	-1.28739	-0.08840
6	0	0.19865	-1.20802	2.72616
6	0	-0.20565	2.44608	0.66118
6	0	-0.34672	2.40910	2.06353
6	0	0.20565	-2.44608	0.66118
6	0	0.34672	-2.40910	2.06353
1	0	-0.19392	3.40030	0.13947
1	0	-0.50955	3.33108	2.61637
1	0	-0.22125	1.16869	3.81377
1	0	0.19392	-3.40030	0.13947
1	0	0.50955	-3.33108	2.61637
1	0	0.22125	-1.16869	3.81377
16	0	0.33411	1.56442	-1.81019
6	0	2.02149	0.91918	-1.92584
1	0	2.37742	1.17667	-2.92746
1	0	2.65862	1.39886	-1.17941
1	0	2.03262	-0.16660	-1.80897
16	0	-0.33411	-1.56442	-1.81019
6	0	-2.02149	-0.91918	-1.92584
1	0	-2.37742	-1.17667	-2.92746
1	0	-2.65862	-1.39886	-1.17941
1	0	-2.03262	0.16660	-1.80897

Adduct **1h** (**AB**)
Symmetry C_1
energy MP2 = –1258.4637719 au
Standard orientation

6	0	0.52560	0.35922	-0.10841
6	0	1.55632	1.35905	0.09221
6	0	0.96859	-1.00528	-0.21198
6	0	2.92085	0.97916	0.19517
6	0	-0.84338	0.82203	-0.15252
6	0	1.23443	2.74123	0.12296
6	0	2.32192	-1.32722	-0.10551
6	0	3.30296	-0.34401	0.12705
6	0	-1.09974	2.19454	-0.14489
6	0	-0.07437	3.15011	0.00207
1	0	3.66354	1.76105	0.34396
1	0	2.60767	-2.37044	-0.22042
1	0	4.35019	-0.62559	0.20540
1	0	-2.11784	2.55442	-0.23379
1	0	-0.32789	4.20772	0.00470
1	0	2.03501	3.46415	0.26582
16	0	-0.09787	-2.36927	-0.61521
6	0	-0.49905	-2.96883	1.04882
1	0	0.41725	-3.20550	1.59465
1	0	-1.09022	-2.22330	1.58579
1	0	-1.09085	-3.87965	0.91900
16	0	-2.21806	-0.30587	-0.18565
6	0	-3.59719	0.75757	0.31548
1	0	-3.37067	1.30012	1.23725
1	0	-3.90164	1.45102	-0.47202
1	0	-4.42136	0.06288	0.50074

Adduct **1h** (**CC**)
Symmetry C_2
energy MP2 = –1258.4623005 au
Standard orientation

6	0	0.00000	0.00000	0.56719
6	0	0.00000	0.00000	2.01373
6	0	0.00000	1.28017	-0.09123
6	0	-0.11549	1.21922	2.73257
6	0	0.00000	-1.28017	-0.09123
6	0	0.11549	-1.21922	2.73257
6	0	-0.16254	2.44605	0.65682
6	0	-0.21754	2.42115	2.06499
6	0	0.16254	-2.44605	0.65682
6	0	0.21754	-2.42115	2.06499
1	0	-0.11251	1.18640	3.82038
1	0	0.11251	-1.18640	3.82038
1	0	-0.21396	3.40386	0.14800
1	0	-0.33357	3.35224	2.61480
1	0	0.21396	-3.40386	0.14800
1	0	0.33357	-3.35224	2.61480
16	0	0.32193	1.42234	-1.83327
6	0	1.27131	2.96722	-1.89467
1	0	0.63352	3.85077	-1.82546
1	0	2.02854	2.98158	-1.10693

1	0	1.76183	2.96692	-2.87207
16	0	-0.32193	-1.42234	-1.83327
6	0	-1.27131	-2.96722	-1.89467
1	0	-0.63352	-3.85077	-1.82546
1	0	-2.02854	-2.98158	-1.10693
1	0	-1.76183	-2.96692	-2.87207

Adduct **1i** (**BB**)
Symmetry C_{2v}
energy MP2 = –5263.1951649 au
Standard orientation

