Supporting Information

The Nature of G---E–Y σ(3c–4e) in *o*-Me$_n$GCH$_2$C$_6$H$_4$EY (Me$_n$G = Me$_2$N and MeE; E = O, S, Se and Te; Y = F, Cl, Br, EMe and Me) with Contributions from CT and Compliance Constants in Noncovalent G---E Interactions†

Satoko Hayashi,*[1] Taro Nishide,[1] Waro Nakanishi,*[1] Luca Sancineto[2] and Claudio Santi*[3]

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

[2]*Department of Heteroorganic Chemistry, Center of Molecular and Macromolecular Studies of the Polish Academy of Sciences, Lódz (Poland)*

[3]*Dipartimento di Chimica e Tecnologia del Farmaco, Università degli Studi di Perugia, Via del Liceo 1, 06123 Perugia (Italy) E-mail: claudio.santi@unipg.it; Tel: +39 075 5855102*

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.

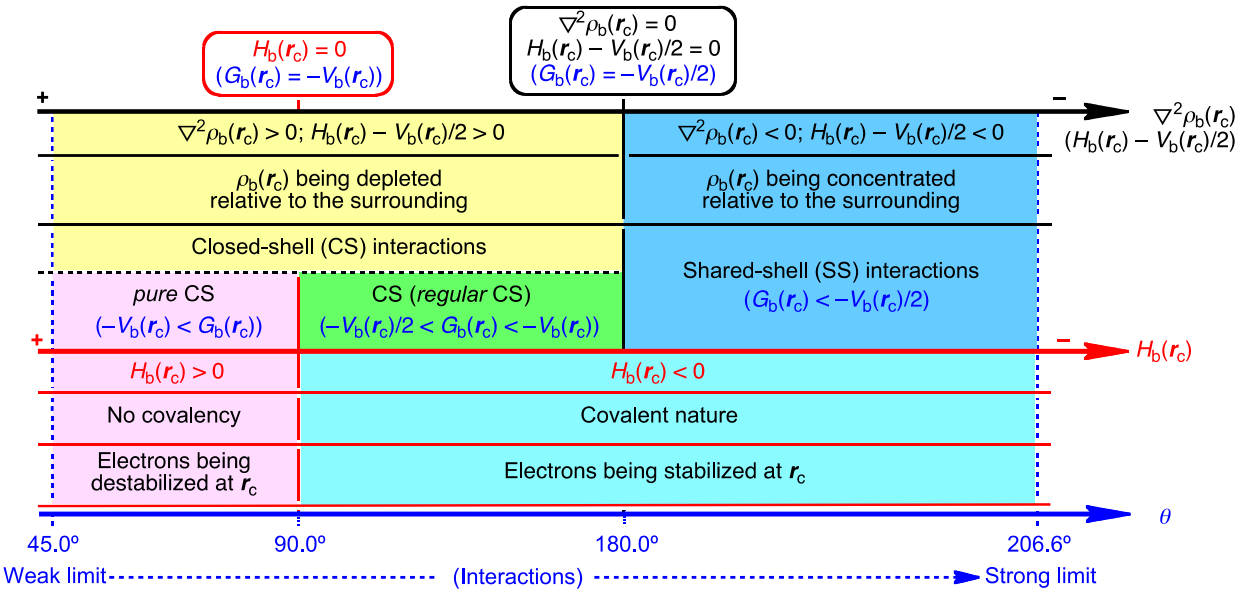
The sign of the Laplacian $\rho_b(\boldsymbol{r}_c)$ ($\nabla^2\rho_b(\boldsymbol{r}_c)$) indicates that $\rho_b(\boldsymbol{r}_c)$ is depleted or concentrated with respect to its surrounding, since $\nabla^2\rho_b(\boldsymbol{r}_c)$ is the second derivative of $\rho_b(\boldsymbol{r}_c)$. $\rho_b(\boldsymbol{r}_c)$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

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

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

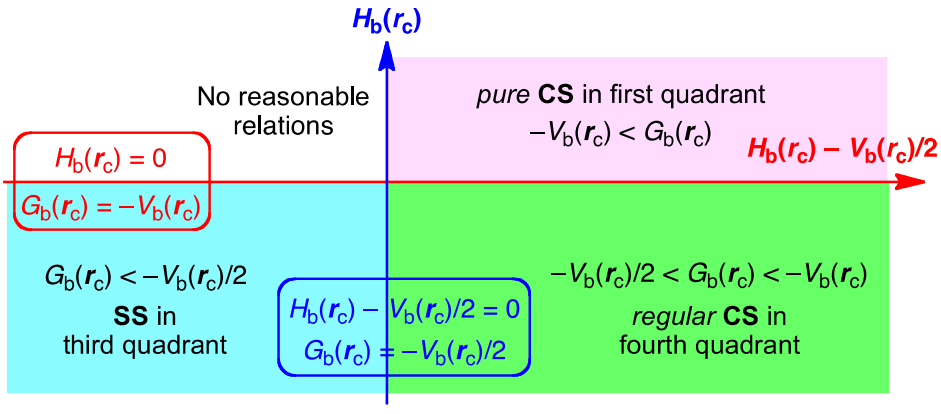
$$= G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2 \quad \text{(S2')}$$

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 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. Indeed, R does not correspond to the usual interaction energy, but it does to the local energy at BCP, expressed by $[(H_b(\boldsymbol{r}_c))^2 + (H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)^2]^{1/2}$ in the plot (cf: Equation (S3)), 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.

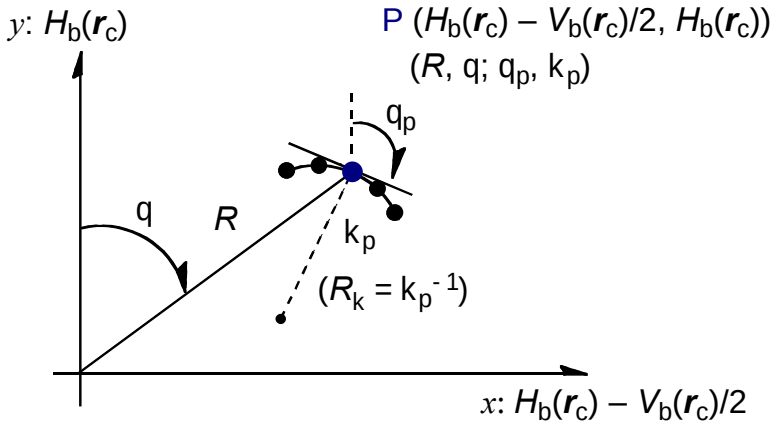


Figure S1. Polar (R, θ) coordinate representation of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, with (θ_p, κ_p) parameters.

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

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

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

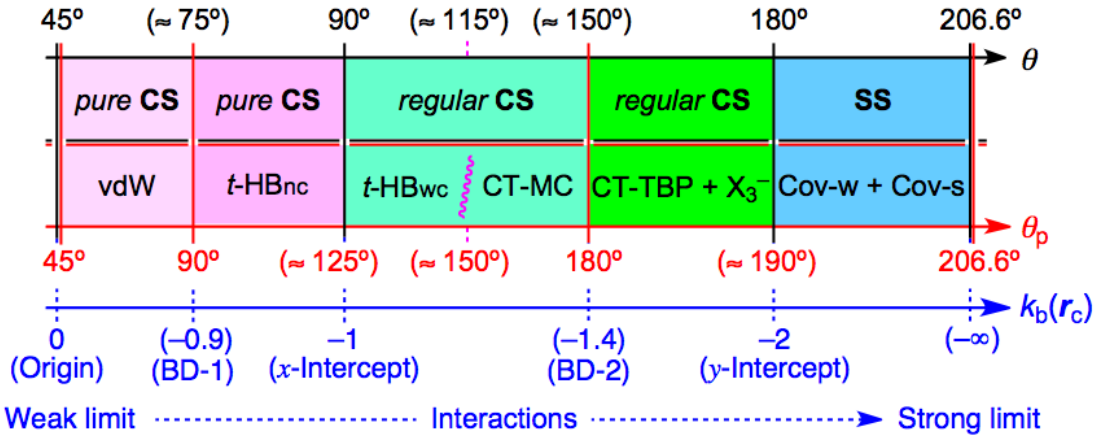
$$\kappa_p = |d^2y/dx^2| /[1 + (dy/dx)^2]^{3/2} \quad \text{(S6)}$$

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

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 θ_p = 150° based on the expectation form the experimental results, where θ_p is defined by [90° – tan^{-1}[d$H_b(\boldsymbol{r}_c)$/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. The plot of $H_b(\boldsymbol{r}_c)$ – $V_b(\boldsymbol{r}_c)$/2 versus *w* in Figure S2 is essentially the same as that of $\nabla^2\rho_b(\boldsymbol{r}_c)$ versus *d*(H---F) in X–H---F–Y, presented by Espinosa and co-workers.[S9]