6	0	0.00000	0.00000	1.08841
6	0	0.00000	0.00000	2.54154
6	0	0.00000	1.29558	0.44792
6	0	0.00000	1.21469	3.27528
6	0	0.00000	-1.29558	0.44792
6	0	0.00000	-1.21469	3.27528
6	0	0.00000	2.45894	1.21749
6	0	0.00000	2.42664	2.62484
6	0	0.00000	-2.45894	1.21749
6	0	0.00000	-2.42664	2.62484
1	0	0.00000	3.42950	0.73698
1	0	0.00000	3.35996	3.18314
1	0	0.00000	1.16496	4.36226
1	0	0.00000	-3.42950	0.73698
1	0	0.00000	-3.35996	3.18314
1	0	0.00000	-1.16496	4.36226
34	0	0.00000	1.49930	-1.46037
6	0	0.00000	3.43343	-1.63312
1	0	0.00000	3.60306	-2.71284
1	0	-0.90100	3.87186	-1.20064
1	0	0.90100	3.87186	-1.20064
34	0	0.00000	-1.49930	-1.46037
6	0	0.00000	-3.43343	-1.63312
1	0	0.00000	-3.60306	-2.71284
1	0	0.90100	-3.87186	-1.20064
1	0	-0.90100	-3.87186	-1.20064

Adduct **1i** (**AA**)
Symmetry C_2
energy MP2 = –5263.198665 au
Standard orientation

6	0	0.00000	0.00000	1.03162
6	0	0.00000	0.00000	2.48299
6	0	0.00000	1.28767	0.39125
6	0	-0.21996	1.20421	3.20215
6	0	0.00000	-1.28767	0.39125
6	0	0.21996	-1.20421	3.20215
6	0	-0.22325	2.44416	1.13812
6	0	-0.38164	2.40321	2.53883
6	0	0.22325	-2.44416	1.13812
6	0	0.38164	-2.40321	2.53883
1	0	-0.20343	3.40342	0.62593
1	0	-0.56145	3.32271	3.09063
1	0	-0.24494	1.16434	4.28975
1	0	0.20343	-3.40342	0.62593

1	0	0.56145	-3.32271	3.09063
1	0	0.24494	-1.16434	4.28975
34	0	0.43960	1.61093	-1.44331
6	0	2.19132	0.77242	-1.44958
1	0	2.67796	1.08511	-2.37676
1	0	2.76574	1.12948	-0.59352
1	0	2.09107	-0.31413	-1.43190
34	0	-0.43960	-1.61093	-1.44331
6	0	-2.19132	-0.77242	-1.44958
1	0	-2.67796	-1.08511	-2.37676
1	0	-2.76574	-1.12948	-0.59352
1	0	-2.09107	0.31413	-1.43190

Adduct **1i** (**AB**)
Symmetry C_1
energy MP2 = –5263.2008851 au
Standard orientation

6	0	0.83726	0.65033	-0.05038
6	0	1.86247	1.67244	-0.00806
6	0	1.27875	-0.69231	-0.29224
6	0	3.20808	1.34909	-0.32690
6	0	-0.52766	1.07434	0.12782
6	0	1.54303	2.99554	0.39510
6	0	2.60775	-0.96539	-0.60861
6	0	3.57012	0.06345	-0.67395
6	0	-0.78530	2.37390	0.56386
6	0	0.24208	3.33131	0.70109
1	0	3.95046	2.14510	-0.30572
1	0	2.90267	-1.99946	-0.77038
1	0	4.60057	-0.17242	-0.92848
1	0	-1.80374	2.68701	0.76433
1	0	-0.00544	4.33451	1.04072
1	0	2.33624	3.73954	0.43577
34	0	0.15836	-2.21657	-0.02563
6	0	-0.02673	-2.01243	1.90329
1	0	0.95928	-2.02986	2.36970
1	0	-0.55158	-1.08165	2.12505
1	0	-0.62079	-2.86109	2.25096
34	0	-2.02145	-0.03797	-0.34680
6	0	-3.38487	1.35169	-0.50608
1	0	-3.70346	1.73698	0.46384
1	0	-3.03918	2.15978	-1.15371
1	0	-4.22983	0.84402	-0.97907

Adduct **1i** (**CC**)
Symmetry C_2
energy MP2 = –5263.1998938 au
Standard orientation

6	0	0.00000	0.00000	1.03345
6	0	0.00000	0.00000	2.47902
6	0	0.00000	1.27194	0.37309
6	0	-0.13831	1.22153	3.19060
6	0	0.00000	-1.27194	0.37309
6	0	0.13831	-1.22153	3.19060
6	0	-0.18406	2.44121	1.10626
6	0	-0.25797	2.41946	2.51577

6	0	0.18406	-2.44121	1.10626
6	0	0.25797	-2.41946	2.51577
1	0	-0.14373	1.19540	4.27880
1	0	0.14373	-1.19540	4.27880
1	0	-0.23562	3.39423	0.58553
1	0	-0.39350	3.34983	3.06237
1	0	0.23562	-3.39423	0.58553
1	0	0.39350	-3.34983	3.06237
34	0	0.44915	1.45473	-1.48316
6	0	1.80935	2.83907	-1.24652
1	0	1.35961	3.81332	-1.05419
1	0	2.47660	2.55442	-0.43167
1	0	2.36640	2.87612	-2.18605
34	0	-0.44915	-1.45473	-1.48316
6	0	-1.80935	-2.83907	-1.24652
1	0	-1.35961	-3.81332	-1.05419
1	0	-2.47660	-2.55442	-0.43167
1	0	-2.36640	-2.87612	-2.18605

Adduct **1j** (**BB**)
Symmetry C_{2v}
energy MP2 = –13686.8213291 au
Standard orientation

6	0	0.00000	0.00000	1.46703
6	0	0.00000	0.00000	2.92320
6	0	0.00000	1.29663	0.83018
6	0	0.00000	1.21228	3.66033
6	0	0.00000	-1.29663	0.83018
6	0	0.00000	-1.21228	3.66033
6	0	0.00000	2.45786	1.60632
6	0	0.00000	2.42577	3.01344
6	0	0.00000	-2.45786	1.60632
6	0	0.00000	-2.42577	3.01344
1	0	0.00000	3.43154	1.13107
1	0	0.00000	3.35842	3.57292
1	0	0.00000	1.15880	4.74726
1	0	0.00000	-3.43154	1.13107
1	0	0.00000	-3.35842	3.57292
1	0	0.00000	-1.15880	4.74726
52	0	0.00000	1.64043	-1.27174
6	0	0.00000	3.78040	-1.22898
1	0	0.00000	4.07733	-2.28112
1	0	-0.90067	4.16543	-0.74898
1	0	0.90067	4.16543	-0.74898
52	0	0.00000	-1.64043	-1.27174
6	0	0.00000	-3.78040	-1.22898
1	0	0.00000	-4.07733	-2.28112
1	0	0.90067	-4.16543	-0.74898
1	0	-0.90067	-4.16543	-0.74898

Adduct **1j** (**AA**)
Symmetry C_2
energy MP2 = –13686.8262908 au
Standard orientation

6	0	0.00000	0.00000	1.39147
6	0	0.00000	0.00000	2.84394

6	0	1.26091	0.25683	0.75016
6	0	1.22451	-0.00632	3.56136
6	0	-1.26091	-0.25683	0.75016
6	0	-1.22451	0.00632	3.56136
6	0	2.44048	0.24485	1.49815
6	0	2.43194	0.05219	2.89527
6	0	-2.44048	-0.24485	1.49815
6	0	-2.43194	-0.05219	2.89527
1	0	3.38304	0.46283	1.00046
1	0	3.37019	0.03356	3.44462
1	0	1.19166	-0.04367	4.64896
1	0	-3.38304	-0.46283	1.00046
1	0	-3.37019	-0.03356	3.44462
1	0	-1.19166	0.04367	4.64896
52	0	1.50952	0.95988	-1.23020
6	0	0.00000	2.46491	-1.12333
1	0	0.26209	3.24767	-1.83856
1	0	-0.97323	2.03535	-1.36748
1	0	-0.00133	2.87890	-0.11357
52	0	-1.50952	-0.95988	-1.23020
6	0	0.00000	-2.46491	-1.12333
1	0	-0.26209	-3.24767	-1.83856
1	0	0.97323	-2.03535	-1.36748
1	0	0.00133	-2.87890	-0.11357