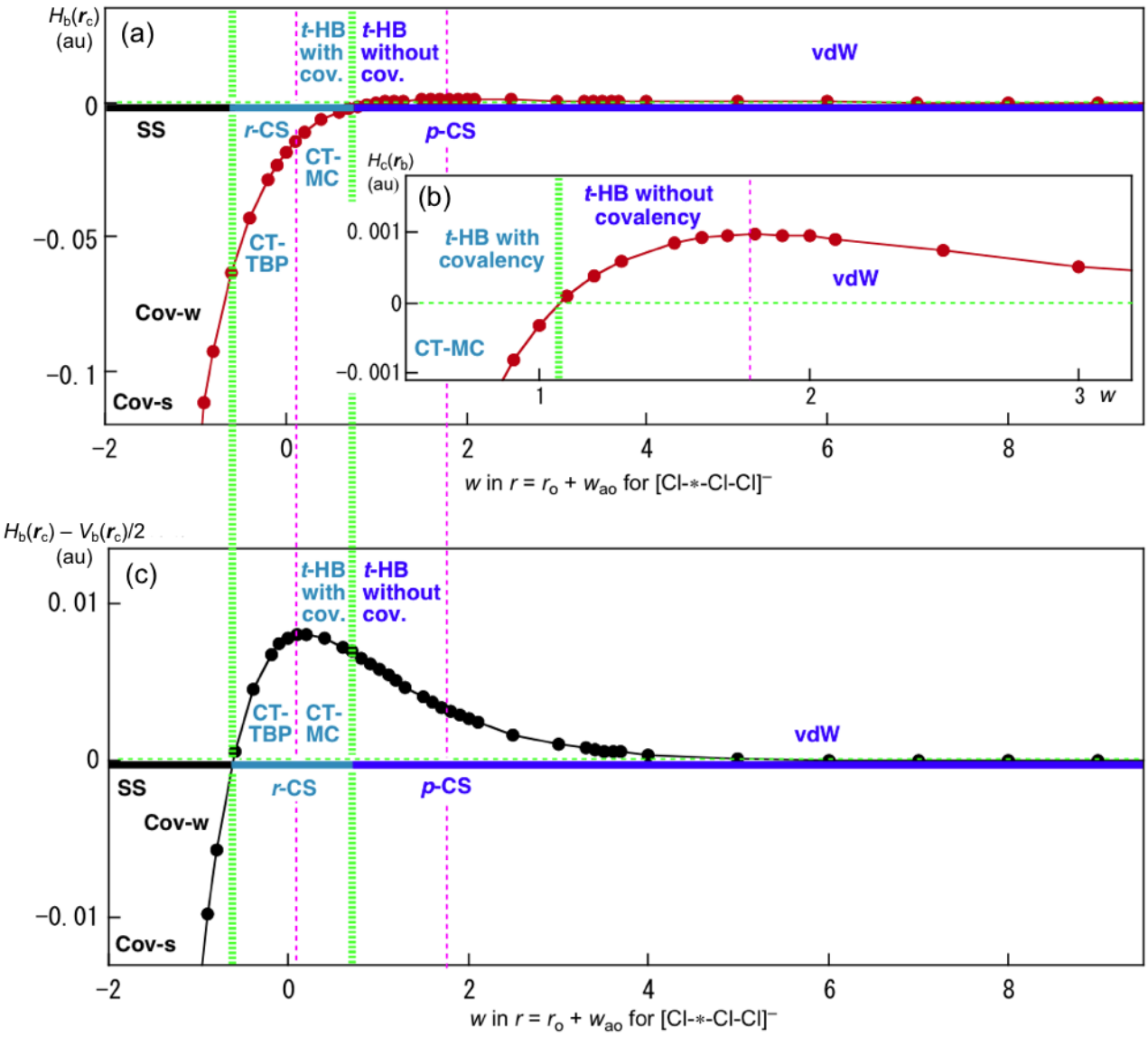


Figure S2. Plot of $H_b(\boldsymbol{r}_c)$ versus *w* in $r(^1\text{Cl-}^2\text{Cl}) = r_o(^1\text{Cl-}^2\text{Cl}) + wa_o$ for $^1\text{Cl-}^2\text{Cl-}^3\text{Cl}^-$ (a) with the magnified picture of (a) (b) and that of $H_b(\boldsymbol{r}_c)$ – $V_b(\boldsymbol{r}_c)$/2 versus *w* (c). Typical hydrogen 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)	$H_b(\boldsymbol{r}_c) = 0$ ($\theta_{pa} = 125^o$)	$G_b(\boldsymbol{r}_c) = -V_b(\boldsymbol{r}_c)$ ($\theta_{pa} = 125^o$)
t-HB$_{\text{with covalency}}$	$H_b(\boldsymbol{r}_c) < 0$; ($125^o <$) $\theta_{pa} < 150^o$	$G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$; ($125^o <$) $\theta_{pb} < 150^o$
Borderline (Tentative)	*$\theta_{pa} = 150^o$*	*$\theta_{pb} = 150^o$*
CT-MC	$d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/d(-r) > 0$;	$dG_b(\boldsymbol{r}_c) > dV_b(\boldsymbol{r}_c)/2$;
	$150^o < \theta_{pa} < 180^o$	$150^o < \theta_{pa} < 180^o$
Borderline (BD-2)	$d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/d(-r) = 0$	$2dG_b(\boldsymbol{r}_c)/d(-r) = -dV_b(\boldsymbol{r}_c)/d(-r)$
	($H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 > 0$; $H_b(\boldsymbol{r}_c) < 0$)	($-V_b(\boldsymbol{r}_c)/2 < G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$)
CT-TBP with X_{3-}	$d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)/d(-r) < 0$	$2dG_b(\boldsymbol{r}_c)/d(-r) < -dV_b(\boldsymbol{r}_c)/d(-r)$
	($H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 > 0$; $H_b(\boldsymbol{r}_c) < 0$)	($-V_b(\boldsymbol{r}_c)/2 < G_b(\boldsymbol{r}_c) < -V_b(\boldsymbol{r}_c)$)
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 $\theta_p = 90^o - \tan^{-1}[dH_b(\boldsymbol{r}_c)/d(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)]$, $\theta_p = 125^o$ is tentatively given for $\theta = 90^o$, where θ is defined by $90^o - \tan^{-1}[H_b(\boldsymbol{r}_c)/(H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2)]$ with $H_b(\boldsymbol{r}_c) = 0$. *b* $\theta_p = 90^o - \tan^{-1}[d(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c))/d(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2)]$, $\theta_p = 125^o$ is tentatively given for $\theta = 90^o$, where θ is defined by $90^o - \tan^{-1}[(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c))/(G_b(\boldsymbol{r}_c) + V_b(\boldsymbol{r}_c)/2)]$ 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, r(G, E), r(E, Y) and ∠GEY, of **1a**, **1b**, **2a**, **2b**, **3a**, **3b**, **4a**, **4b** and **5c** (**1**–**5**), together with the Δr(G, E), Δr(E, Y) and Δ∠GEY values, evaluated with MP2/BSS-A.[a] The Δr(G, E), Δr(E, Y) and Δ∠GEY values are defined in the footnotes of the Table.

Species No	(G, E, Y)	r(G, E) (Å)	Δr(G, E)[b] (Å)	r(E, Y) (Å)	Δr(E, Y)[c] (Å)	∠GEY (º)	Δ∠GEY[d] (º)
1a	(N, S, F)	2.1619	-1.188	1.7167	0.037	175.20	-4.80
1a	(N, S, Cl)	2.2218	-1.128	2.1630	0.134	178.00	-2.00
1a	(N, S, Br)	2.2425	-1.107	2.3147	0.135	177.80	-2.20
1a	(N, S, I)	2.3525	-0.998	2.4827	0.113	175.73	-4.27
1a	(N, S, SMe)	2.8599	-0.490	2.0538	-0.026	172.52	-7.48
1a	(N, S, C_{Me})	2.9873	-0.363	1.8121	0.000	174.14	-5.86
1b	(N, Se, F)	2.2604	-1.190	1.8370	0.027	170.58	-9.42
1b	(N, Se, Cl)	2.2954	-1.155	2.2816	0.122	174.00	-6.00
1b	(N, Se, Br)	2.3128	-1.137	2.4284	0.118	174.85	-5.15
1b	(N, Se, I)	2.3700	-1.080	2.6143	0.114	175.41	-4.59
1b	(N, Se, SeMe)	2.6873	-0.763	2.3351	-0.005	171.86	-8.14
1b	(N, Se, C_{Me})	2.8849	-0.565	1.9522	0.010	168.90	-11.10
2a	(O, S, F)	2.4796	-0.840	1.6475	-0.033	176.37	-3.63
2a	(O, S, Cl)	2.7094	-0.611	2.0453	0.015	175.20	-4.80
2a	(O, S, Br)	2.7564	-0.564	2.1950	0.015	173.29	-6.71
2a	(O, S, I)	2.8547	-0.465	2.3863	0.016	169.18	-10.82
2a	(O, S, SMe)	2.9638	-0.356	2.0437	-0.036	174.34	-5.67
2a	(O, S, C_{Me})	3.1040	-0.216	1.8080	-0.004	176.46	-3.5
2b	(O, Se, F)	2.4354	-0.985	1.7844	-0.026	171.20	-8.80
2b	(O, Se, Cl)	2.5569	-0.863	2.1884	0.028	174.11	-5.89
2b	(O, Se, Br)	2.5980	-0.822	2.3322	0.022	174.47	-5.53
2b	(O, Se, I)	2.6947	-0.725	2.5195	0.019	173.55	-6.45
2b	(O, Se, SeMe)	2.8787	-0.541	2.3086	-0.031	172.37	-7.63
2b	(O, Se, C_{Me})	2.9614	-0.457	1.9450	0.003	170.80	-9.20
3a	(S, S, F)	2.7254	-0.875	1.6715	-0.009	176.31	-3.69
3a	(S, S, Cl)	3.0214	-0.579	2.0612	0.031	170.94	-9.06
3a	(S, S, Br)	3.0535	-0.547	2.2112	0.031	168.98	-11.02
3a	(S, S, I)	3.1736	-0.426	2.3978	0.028	163.26	-16.74
3a	(S, S, SMe)	3.3364	-0.264	2.0488	-0.031	169.34	-10.66
3a	(S, S, C_{Me})	3.4257	-0.174	1.8094	-0.003	176.13	-3.87
3b	(S, Se, F)	2.6507	-1.049	1.8195	0.010	172.64	-7.36
3b	(S, Se, Cl)	2.7802	-0.920	2.2325	0.072	173.59	-6.41
3b	(S, Se, Br)	2.8216	-0.878	2.3745	0.065	173.16	-6.84
3b	(S, Se, I)	2.9507	-0.749	2.5494	0.049	170.72	-9.28
3b	(S, Se, SeMe)	3.2512	-0.449	2.3169	-0.023	167.40	-12.60
3b	(S, Se, C_{Me})	3.3731	-0.327	1.9494	0.007	168.10	-11.90
4a	(Se, S, F)	2.8493	-0.851	1.6728	-0.007	175.40	-4.60
4a	(Se, S, Cl)	3.1043	-0.596	2.0660	0.036	170.49	-9.51
4a	(Se, S, Br)	3.1244	-0.576	2.2169	0.037	168.80	-11.20
4a	(Se, S, I)	3.2417	-0.458	2.4018	0.032	163.29	-16.71
4a	(Se, S, SMe)	3.4323	-0.268	2.0500	-0.030	168.87	-11.13
4a	(Se, S, C_{Me})	3.5507	-0.149	1.8080	-0.004	171.83	-8.17

[a] See text for BSS-A. [b] Δr(G, E) = r(G, E) – (r_{vdW}(G) + r_{vdW}(E)) (A. Bondi, *J. Phys. Chem.* **1964**, *68*, 441–451). [c] Δr(E, Y) = r(E, Y) – (r_{co}(E) + r_{co}(Y)) (P. Pyykkö, M. Atsumi, *Chem. Eur. J.* **2009**, *15*, 186 – 197). [d] Δ∠GEY = ∠GEY – 180.00º.

Table S2 (continued)

Species No	(G, E, Y)	r(G, E) (Å)	Δr(G, E)[b] (Å)	r(E, Y) (Å)	Δr(E, Y)[c] (Å)	∠GEY (º)	Δ∠GEY[d] (º)
4b	(Se, Se, F)	2.7512	-1.049	1.8249	0.015	172.73	-7.27
4b	(Se, Se, Cl)	2.8662	-0.934	2.2427	0.083	172.87	-7.14
4b	(Se, Se, Br)	2.8995	-0.900	2.3861	0.076	172.45	-7.56
4b	(Se, Se, I)	3.0175	-0.783	2.5601	0.060	170.29	-9.71
4b	(Se, Se, SeMe)	3.3569	-0.443	2.3132	-0.027	175.11	-4.89
4b	(Se, Se, C_{Me})	3.4859	-0.314	1.9502	0.008	167.93	-12.07
5c	(Te, Te, F)	3.0154	-1.105	1.9858	-0.024	164.79	-15.21
5c	(Te, Te, Cl)	3.0880	-1.032	2.4312	0.071	166.33	-13.67
5c	(Te, Te, Br)	3.1128	-1.007	2.5791	0.069	166.55	-13.45
5c	(Te, Te, I)	3.1820	-0.938	2.7777	0.078	166.17	-13.83
5c	(Te, Te, TeMe)	3.6034	-0.517	2.6968	-0.043	162.34	-17.66
5c	(Te, Te, C_{Me})	3.7115	-0.409	2.1511	0.009	160.85	-19.15

[a] See text for BSS-A. [b] Δr(G, E) = r(G, E) – (r_{vdW}(G) + r_{vdW}(E)) (A. Bondi, *J. Phys. Chem.* **1964**, *68*, 441–451). [c] Δr(E, Y) = r(E, Y) – (r_{co}(E) + r_{co}(Y)) (P. Pyykkö, M. Atsumi, *Chem. Eur. J.* **2009**, *15*, 186–197). [d] Δ∠GEY = ∠GEY – 180.00º.

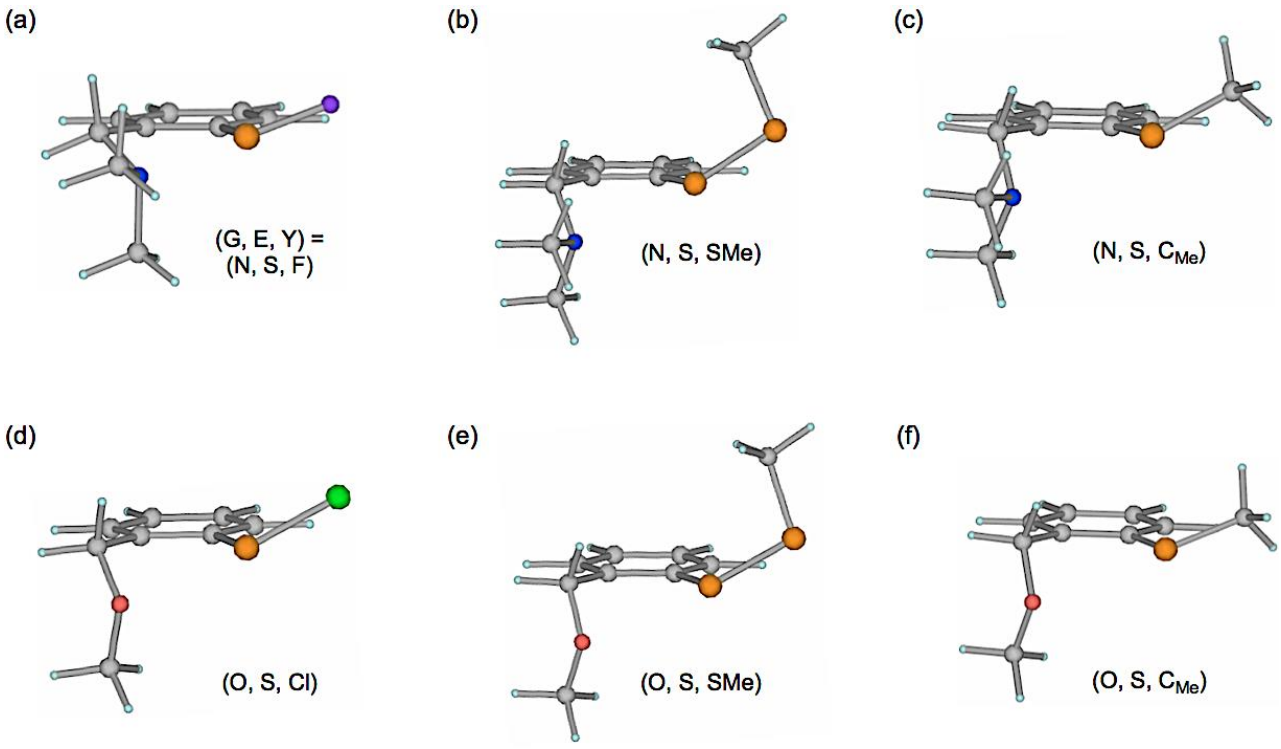


Figure S3. Optimized structures in **1a** (a–c) and **2a** (d–f) calculated with MP2/BSS-A.

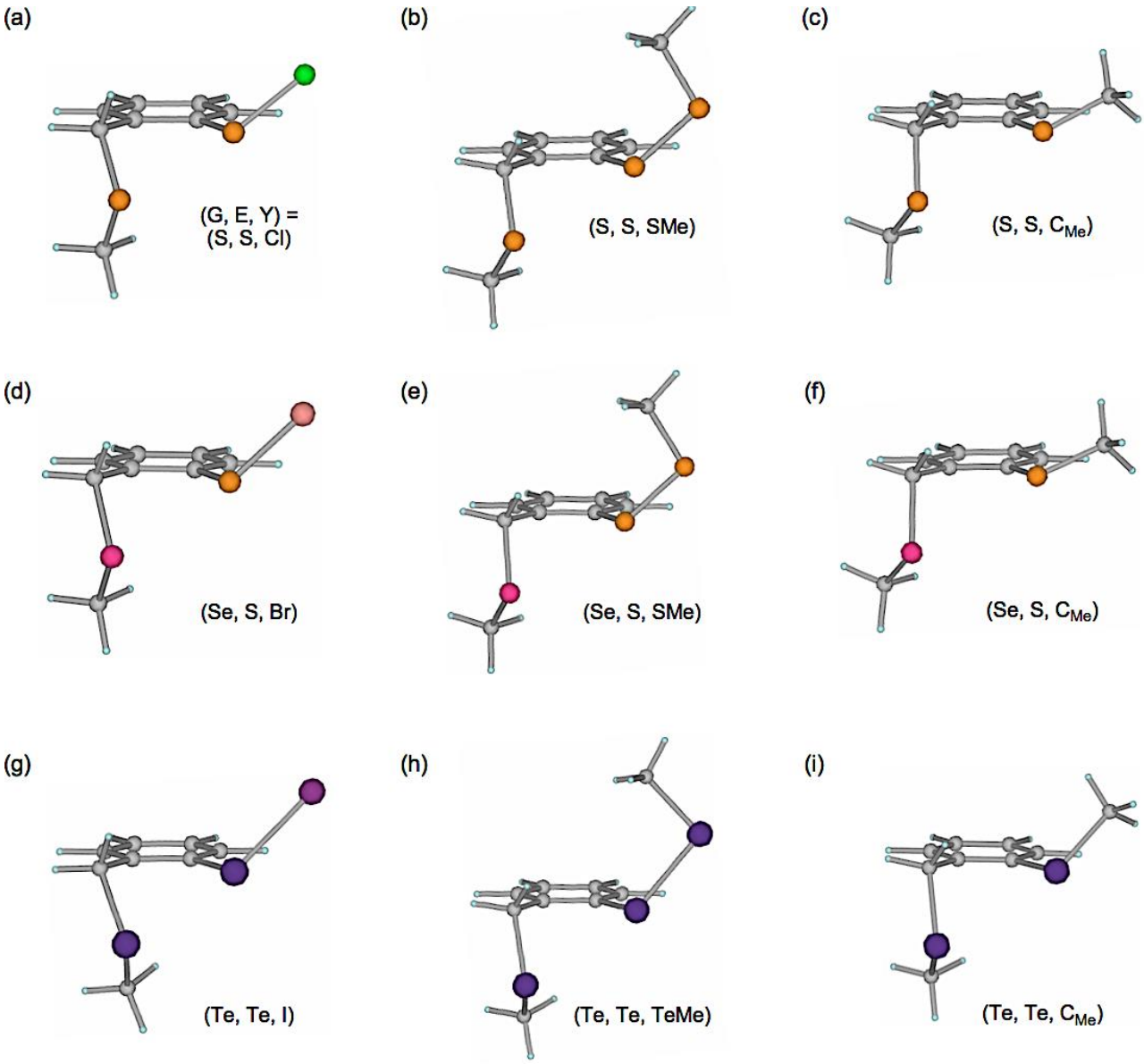


Figure S4. Optimized structures in **3a** (a–c), **4a** (d–f) and **5c** (g–i) calculated with MP2/BSS-A.

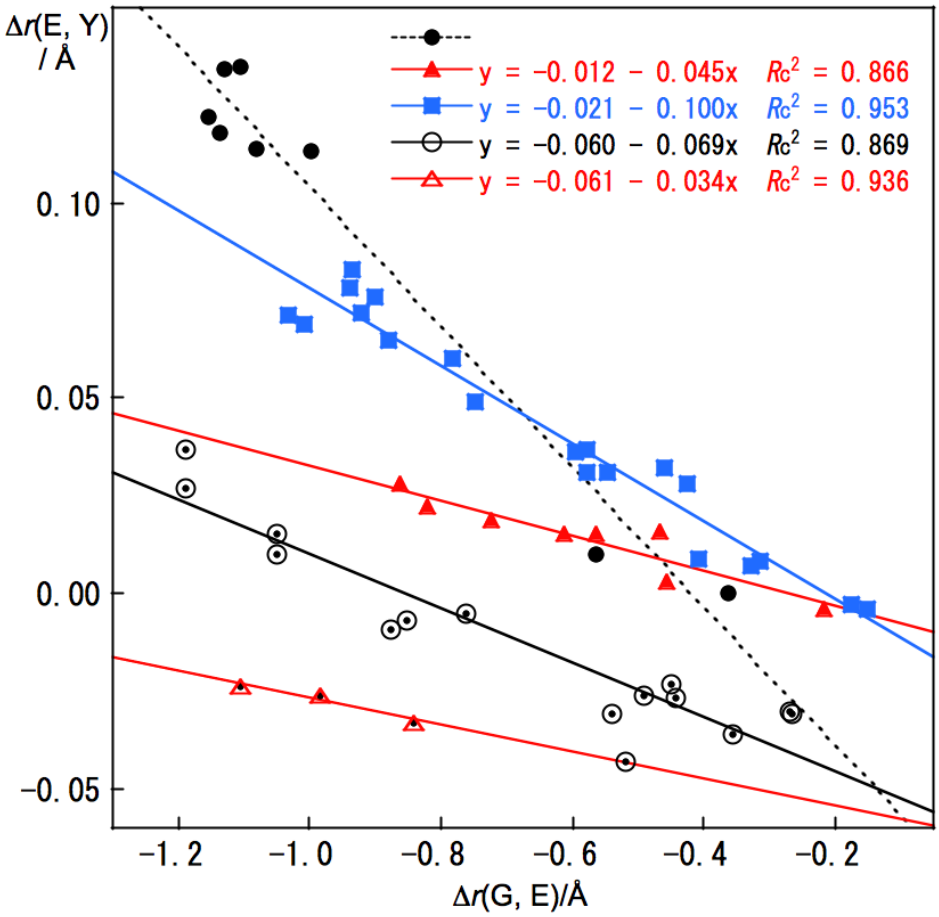


Figure S5. Plots of Δ*r*(E, Y) versus Δ*r*(G, E), separately by **1** (●), **2** (▲) and **3**–**5** (■), although data for Y = F and EMe in **1**–**5** being omitted from the correlations, which were plotted separately. The data for Y = F and EMe in **1**–**5**, are analyzed as two correlations for Y = F in **2a**, **2b** and **3c** (△) and for Y = F and EMe in **1**–**5**, other than the data for Y = F in **2a**, **2b** and **3c** (○). In the case of **1** (●), data are separated widely as two groups (the upper left group of six points and two points at the lower right part). Therefore, the data may not be appropriate for the fitting from the statistic point of view. Nevertheless, the plot for **1** is tentatively shown by the dotted line, where the correlation is not given.