Adduct **1j** (**AB**)
Symmetry C_1
energy MP2 = –13686.8308478 au
Standard orientation

6	0	-0.76277	1.18189	-0.06919
6	0	-1.43282	2.46443	-0.01234
6	0	0.63299	1.14183	0.27093
6	0	-0.75847	3.60475	0.49862
6	0	-1.57502	0.04856	-0.40355
6	0	-2.75606	2.59693	-0.51054
6	0	1.23086	2.27399	0.82616
6	0	0.53261	3.49309	0.96945
6	0	-2.87736	0.21676	-0.87334
6	0	-3.45923	1.49909	-0.96436
1	0	2.26926	2.23729	1.14042
1	0	1.03913	4.35163	1.40480
1	0	-1.28889	4.55428	0.54154
1	0	-3.47383	-0.66103	-1.11045
1	0	-4.47004	1.60960	-1.34962
1	0	-3.22093	3.58139	-0.49382
52	0	1.96649	-0.41579	-0.31433
6	0	3.65230	0.91958	-0.50759
1	0	4.39135	0.36865	-1.09614
1	0	3.35630	1.81889	-1.05122
1	0	4.09176	1.17813	0.45672
52	0	-0.98635	-1.92677	0.04188
6	0	-0.91912	-1.55778	2.14966
1	0	-0.68002	-2.50252	2.64302
1	0	-0.13717	-0.82496	2.35422
1	0	-1.89187	-1.19644	2.48438

Adduct **1j** (**CC**)
Symmetry C_1
energy MP2 = –13686.8313053 au
Standard orientation

6	0	-0.00515	1.38614	0.00571
6	0	-0.00149	2.83206	-0.00897
6	0	-1.19963	0.72284	-0.42557
6	0	-1.11318	3.54223	-0.53614
6	0	1.19863	0.72829	0.41970
6	0	1.09576	3.54613	0.54304
6	0	-2.24792	1.45645	-0.97842
6	0	-2.19920	2.86618	-1.05398
6	0	2.24055	1.46466	0.98079
6	0	2.19028	2.87477	1.04868
1	0	-3.13191	0.93601	-1.34103
1	0	-3.03434	3.41201	-1.48693
1	0	-1.08195	4.63045	-0.54506
1	0	3.12954	0.94829	1.33690
1	0	3.01728	3.42324	1.49378
1	0	1.06523	4.63441	0.54192
52	0	-1.64732	-1.29326	0.05533
6	0	-3.39443	-0.71520	1.17097
1	0	-3.72938	-1.59423	1.72734
1	0	-3.11912	0.07753	1.86788
1	0	-4.18945	-0.37975	0.50470
52	0	1.65136	-1.28764	-0.05599
6	0	3.40243	-0.70656	-1.16403
1	0	3.73910	-1.58418	-1.72157
1	0	3.12956	0.08797	-1.85986
1	0	4.19543	-0.37302	-0.49440

Adduct **2'b** (**BB**)
Symmetry C_1
energy MP2 = –3129.4526195 au
Standard orientation

6	0	-1.16748	0.92553	0.00001
6	0	-1.90331	2.16547	0.00001
6	0	0.25745	1.03123	0.00001
6	0	-1.21161	3.40726	0.00003
6	0	-1.89226	-0.31750	-0.00001
6	0	-3.32167	2.14029	0.00001
6	0	0.91531	2.25031	0.00002
6	0	0.16666	3.44766	0.00003
6	0	-3.28562	-0.28098	-0.00001
6	0	-3.99667	0.93827	-0.00001
1	0	-1.79170	4.32770	0.00003
1	0	2.00046	2.27985	0.00003
1	0	0.68890	4.40132	0.00004
1	0	-3.86484	3.08324	0.00001
1	0	-3.85827	-1.20105	-0.00002
1	0	-5.08426	0.91780	-0.00001
34	0	-0.98172	-2.00581	-0.00003
6	0	-2.50905	-3.20432	-0.00005
1	0	-3.11594	-3.08420	0.89899
1	0	-3.11594	-3.08417	-0.89909
1	0	-2.06857	-4.20467	-0.00007
8	0	0.92793	-0.17035	0.00001
6	0	2.31405	-0.15845	0.00001