Table S3. Lengths of bond paths (BPs: r_{BP}) and the corresponding straight-line distances (R_{SL}), corresponding to the intramolecular G-∗-E interactions in G-∗-E-∗-Y σ(3c–4e) of **1**–**5**, evaluated with MP2/BSS-A, together with the differences between the two ($\Delta r_{BP} = r_{BP} - R_{SL}$)[a]

Species (symm)		G-∗-E	r_{BP} (Å)	R_{SL} (Å)	Δr_{BP}[b] (Å)
1a	(N, S, F)	N-∗-S	2.1678	2.1619	0.0059
1a	(N, S, Cl)	N-∗-S	2.2278	2.2218	0.0060
1a	(N, S, Br)	N-∗-S	2.2485	2.2425	0.0060
1a	(N, S, I)	N-∗-S	2.3595	2.3525	0.0070
1a	(N, S, SMe)	N-∗-S	2.8737	2.8599	0.0138
1a	(N, S, C_{Me})	N-∗-S	2.9985	2.9873	0.0112
1b	(N, Se, F)	N-∗-Se	2.2618	2.2604	0.0013
1b	(N, Se, Cl)	N-∗-Se	2.2968	2.2954	0.0014
1b	(N, Se, Br)	N-∗-Se	2.3143	2.3128	0.0015
1b	(N, Se, I)	N-∗-Se	2.3718	2.3700	0.0018
1b	(N, Se, SeMe)	N-∗-Se	2.6911	2.6873	0.0038
1b	(N, Se, C_{Me})	N-∗-Se	2.8900	2.8849	0.0050
2a	(O, S, F)	O-∗-S	2.4911	2.4796	0.0116
2a	(O, S, Cl)	O-∗-S	2.7221	2.7094	0.0127
2a	(O, S, Br)	O-∗-S	2.7692	2.7564	0.0128
2a	(O, S, I)	O-∗-S	2.8683	2.8547	0.0136
2a	(O, S, SMe)	O-∗-S	2.9752	2.9638	0.0114
2a	(O, S, C_{Me})	O-∗-S	3.0226	3.0140	0.0086
2b	(O, Se, F)	O-∗-Se	2.4373	2.4354	0.0019
2b	(O, Se, Cl)	O-∗-Se	2.5592	2.5569	0.0023
2b	(O, Se, Br)	O-∗-Se	2.6005	2.5980	0.0025
2b	(O, Se, I)	O-∗-Se	2.6978	2.6947	0.0031
2b	(O, Se, SeMe)	O-∗-Se	2.8820	2.8787	0.0033
2b	(O, Se, C_{Me})	O-∗-Se	2.9646	2.9614	0.0032
3a	(S, S, F)	S-∗-S	2.7393	2.7254	0.0139
3a	(S, S, Cl)	S-∗-S	3.0421	3.0214	0.0207
3a	(S, S, Br)	S-∗-S	3.0737	3.0535	0.0202
3a	(S, S, I)	S-∗-S	3.1953	3.1736	0.0217
3a	(S, S, SMe)	S-∗-S	3.3551	3.3364	0.0187
3a	(S, S, C_{Me})	S-∗-S	3.4392	3.4257	0.0136
3b	(S, Se, F)	S-∗-Se	2.6535	2.6507	0.0028
3b	(S, Se, Cl)	S-∗-Se	2.7851	2.7802	0.0049
3b	(S, Se, Br)	S-∗-Se	2.8272	2.8216	0.0056
3b	(S, Se, I)	S-∗-Se	2.9580	2.9507	0.0073
3b	(S, Se, SeMe)	S-∗-Se	3.2611	3.2512	0.0100
3b	(S, Se, C_{Me})	S-∗-Se	3.3825	3.3731	0.0094
4a	(Se, S, F)	Se-∗-S	2.8637	2.8493	0.0144
4a	(Se, S, Cl)	Se-∗-S	3.1228	3.1043	0.0185
4a	(Se, S, Br)	Se-∗-S	3.1421	3.1244	0.0177
4a	(Se, S, I)	Se-∗-S	3.2601	3.2417	0.0184
4a	(Se, S, SMe)	Se-∗-S	3.4482	3.4323	0.0159
4a	(Se, S, C_{Me})	Se-∗-S	*c*	3.5507	*c*

[a] See text for BSS-A. [b] $\Delta r_{BP} = r_{BP} - R_{SL}$. [c] The bond path corresponding to the interaction being not detected.

Table S3 (continued)

Species (symm)		G-∗-E	r_{BP} (Å)	R_{SL} (Å)	Δr_{BP}[b] (Å)
4b	(Se, Se, F)	Se-∗-Se	2.7538	2.7512	0.0026
4b	(Se, Se, Cl)	Se-∗-Se	2.8703	2.8662	0.0041
4b	(Se, Se, Br)	Se-∗-Se	2.9040	2.8995	0.0045
4b	(Se, Se, I)	Se-∗-Se	3.0231	3.0175	0.0057
4b	(Se, Se, SeMe)	Se-∗-Se	3.3541	3.3468	0.0072
4b	(Se, Se, C_{Me})	Se-∗-Se	3.4918	3.4859	0.0059
5c	(Te, Te, F)	Te-∗-Te	3.0180	3.0154	0.0025
5c	(Te, Te, Cl)	Te-∗-Te	3.0915	3.0880	0.0036
5c	(Te, Te, Br)	Te-∗-Te	3.1167	3.1128	0.0039
5c	(Te, Te, I)	Te-∗-Te	3.1868	3.1820	0.0048
5c	(Te, Te, TeMe)	Te-∗-Te	3.6115	3.6034	0.0081
5c	(Te, Te, C_{Me})	Te-∗-Te	3.7190	3.7115	0.0075

[a] See text for BSS-A. [b] $\Delta r_{BP} = r_{BP} - R_{SL}$. [c] The bond path corresponding to the interaction being not detected.

Table S4. The QTAIM functions, QTAIM-DFA parameters and the C_{ii} values for the E-∗-Y bonds in G---E–Y σ(3c–4e) of **1**–**5**, calculated with MP2/BSS-A[a]

Species: E-∗-Y (No)	$\rho_b(\boldsymbol{r}_c)$ (au)	$c\nabla^2\rho_b(\boldsymbol{r}_c)$[b] (au)	$H_b(\boldsymbol{r}_c)$ (au)	$k_b(\boldsymbol{r}_c)$[c]	R[d] (au)	θ[e] (º)	C_{iif}[f] (Å mdyn^{-1})	θ_p[g] (º)	κ_p[h] (au^{-1})
1a: NS-∗-F	0.1578	-0.0081	-0.1554	-2.116	0.1556	183.0	0.434	175.2	11.5
1a: NS-∗-Cl	0.1141	-0.0004	-0.0536	-2.016	0.0536	180.5	0.863	195.6	1.8
1a: NS-∗-Br	0.0979	0.0022	-0.0374	-1.896	0.0375	176.7	0.933	193.9	3.5
1a: NS-∗-I	0.0873	-0.0002	-0.0340	-2.010	0.0340	180.3	1.170	192.8	0.7
1b: NSe-∗-F	0.1315	0.0351	-0.0752	-1.517	0.0830	155.0	0.407	146.9	5.9
1b: NSe-∗-Cl	0.0955	0.0038	-0.0415	-1.844	0.0417	174.7	0.731	187.3	1.2
1b: NSe-∗-Br	0.0844	0.0036	-0.0305	-1.809	0.0307	173.3	0.791	189.5	3.5
1b: NSe-∗-I	0.0753	0.0012	-0.0259	-1.914	0.0260	177.3	0.897	191.7	3.5
2a: OS-∗-F	0.1770	0.0103	-0.1961	-1.905	0.1964	177.0	0.270	136.3	18.4
2a: OS-∗-Cl	0.1441	-0.0125	-0.0881	-2.396	0.0890	188.1	0.388	196.4	0.3
2a: OS-*-Br	0.1228	-0.0057	-0.0608	-2.229	0.0611	185.3	0.434	195.2	1.0
2a: OS-∗-I	0.1022	-0.0033	-0.0482	-2.158	0.0483	183.9	0.483	187.9	4.8
2b: OSe-∗-F	0.1466	0.0450	-0.0913	-1.503	0.1018	153.7	0.297	141.8	3.1
2b: OSe-∗-Cl	0.1142	-0.0004	-0.0603	-2.015	0.0603	180.4	0.457	184.4	7.6
2b: OSe-∗-Br	0.1010	-0.0008	-0.0448	-2.039	0.0448	181.1	0.503	190.8	0.3
2b: OSe-∗-I	0.0885	-0.0021	-0.0367	-2.132	0.0367	183.3	0.552	191.7	0.5
3a: SS-∗-F	0.1705	-0.0006	-0.1840	-2.006	0.1840	180.2	0.390	150.0	17.0
3a: SS-∗-Cl	0.1394	-0.0103	-0.0819	-2.336	0.0825	187.2	0.467	196.8	0.2
3a: SS-∗-Br	0.1188	-0.0042	-0.0567	-2.174	0.0569	184.2	0.514	195.5	0.9
3a: SS-∗-I	0.1000	-0.0029	-0.0460	-2.144	0.0461	183.6	0.527	188.7	4.6
3a: SS-∗-SMe	0.1514	-0.0184	-0.0931	-2.652	0.0949	191.2	0.403	197.5	0.2
3a: SS-∗-C$_{Me}$	0.1812	-0.0359	-0.1255	-3.335	0.1305	196.0	0.338	199.7	0.2
3b: SeS-∗-F	0.1367	0.0374	-0.0805	-1.518	0.0888	155.1	0.400	145.3	5.4
3b: SSe-∗-Cl	0.1050	0.0017	-0.0503	-1.935	0.0503	178.0	0.693	188.0	3.6
3b: SSe-∗-Br	0.0932	0.0015	-0.0374	-1.924	0.0375	177.7	0.740	191.9	0.9
3b: SSe-∗-I	0.0838	-0.0008	-0.0327	-2.052	0.0327	181.4	0.732	192.7	0.4
3b: SSe-∗-SeMe	0.1073	-0.0056	-0.0511	-2.283	0.0515	186.3	0.510	194.0	0.5
3b: SSe-∗-C$_{Me}$	0.1483	-0.0228	-0.0967	-2.890	0.0994	193.3	0.386	193.2	3.1
4a: SeS-∗-F	0.1701	-0.0013	-0.1831	-2.014	0.1831	180.4	0.402	151.3	17.0
4a: SeS-∗-Cl	0.1380	-0.0096	-0.0801	-2.316	0.0807	186.8	0.500	196.9	0.2
4a: SeS-∗-Br	0.1174	-0.0037	-0.0553	-2.157	0.0554	183.9	0.555	195.7	0.7
4a: SeS-∗-I	0.0993	-0.0027	-0.0453	-2.138	0.0454	183.5	0.553	189.0	4.6
4a: SeS-∗-SMe	0.1510	-0.0183	-0.0926	-2.652	0.0944	191.2	0.408	197.5	0.2
4a: SeS-∗-C$_{Me}$	0.1815	-0.0359	-0.1257	-3.331	0.1308	195.9	0.345	199.7	0.2

[a] See text for MP2/BSS-A. [b] $c\nabla^2\rho_b(\boldsymbol{r}_c) = H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, where $c = \hbar^2/8m$. [c] $k_b(\boldsymbol{r}_c) = V_b(\boldsymbol{r}_c)/G_b(\boldsymbol{r}_c)$. [d] $R = (x^2 + y^2)^{1/2}$, where $(x, y) = (H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2, H_b(\boldsymbol{r}_c))$. [e] $\theta = 90° - \tan^{-1}(y/x)$. [f] Defined in eqn (3) in the text. [g] $\theta_p = 90° - \tan^{-1}(dy/dx)$. [h] $\kappa_p = |d^2y/dx^2| /[1 + (dy/dx)^2]^{3/2}$.

Table S4 (continued)

Species: E-*-Y (No)	$\rho_b(\boldsymbol{r}_c)$ (au)	$c\nabla^2\rho_b(\boldsymbol{r}_c)_b$ (au)	$H_b(\boldsymbol{r}_c)$ (au)	$k_b(\boldsymbol{r}_c)_c$	R_d (au)	θ_e (º)	C_{iif} (Å mdyn^{-1})	θ_{pg} (º)	κ_{ph} (au^{-1})
4b: SeSe-*-F	0.1353	0.0362	-0.0790	-1.522	0.0869	155.4	0.421	146.0	5.9
4b: SeSe-*-Cl	0.1030	0.0022	-0.0481	-1.916	0.0482	177.4	0.754	188.5	3.2
4b: SeSe-*-Br	0.0911	0.0021	-0.0356	-1.896	0.0357	176.7	0.808	192.0	1.1
4b: SeSe-*-I	0.0822	-0.0004	-0.0313	-2.026	0.0313	180.7	0.807	192.9	0.4
4b: SeSe-*-SeMe	0.1068	-0.0055	-0.0507	-2.277	0.0510	186.2	0.520	194.0	0.5
4b: SeSe-*-C$_{Me}$	0.1480	-0.0226	-0.0967	-2.876	0.0993	193.1	0.389	193.2	3.1
5c: TeTe-*-F	0.1069	0.0561	-0.0338	-1.231	0.0655	121.1	0.397	115.8	1.7
5c: TeTe-*-Cl	0.0805	0.0093	-0.0317	-1.629	0.0331	163.6	0.729	154.9	25.9
5c: TeTe-*-Br	0.073	0.0044	-0.0270	-1.753	0.0274	170.7	0.820	173.0	21.0
5c: TeTe-*-I	0.0662	0.0006	-0.0236	-1.949	0.0236	178.5	0.967	188.3	2.5
5c: TeTe-*-TeMe	0.0775	-0.0040	-0.0330	-2.322	0.0332	186.9	0.679	190.8	2.3
5c: TeTe-*-C$_{Me}$	0.1142	-0.0007	-0.0615	-2.023	0.0615	180.6	0.451	163.8	11.9

[a] See text for MP2/BSS-A. [b] $c\nabla^2\rho_b(\boldsymbol{r}_c) = H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, where $c = \hbar^2/8m$. [c] $k_b(\boldsymbol{r}_c) = V_b(\boldsymbol{r}_c)/G_b(\boldsymbol{r}_c)$. [d] $R = (x^2 + y^2)^{1/2}$, where $(x, y) = (H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2, H_b(\boldsymbol{r}_c))$. [e] $\theta = 90° - \tan^{-1}(y/x)$. [f] Defined in eqn (3) in the text. [g] $\theta_p = 90° - \tan^{-1}(dy/dx)$. [h] $\kappa_p = |d^2y/dx^2| /[1 + (dy/dx)^2]^{3/2}$.

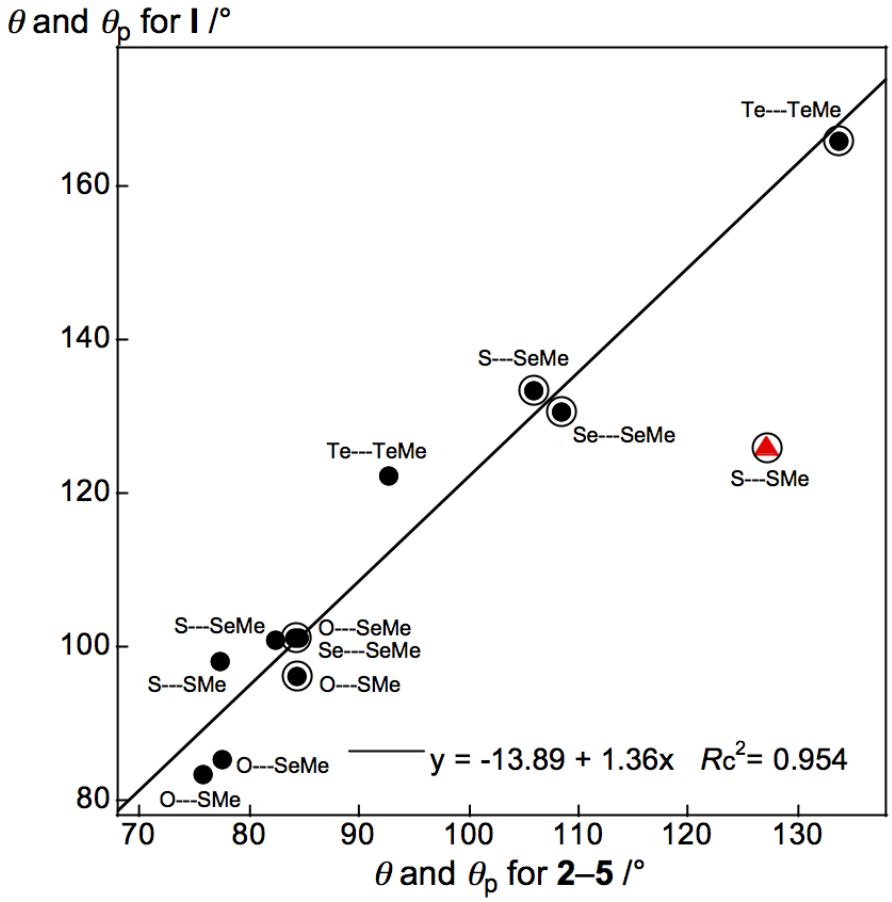


Figure S6. Plots of θ (●) and θ_p (◎) of **I** versus the corresponding values of **2**–**5**, although data for S---SMe being omitted from the correlations.