6	0	2.99125	-0.18963	-1.22039
6	0	2.99124	-0.18965	1.22042
6	0	4.38924	-0.24020	-1.21310
6	0	4.38923	-0.24022	1.21314
6	0	5.08797	-0.2644	0.00002
1	0	2.42063	-0.1771	-2.14533
1	0	2.42061	-0.17714	2.14535
1	0	4.93088	-0.26894	-2.15507
1	0	4.93086	-0.26898	2.15511
1	0	6.17375	-0.30732	0.00003

Adduct **2'b** (**AA**)
Symmetry C_1
energy MP2 = –3129.4543488 au
Standard orientation

6	0	1.37913	0.30931	0.08462
6	0	2.67390	0.86170	-0.25458
6	0	0.52879	1.14620	0.87322
6	0	3.04647	2.15725	0.19463
6	0	1.08882	-1.03190	-0.34085
6	0	3.54319	0.14421	-1.11843
6	0	0.92577	2.39761	1.31324
6	0	2.20452	2.90034	0.99730
6	0	1.98111	-1.69446	-1.18224
6	0	3.20290	-1.11040	-1.58006
1	0	4.02759	2.54016	-0.07947
1	0	0.21901	2.97329	1.90574
1	0	2.50112	3.88573	1.34728
1	0	4.50121	0.58929	-1.38118
1	0	1.74104	-2.70857	-1.49244
1	0	3.87201	-1.65613	-2.24105
34	0	-0.47425	-2.03458	0.12612
6	0	-0.11851	-2.20977	2.03176
1	0	0.86274	-2.66117	2.18402
1	0	-0.18462	-1.23305	2.51048
1	0	-0.89222	-2.87194	2.42851
8	0	-0.74405	0.74697	1.23942
6	0	-1.74736	0.90394	0.29800
6	0	-1.52205	1.37688	-0.99776
6	0	-3.02691	0.53086	0.72107
6	0	-2.60843	1.46617	-1.87873
6	0	-4.09726	0.62684	-0.16901
6	0	-3.89205	1.08882	-1.47581
1	0	-0.52734	1.67048	-1.31955
1	0	-3.15837	0.1656	1.73631
1	0	-2.43947	1.83042	-2.88928
1	0	-5.09204	0.33427	0.15796
1	0	-4.72575	1.15997	-2.16884

Adduct **2'b** (**AB**)
Symmetry C_1
energy MP2 = –3129.4565006 au
Standard orientation

6	0	1.38429	-0.56867	-0.15606
6	0	2.57055	-1.32183	0.17838
6	0	0.30701	-1.30696	-0.72329

6	0	2.58270	-2.73325	0.01883
6	0	1.39135	0.85829	0.02052
6	0	3.68646	-0.65644	0.74937
6	0	0.34705	-2.68013	-0.88862
6	0	1.50356	-3.40121	-0.52773
6	0	2.51944	1.46099	0.57238
6	0	3.66628	0.71203	0.91723
1	0	3.48372	-3.27852	0.29334
1	0	-0.51870	-3.17286	-1.32463
1	0	1.53095	-4.48019	-0.65699
1	0	4.57062	-1.23563	1.00819
1	0	2.55092	2.53494	0.71740
1	0	4.52412	1.22509	1.34634
34	0	-0.14010	1.90354	-0.44623
6	0	0.45060	3.64413	0.17569
1	0	0.65760	3.63404	1.24734
1	0	1.31466	4.00284	-0.38622
1	0	-0.39756	4.30572	-0.01764
8	0	-0.82798	-0.63193	-1.14162
6	0	-1.94090	-0.69572	-0.31586
6	0	-1.87599	-1.10424	1.01949
6	0	-3.13675	-0.24736	-0.88384
6	0	-3.04827	-1.08064	1.78506
6	0	-4.29526	-0.22698	-0.10385
6	0	-4.2556	-0.64105	1.23347
1	0	-0.93567	-1.43092	1.45377
1	0	-3.1377	0.07132	-1.92283
1	0	-3.00745	-1.39723	2.82447
1	0	-5.22872	0.1168	-0.54249
1	0	-5.15853	-0.62618	1.83757