Table S5. NBO analysis for **1**–**5** evaluated with MP2/BSS-A

Species G-*-EY	NBO(*i*)→NBO(*j*)	$E(2)_a$ (kcal mol^{-1})	ΔE_b (au)	$F(i,j)_c$ (au)	NBO(*i*)→NBO(*j*)	$E(2)_a$ (kcal mol^{-1})	ΔE_b (au)	$F(i,j)_c$ (au)
1a: N-*-SF	n_s(N)→n_p(S+)	84.37	0.50	0.198	n_p(N)→n_p(S+)	*d*	*d*	*d*
1a: N-*-SCl	n_s(N)→σ*(S–Cl)	48.32	0.65	0.161	n_p(N)→σ*(S–Cl)	*d*	*d*	*d*
1a: N-*-SBr	n_s(N)→σ*(S–Br)	48.08	0.60	0.154	n_p(N)→σ*(S–Br)	*d*	*d*	*d*
1a: N-*-SI	n_s(N)→σ*(S–I)	31.71	0.56	0.121	n_p(N)→σ*(S–I)	*d*	*d*	*d*
1a: N-*-SSMe	n_s(N)→σ*(S–S)	3.56	0.71	0.046	n_p(N)→σ*(S–S)	*d*	*d*	*d*
1a: N-*-SC$_{Me}$	n_s(N)→σ*(S–C)	1.70	0.85	0.035	n_p(N)→σ*(S–C)	*d*	*d*	*d*
1b: N-*-SeF	n_s(N)→n_p(Se+)	76.84	0.52	0.189	n_p(N)→n_p(Se+)	*d*	*d*	*d*
1b: N-*-SeCl	n_s(N)→σ*(Se–Cl)	49.04	0.65	0.162	n_p(N)→σ*(Se–Cl)	*d*	*d*	*d*
1b: N-*-SeBr	n_s(N)→σ*(Se–Br)	47.94	0.61	0.155	n_p(N)→σ*(Se–Br)	*d*	*d*	*d*
1b: N-*-SeI	n_s(N)→σ*(Se–I)	39.27	0.58	0.137	n_p(N)→σ*(Se–I)	*d*	*d*	*d*
1b: N-*-SeSeMe	n_s(N)→σ*(Se–Se)	10.42	0.63	0.073	n_p(N)→σ*(Se–Se)	*d*	*d*	*d*
1b: N-*-SeC$_{Me}$	n_s(N)→σ*(Se–C)	4.16	0.77	0.052	n_p(N)→σ*(Se–C)	*d*	*d*	*d*
2a: O-*-SF	n_s(O)→σ*(S–F)	1.67	1.09	0.038	n_p(O)→σ*(S–F)	9.78	0.87	0.083
2a: O-*-SCl	n_s(O)→σ*(S–Cl)	1.11	1.00	0.030	n_p(O)→σ*(S–Cl)	4.31	0.72	0.050
2a: O-*-SBr	n_s(O)→σ*(S–Br)	1.03	0.95	0.028	n_p(O)→σ*(S–Br)	3.76	0.66	0.040
2a: O-*-SI	n_s(O)→σ*(S–I)	0.78	0.91	0.024	n_p(O)→σ*(S–I)	2.40	0.61	0.035
2a: O-*-SSMe	n_s(O)→σ*(S–S)	*e*	*e*	*e*	n_p(O)→σ*(S–S)	1.15	0.75	0.026
2a: O-*-SC$_{Me}$	n_s(O)→σ*(S–C)	*e*	*e*	*e*	n_p(O)→σ*(S–C)	0.75	0.89	0.023
2b: O-*-SeF	n_s(O)→n_p(Se+)	2.48	0.77	0.043	n_p(O)→n_p(Se+)	22.34	0.62	0.114
2b: O-*-SeCl	n_s(O)→σ*(Se–Cl)	2.13	0.94	0.040	n_p(O)→σ*(Se–Cl)	11.65	0.74	0.083
2b: O-*-SeBr	n_s(O)→σ*(Se–Br)	2.08	0.91	0.039	n_p(O)→σ*(Se–Br)	10.31	0.69	0.076
2b: O-*-SeI	n_s(O)→σ*(Se–I)	1.87	0.89	0.036	n_p(O)→σ*(Se–I)	6.97	0.63	0.060
2a: O-*-SeSeMe	n_s(O)→σ*(Se–Se)	1.03	0.97	0.028	n_p(O)→σ*(Se–Se)	2.60	0.67	0.038
2a: O-*-SeC$_{Me}$	n_s(O)→σ*(Se–C)	0.67	1.12	0.025	n_p(O)→σ*(Se–C)	1.49	0.82	0.031
3a: S-*-SF	n_s(S)→n_p(S+)	2.35	0.74	0.043	n_p(S)→n_p(S+)	43.42	0.38	0.125
3a: S-*-SCl	n_s(S)→σ*(S–Cl)	0.95	0.98	0.027	n_p(S)→σ*(S–Cl)	9.56	0.56	0.066
3a: S-*-SBr	n_s(S)→σ*(S–Br)	0.89	0.93	0.026	n_p(S)→σ*(S–Br)	9.03	0.51	0.061
3a: S-*-SI	n_s(S)→σ*((S–I)	0.66	0.90	0.022	n_p(S)→σ*(S–I)	5.40	0.47	0.045
3a: S-*-SSMe	n_s(S)→σ*(S–S)	*e*	*e*	*e*	n_p(S)→σ*(S–S)	1.85	0.60	0.030
3a: S-*-SC$_{Me}$	n_s(S)→σ*(S–C)	*e*	*e*	*e*	n_p(S)→σ*(S–C)	0.85	0.74	0.023
3b: S-*-SeF	n_s(S)→n_p(Se+)	3.98	0.72	0.055	n_p(S)→n_p(Se+)	84.08	0.40	0.174
3b: S-*-SeCl	n_s(S)→σ*(Se–Cl)	2.84	0.90	0.046	n_p(S)→σ*(Se–Cl)	36.92	0.55	0.129
3b: S-*-SeBr	n_s(S)→σ*(Se–Br)	2.70	0.88	0.045	n_p(S)→σ*(Se–Br)	33.34	0.51	0.118
3b: S-*-SeI	n_s(S)→σ*(Se–I)	2.07	0.86	0.038	n_p(S)→σ*(Se–I)	21.03	0.48	0.090
3b: S-*-SeSeMe	n_s(S)→σ*(Se–Se)	0.81	0.96	0.025	n_p(S)→σ*(Se–Se)	5.10	0.52	0.047
3b: S-*-SeC$_{Me}$	n_s(S)→σ*(Se–C)	0.54	1.11	0.022	n_p(S)→σ*(Se–C)	2.32	0.67	0.036
4a: Se-*-SF	n_s(Se)→σ*(S–F)	1.78	1.10	0.040	n_p(Se)→σ*(S–F)	26.24	0.65	0.118
4a: Se-*-SCl	n_s(Se)→σ*(S–Cl)	0.80	1.02	0.026	n_p(Se)→σ*(S–Cl)	11.04	0.53	0.069
4a: Se-*-SBr	n_s(Se)→σ*(S–Br)	0.79	0.98	0.025	n_p(Se)→σ*(S–Br)	10.97	0.49	0.066
4a: Se-*-SI	n_s(Se)→σ*(S–I)	0.58	0.95	0.021	n_p(Se)→σ*(S–I)	6.75	0.45	0.049
4a: Se-*-SSMe	n_s(Se)→σ*(S–S)	*e*	*e*	*e*	n_p(Se)→σ*(S–S)	2.10	0.58	0.031
4a: Se-*SC$_{Me}$	n_s(Se)→σ*(S–C)	*e*	*e*	*e*	n_p(Se)→σ*(S–C)	0.70	0.72	0.020
4b: Se-*-SeF	n_s(Se)→n_p(Se+)	4.03	0.76	0.057	n_p(Se)→n_p(Se+)	92.76	0.35	0.173
4b: Se-*-SeCl	n_s(Se)→σ*(Se–Cl)	2.91	0.95	0.048	n_p(Se)→σ*(Se–Cl)	42.05	0.51	0.133
4b: Se-*-SeBr	n_s(Se)→σ*(Se–Br)	2.75	0.92	0.046	n_p(Se)→σ*(Se–Br)	39.25	0.48	0.124
4b: Se-*-SeI	n_s(Se)→σ*(Se–I)	2.05	0.90	0.039	n_p(Se)→σ*(Se–I)	25.97	0.45	0.097
4b: Se-*-SeSeMe	n_s(Se)→σ*(Se–Se)	0.65	1.01	0.023	n_p(Se)→σ*(Se–Se)	5.90	0.50	0.049
4b: Se-*-SeC$_{Me}$	n_s(Se)→σ*(Se–C)	*e*	*e*	*e*	n_p(Se)→σ*(Se–C)	2.52	0.65	0.036
5c: Te-*-TeF	n_s(Te)→n_p(Te+)	4.56	0.67	0.056	N_p(Te)→n_p(Te+)	125.85	0.32	0.188
5c: Te-*-TeCl	n_s(Te)→σ*(Se–Cl)	3.43	0.83	0.050	n_p(Te)→σ*(Te–Cl)	60.71	0.47	0.153
5c: Te-*-TeBr	n_s(Te)→σ*(Te–Br)	0.83	1.38	0.030	n_p(Te)→σ*(Te–Br)	58.03	0.44	0.145
5c: Te-*-TeI	n_s(Te)→σ*(Te–I)	3.00	0.79	0.045	n_p(Te)→σ*(Te–I)	47.90	0.42	0.128
5c: Te-*-TeTeMe	n_s(Te)→σ*(Te–Te)	0.76	0.85	0.023	n_p(Te)→σ*(Te–Te)	9.76	0.44	0.059
5c: Te-*-TeC$_{Me}$	n_s(Te)→σ*(Te–C)	*e*	*e*	*e*	n_p(Te)→σ*(Te–C)	5.87	0.56	0.052

a Second-order perturbation energy of the NBO analysis. *b* $\Delta E = E(j) - E(i)$. *c* The off-diagonal NBO Fock matrix element. See Eqn (5) in the text. *d* Not detected due to the only one n_s(G): lone pair orbital of N (G = N) being characterized as n_s(N). *e* Not printed, possibly because the evaluated $E(2)$ was less than the threshold value of 0.5 kcal mol^{-1}.

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.

S9 E. Espinosa, I. Alkorta, J. Elguero, E. Molins, *J. Chem. Phys.* **2002**, *117*, 5529. See also R. Bianchi, G. Gervasio and D. Marabello, *C. R. Chim.*, 2005, **8**, 1392.

Optimized structures given by Cartesian coordinates

Gaussian 09 programs were employed for the calculations, containing the NBO analysis. 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, as implemented from the Sapporo Basis Set Factory, with the 6-311G(d) basis set for C and H. The basis set system is called A (BSS-A). The Møller-Plesset second order energy correlation (MP2) level was applied to the calculations (MP2/BSS-A).

All positive frequencies were obtained for all compounds.

1a (N---S–F)
Symmetry C_1
energy MP2 = –901.1066934 au
Standard orientation

6	0	0.588374	-0.963982	-0.343452
6	0	0.655338	0.417433	-0.050453
6	0	1.900824	1.002765	0.251740
6	0	3.055492	0.201879	0.264915
6	0	2.987005	-1.175173	-0.011435
6	0	1.744107	-1.756185	-0.315171
1	0	1.959059	2.068522	0.466488
1	0	4.017245	0.661230	0.503090
1	0	3.889383	-1.788540	0.010490
1	0	1.671484	-2.824333	-0.536702
6	0	-0.784525	-1.459665	-0.703049
1	0	-0.993301	-1.262873	-1.767275
1	0	-0.921113	-2.539124	-0.506989
7	0	-1.712837	-0.637392	0.080617
6	0	-1.738939	-1.032184	1.493125
1	0	-2.184139	-2.037156	1.609823
1	0	-0.713569	-1.039723	1.884249
1	0	-2.331408	-0.297911	2.054006
6	0	-3.062197	-0.571645	-0.479379
1	0	-3.558033	-1.557512	-0.441405
1	0	-3.651982	0.150400	0.102265
1	0	-3.002802	-0.224512	-1.518717
16	0	-0.860733	1.342944	-0.080503
9	0	-0.054678	2.854081	-0.197405

1a (N---S–Cl)
Symmetry C_1
energy MP2 = –1261.0673823 au
Standard orientation

6	0	0.484442	-1.235180	-0.414209
6	0	0.671090	0.111491	-0.016369
6	0	1.954964	0.544736	0.366555
6	0	3.032205	-0.357483	0.337114
6	0	2.848280	-1.693182	-0.058625
6	0	1.564885	-2.128311	-0.428450
1	0	2.110738	1.576987	0.676376
1	0	4.022612	-0.008617	0.636873
1	0	3.690157	-2.387438	-0.072882
1	0	1.398302	-3.165391	-0.731728
6	0	-0.920522	-1.606627	-0.798101
1	0	-1.136063	-1.278210	-1.827925
1	0	-1.108218	-2.694570	-0.725191

7	0	-1.791123	-0.835518	0.091904
6	0	-1.790159	-1.347320	1.463690
1	0	-2.280443	-2.337752	1.514268
1	0	-0.755089	-1.437307	1.817438
1	0	-2.328971	-0.639017	2.106843
6	0	-3.147338	-0.649719	-0.416652
1	0	-3.691596	-1.610122	-0.466847
1	0	-3.687997	0.033787	0.252833
1	0	-3.098031	-0.200361	-1.417065
16	0	-0.788734	1.145163	-0.001372
17	0	0.225596	3.049623	-0.152593

1a (N---S–Br)
Symmetry C_1
energy MP2 = –3374.0390045 au
Standard orientation

6	0	1.637525	0.637986	-0.436163
6	0	0.291251	0.670838	0.005451
6	0	-0.268695	1.896730	0.412926
6	0	0.504503	3.069125	0.361699
6	0	1.837705	3.038450	-0.080747
6	0	2.401581	1.812958	-0.472401
1	0	-1.300612	1.935093	0.759695
1	0	0.056399	4.012509	0.681079
1	0	2.432133	3.953258	-0.112726
1	0	3.440709	1.764770	-0.809173
6	0	2.159473	-0.714653	-0.832999
1	0	1.814938	-0.976463	-1.846739
1	0	3.264756	-0.765726	-0.809009
7	0	1.542861	-1.667870	0.091013
6	0	2.099322	-1.589230	1.441992
1	0	3.145535	-1.949512	1.458783
1	0	2.070195	-0.548016	1.787938
1	0	1.489542	-2.207943	2.113705
6	0	1.505980	-3.040120	-0.404719
1	0	2.523660	-3.462353	-0.493453
1	0	0.922911	-3.655906	0.294284
1	0	1.013748	-3.055337	-1.385977
16	0	-0.563949	-0.900796	0.047531
35	0	-2.733218	-0.104259	-0.085892

1a (N---S–I)
Symmetry C_1
energy MP2 = –7719.4831762 au
Standard orientation

6	0	2.009789	0.637855	-0.477053
6	0	0.685718	0.685321	0.028926
6	0	0.164695	1.913855	0.478149
6	0	0.944434	3.079893	0.396829
6	0	2.251560	3.037663	-0.115840
6	0	2.780276	1.808211	-0.542275
1	0	-0.846232	1.962922	0.882728
1	0	0.523480	4.024488	0.747881
1	0	2.854008	3.945983	-0.173350
1	0	3.801622	1.751085	-0.928449
6	0	2.521446	-0.714019	-0.892336

1	0	2.086927	-1.003789	-1.863195
1	0	3.625820	-0.728348	-0.982769
7	0	2.031399	-1.666571	0.100383
6	0	2.694220	-1.530736	1.393470
1	0	3.757348	-1.838400	1.334389
1	0	2.643745	-0.484894	1.723778
1	0	2.177644	-2.162569	2.128783
6	0	2.011507	-3.046052	-0.365427
1	0	3.033174	-3.430027	-0.551198
1	0	1.530540	-3.675354	0.396661
1	0	1.426781	-3.106023	-1.293452
16	0	-0.185046	-0.878191	0.108728
53	0	-2.533128	-0.089999	-0.062090

1a (N---S–SMe)
Symmetry C_1
energy MP2 = –1238.8576566 au
Standard orientation

6	0	-0.879263	0.869148	0.502731
6	0	0.303599	0.557314	-0.212788
6	0	1.120464	1.590877	-0.709439
6	0	0.775163	2.932668	-0.481186
6	0	-0.392452	3.253923	0.231976
6	0	-1.212492	2.219548	0.710920
1	0	2.029014	1.340281	-1.259683
1	0	1.416616	3.725618	-0.872064
1	0	-0.664057	4.296535	0.407806
1	0	-2.128815	2.456204	1.258521
6	0	-1.761436	-0.248641	0.994194
1	0	-1.203508	-0.870771	1.713873
1	0	-2.649839	0.166158	1.519424
7	0	-2.137133	-1.108005	-0.122489
6	0	-3.022041	-0.420081	-1.050806
1	0	-3.986015	-0.134940	-0.574347
1	0	-2.535699	0.491871	-1.423809
1	0	-3.235759	-1.077949	-1.904868
6	0	-2.724543	-2.353588	0.342274
1	0	-3.662360	-2.190568	0.916639
1	0	-2.954748	-2.993966	-0.520941
1	0	-2.005545	-2.880002	0.986358
16	0	0.702399	-1.172872	-0.456955
16	0	2.756032	-1.151800	-0.438211
6	0	3.080116	-0.883100	1.326174
1	0	2.624874	-1.685889	1.920642
1	0	4.172755	-0.895236	1.453468
1	0	2.685428	0.095027	1.634765

1a (N---S–C_{Me})
Symmetry C_1
energy MP2 = –841.168204 au
Standard orientation

6	0	0.097589	-0.834414	-0.472046
6	0	0.882448	0.250186	0.001036
6	0	2.212765	0.015914	0.408667
6	0	2.766681	-1.272867	0.335410
6	0	1.995960	-2.348608	-0.132895

6	0	0.667890	-2.118205	-0.527330
1	0	2.823943	0.834342	0.789599
1	0	3.798940	-1.431654	0.655043
1	0	2.421147	-3.352399	-0.188975
1	0	0.055195	-2.946949	-0.892350
6	0	-1.326066	-0.598759	-0.905708
1	0	-1.342578	0.158815	-1.706626
1	0	-1.754981	-1.539975	-1.316892
7	0	-2.124205	-0.080533	0.199177
6	0	-2.286733	-1.075505	1.247379
1	0	-2.828243	-1.978712	0.886451
1	0	-1.302354	-1.388272	1.622310
1	0	-2.855702	-0.638251	2.080039
6	0	-3.412475	0.399327	-0.271039
1	0	-4.023039	-0.408543	-0.731761
1	0	-3.977819	0.820000	0.572763
1	0	-3.259129	1.190959	-1.018498
16	0	0.143212	1.859828	0.066326
6	0	1.601008	2.918125	-0.130006
1	0	1.205629	3.928680	-0.302636
1	0	2.223931	2.938511	0.773768
1	0	2.198712	2.608771	-0.998500

1b (N---Se–F)
Symmetry C_1
energy MP2 = –2903.4919973 au
Standard orientation

6	0	0.886453	-1.075117	-0.340482
6	0	0.804473	0.301248	-0.038662
6	0	1.970261	1.029554	0.259973
6	0	3.210655	0.368455	0.260880
6	0	3.296708	-1.006671	-0.022459
6	0	2.128350	-1.727253	-0.323466
1	0	1.900329	2.094670	0.478717
1	0	4.115843	0.932997	0.494805
1	0	4.263780	-1.512433	-0.009649
1	0	2.181301	-2.795257	-0.551821
6	0	-0.411614	-1.737723	-0.714012
1	0	-0.646069	-1.535991	-1.772379
1	0	-0.392458	-2.832266	-0.556725
7	0	-1.464298	-1.097249	0.088517
6	0	-1.409473	-1.530733	1.491248
1	0	-1.648432	-2.606960	1.574544
1	0	-0.401847	-1.349105	1.886039
1	0	-2.133777	-0.945979	2.072702
6	0	-2.804559	-1.294644	-0.469266
1	0	-3.087213	-2.362338	-0.452186
1	0	-3.528185	-0.723402	0.128586
1	0	-2.823289	-0.923219	-1.501876
34	0	-0.931421	1.095122	-0.049783
9	0	-0.212120	2.782577	-0.148922

1b (N---Se–Cl)
Symmetry C_1
energy MP2 = –3263.4546782 au
Standard orientation

6	0	1.151424	-1.052524	-0.393290
6	0	0.785899	0.261189	-0.019550
6	0	1.779005	1.189678	0.338831
6	0	3.129868	0.801336	0.313624
6	0	3.499140	-0.504497	-0.052895
6	0	2.502538	-1.430810	-0.402548
1	0	1.499542	2.203367	0.624817
1	0	3.896572	1.526951	0.593362
1	0	4.549932	-0.799183	-0.063026
1	0	2.772552	-2.451282	-0.687615
6	0	0.027952	-1.972265	-0.785419
1	0	-0.291449	-1.762245	-1.819624
1	0	0.311894	-3.039094	-0.711224
7	0	-1.109482	-1.654187	0.087055
6	0	-0.893328	-2.118542	1.462068
1	0	-0.866341	-3.223657	1.500181
1	0	0.058194	-1.718985	1.835127
1	0	-1.711166	-1.749776	2.094784
6	0	-2.387562	-2.134348	-0.440235
1	0	-2.409979	-3.238409	-0.480820
1	0	-3.198795	-1.784251	0.213014
1	0	-2.538901	-1.725390	-1.447705
34	0	-1.098745	0.639391	-0.002379
17	0	-0.853998	2.903921	-0.135489

1b (N---Se–Br)
Symmetry C_1
energy MP2 = –5376.4263458 au
Standard orientation

6	0	1.771558	0.735070	-0.412796
6	0	0.418986	0.810283	-0.005831
6	0	-0.128748	2.047990	0.374474
6	0	0.672568	3.202246	0.335195
6	0	2.017303	3.133657	-0.067625
6	0	2.563515	1.893213	-0.436798
1	0	-1.170359	2.110189	0.689023
1	0	0.239523	4.159808	0.632121
1	0	2.634411	4.033545	-0.089684
1	0	3.609206	1.821157	-0.748076
6	0	2.277688	-0.622224	-0.817176
1	0	1.944283	-0.863123	-1.840184
1	0	3.381942	-0.685740	-0.779802
7	0	1.649283	-1.599588	0.079081
6	0	2.193065	-1.531754	1.439230
1	0	3.252377	-1.850745	1.452409
1	0	2.120136	-0.501291	1.809533
1	0	1.604510	-2.190723	2.090955
6	0	1.687984	-2.965526	-0.442907
1	0	2.727508	-3.334479	-0.513196
1	0	1.120620	-3.622732	0.230629
1	0	1.222452	-2.985695	-1.436991
34	0	-0.540659	-0.857446	0.031379
35	0	-2.762649	0.115496	-0.083194

1b (N---Se–I)
Symmetry C_1

energy MP2 = –9721.8695846 au
Standard orientation

6	0	2.105230	0.773062	-0.443478
6	0	0.764263	0.815871	0.007510
6	0	0.207158	2.038898	0.420796
6	0	0.979179	3.212082	0.363335
6	0	2.308847	3.176794	-0.089327
6	0	2.867895	1.950620	-0.485438
1	0	-0.822532	2.079589	0.776637
1	0	0.535263	4.156396	0.685502
1	0	2.904990	4.090196	-0.127133
1	0	3.904157	1.903258	-0.831116
6	0	2.644304	-0.567731	-0.861523
1	0	2.266177	-0.833904	-1.862579
1	0	3.751442	-0.577671	-0.888509
7	0	2.113550	-1.561268	0.074906
6	0	2.709519	-1.446297	1.406923
1	0	3.784267	-1.711568	1.382737
1	0	2.601258	-0.415670	1.768551
1	0	2.183860	-2.124112	2.092676
6	0	2.191465	-2.928526	-0.432515
1	0	3.242226	-3.252251	-0.554019
1	0	1.691338	-3.603655	0.275875
1	0	1.677592	-2.984984	-1.401419
34	0	-0.155688	-0.877669	0.067084
53	0	-2.601673	0.035762	-0.064907

1b (N---Se–SeMe)
Symmetry C_1
energy MP2 = –5243.610077 au
Standard orientation

6	0	-1.697522	0.885150	0.485690
6	0	-0.426769	0.808343	-0.132937
6	0	0.175678	1.970531	-0.647360
6	0	-0.474710	3.210513	-0.529850
6	0	-1.733602	3.298283	0.088575
6	0	-2.338362	2.132357	0.586060
1	0	1.155314	1.905101	-1.124820
1	0	0.002345	4.106232	-0.934221
1	0	-2.241466	4.260729	0.176016
1	0	-3.323048	2.184215	1.059008
6	0	-2.328076	-0.379608	1.007750
1	0	-1.772426	-0.732976	1.893303
1	0	-3.380110	-0.196430	1.314794
7	0	-2.221876	-1.418157	-0.009728
6	0	-3.054424	-1.134224	-1.170448
1	0	-4.135689	-1.141184	-0.915159
1	0	-2.797538	-0.147321	-1.578794
1	0	-2.869785	-1.893937	-1.942791
6	0	-2.484213	-2.743050	0.528418
1	0	-3.522870	-2.843969	0.907349
1	0	-2.326848	-3.493569	-0.259182
1	0	-1.785534	-2.947364	1.352305
34	0	0.409843	-0.930189	-0.249878
34	0	2.646335	-0.258826	-0.243753
6	0	2.747129	0.298795	1.622957
1	0	2.482238	-0.544970	2.271798
1	0	3.783270	0.613456	1.812234

1	0	2.064431	1.143071	1.786577

1b (N---Se–C_{Me})
Symmetry C_1
energy MP2 = –2843.5385263 au
Standard orientation

6	0	0.277328	-1.192703	-0.465094
6	0	0.859970	0.014428	-0.005380
6	0	2.207953	0.022520	0.406478
6	0	2.978297	-1.151226	0.346589
6	0	2.406910	-2.349757	-0.110356
6	0	1.059377	-2.360239	-0.506500
1	0	2.665173	0.939229	0.780449
1	0	4.021463	-1.126079	0.669635
1	0	3.000075	-3.265240	-0.152782
1	0	0.600162	-3.288337	-0.857970
6	0	-1.165089	-1.200786	-0.901093
1	0	-1.283352	-0.547446	-1.782251
1	0	-1.471055	-2.229255	-1.194700
7	0	-2.010866	-0.659906	0.154848
6	0	-2.043961	-1.534681	1.316547
1	0	-2.493059	-2.524808	1.080819
1	0	-1.023418	-1.696227	1.690441
1	0	-2.637966	-1.061944	2.111454
6	0	-3.349336	-0.371663	-0.330909
1	0	-3.877268	-1.284318	-0.683550
1	0	-3.942427	0.080144	0.477007
1	0	-3.290411	0.343606	-1.163904
34	0	-0.215162	1.595475	0.047448
6	0	1.222266	2.888576	-0.222242
1	0	0.721154	3.843247	-0.433836
1	0	1.840536	3.004262	0.676503
1	0	1.839659	2.599547	-1.082738

2a (O---S–F)
Symmetry C_1
energy MP2 = –881.7703824 au
Standard orientation

6	0	0.422629	-0.895070	-0.423271
6	0	0.314354	0.469734	-0.065908
6	0	1.455075	1.180399	0.358331
6	0	2.697144	0.527345	0.415769
6	0	2.810685	-0.831695	0.077744
6	0	1.667203	-1.537247	-0.331462
1	0	1.371979	2.231955	0.630465
1	0	3.577269	1.085927	0.740617
1	0	3.775896	-1.337169	0.137991
1	0	1.739211	-2.595965	-0.594447
6	0	-0.827117	-1.588619	-0.898351
1	0	-1.065079	-1.296815	-1.932730
1	0	-0.727818	-2.686582	-0.845322
8	0	-1.942162	-1.143690	-0.126178
6	0	-1.924106	-1.660002	1.204489
1	0	-2.017653	-2.758842	1.184596
1	0	-0.994438	-1.380529	1.726812
1	0	-2.785151	-1.222060	1.721836

16	0	-1.276345	1.244738	-0.147683
9	0	-0.734509	2.800524	-0.157946

2a (O---S–Cl)
Symmetry C_1
energy MP2 = –1241.7356157 au
Standard orientation

6	0	1.159629	0.169811	-0.496553
6	0	-0.150352	0.418859	-0.014610
6	0	-0.495948	1.695398	0.468603
6	0	0.454916	2.728455	0.454266
6	0	1.757304	2.493630	-0.016619
6	0	2.101527	1.212442	-0.476502
1	0	-1.502367	1.883121	0.842694
1	0	0.174223	3.716636	0.824098
1	0	2.497241	3.295760	-0.018971
1	0	3.113708	1.013980	-0.838867
6	0	1.511113	-1.209788	-0.994634
1	0	0.941410	-1.449124	-1.905020
1	0	2.591420	-1.275751	-1.216374
8	0	1.132622	-2.207661	-0.050742
6	0	1.899314	-2.139214	1.146109
1	0	2.972730	-2.278884	0.926629
1	0	1.760347	-1.172631	1.658876
1	0	1.547158	-2.951954	1.791890
16	0	-1.272609	-0.961508	0.003107
17	0	-3.071772	0.002748	-0.125241

2a (O---S–Br)
Symmetry C_1
energy MP2 = –3354.7079255 au
Standard orientation

6	0	1.645000	0.185479	-0.511830
6	0	0.349102	0.416644	0.016409
6	0	0.005018	1.687740	0.515057
6	0	0.939121	2.734577	0.467944
6	0	2.226385	2.518601	-0.051465
6	0	2.571236	1.242795	-0.525193
1	0	-0.990047	1.860570	0.926028
1	0	0.658291	3.718115	0.850323
1	0	2.954317	3.331302	-0.080903
1	0	3.572537	1.058903	-0.924076
6	0	2.007258	-1.189214	-1.017070
1	0	1.384875	-1.459484	-1.882984
1	0	3.071440	-1.218983	-1.313250
8	0	1.734356	-2.189344	-0.040062
6	0	2.571567	-2.070751	1.103531
1	0	3.635121	-2.155551	0.816949
1	0	2.415373	-1.108709	1.620102
1	0	2.305504	-2.895423	1.775008
16	0	-0.742898	-0.986776	0.081395
35	0	-2.710972	-0.028080	-0.078666

2a (O---S–I)

Symmetry C_1
energy MP2 = –7700.1552981 au
Standard orientation

6	0	2.036750	0.187974	-0.528370
6	0	0.767499	0.418342	0.061989
6	0	0.447051	1.689500	0.576567
6	0	1.372356	2.740236	0.480757
6	0	2.631242	2.527096	-0.105731
6	0	2.955168	1.251452	-0.593571
1	0	-0.526267	1.859896	1.039102
1	0	1.108352	3.723257	0.876257
1	0	3.353322	3.342518	-0.176609
1	0	3.935152	1.070883	-1.043658
6	0	2.394586	-1.186757	-1.039236
1	0	1.693789	-1.501598	-1.825974
1	0	3.420498	-1.179531	-1.450730
8	0	2.277837	-2.175089	-0.020905
6	0	3.219870	-1.985578	1.025854
1	0	4.252045	-2.004471	0.631345
1	0	3.055753	-1.028762	1.550080
1	0	3.081644	-2.816031	1.728193
16	0	-0.311358	-0.992841	0.197814
53	0	-2.482309	-0.038370	-0.067837

2a (O---S–SMe)
Symmetry C_1
energy MP2 = –1219.5337671 au
Standard orientation

6	0	-1.269727	0.251383	0.520412
6	0	-0.040527	0.371690	-0.175460
6	0	0.342015	1.609568	-0.726073
6	0	-0.483868	2.734398	-0.572342
6	0	-1.704521	2.629742	0.115924
6	0	-2.089400	1.388531	0.646812
1	0	1.290193	1.688992	-1.260848
1	0	-0.174751	3.689642	-1.002339
1	0	-2.350463	3.501882	0.232840
1	0	-3.040069	1.293483	1.178832
6	0	-1.699250	-1.078541	1.094580
1	0	-0.951376	-1.450171	1.810194
1	0	-2.667541	-0.961572	1.616025
8	0	-1.795618	-2.091670	0.101040
6	0	-2.803881	-1.811908	-0.858271
1	0	-3.787644	-1.686846	-0.369517
1	0	-2.574204	-0.899115	-1.433905
1	0	-2.840662	-2.672130	-1.537191
16	0	0.962219	-1.101252	-0.343615
16	0	2.864731	-0.363228	-0.455936
6	0	3.166458	0.089280	1.274902
1	0	3.058357	-0.792149	1.919816
1	0	4.198399	0.467248	1.324669
1	0	2.469726	0.880903	1.583013

2a (O---S–C_{Me})
Symmetry C_1
energy MP2 = –821.8455735 au

Standard orientation

6	0	0.704325	0.456254	-0.489223
6	0	-0.611820	0.168552	-0.038989
6	0	-1.434778	1.222235	0.411789
6	0	-0.966757	2.546767	0.407293
6	0	0.333771	2.837427	-0.032812
6	0	1.157205	1.787233	-0.470037
1	0	-2.443318	1.019802	0.772049
1	0	-1.622037	3.346973	0.758229
1	0	0.702547	3.864699	-0.033783
1	0	2.172914	1.998929	-0.815462
6	0	1.606637	-0.649883	-0.985306
1	0	1.125221	-1.195188	-1.810236
1	0	2.555927	-0.213145	-1.348454
8	0	1.871021	-1.635965	0.004365
6	0	2.561318	-1.104671	1.123383
1	0	3.509334	-0.627532	0.812265
1	0	1.950083	-0.360612	1.662119
1	0	2.779953	-1.947953	1.789481
16	0	-1.140270	-1.520215	-0.049359
6	0	-2.939261	-1.340942	-0.062094
1	0	-3.329258	-2.351914	-0.242791
1	0	-3.325425	-0.984557	0.901817
1	0	-3.263621	-0.676167	-0.874427

2b (O---Se–F)
Symmetry C_1
energy MP2 = –2884.1538704 au
Standard orientation

6	0	-1.083655	0.762176	-0.402523
6	0	-0.435507	-0.438628	-0.040596
6	0	-1.186172	-1.557362	0.365722
6	0	-2.587843	-1.467515	0.405270
6	0	-3.241617	-0.270978	0.062542
6	0	-2.483600	0.843087	-0.334628
1	0	-0.680451	-2.483651	0.637887
1	0	-3.169489	-2.336928	0.718667
1	0	-4.329966	-0.204917	0.108615
1	0	-2.980211	1.779452	-0.603165
6	0	-0.210341	1.895723	-0.872194
1	0	0.111240	1.736976	-1.913033
1	0	-0.716880	2.871938	-0.791461
8	0	1.005009	1.901511	-0.112125
6	0	0.809957	2.390856	1.219552
1	0	0.498496	3.447290	1.183388
1	0	0.049063	1.795826	1.749315
1	0	1.775176	2.300861	1.729870
34	0	1.471598	-0.488796	-0.106628
9	0	1.542366	-2.271560	-0.079624

2b (O---Se–Cl)
Symmetry C_1
energy MP2 = –3244.1186462 au
Standard orientation

6	0	1.501395	-0.075041	-0.455752
6	0	0.299442	0.534250	-0.025100

6	0	0.304874	1.864646	0.430917
6	0	1.508111	2.590359	0.442016
6	0	2.708402	1.993976	0.020754
6	0	2.698117	0.659599	-0.416874
1	0	-0.620365	2.333540	0.765947
1	0	1.503516	3.624144	0.793576
1	0	3.642253	2.558384	0.040038
1	0	3.626127	0.180384	-0.740439
6	0	1.446117	-1.500121	-0.942626
1	0	0.969421	-1.556291	-1.933280
1	0	2.454760	-1.944585	-0.999216
8	0	0.604766	-2.278274	-0.088112
6	0	1.191044	-2.502983	1.194782
1	0	2.120634	-3.086998	1.087506
1	0	1.412893	-1.550439	1.702906
1	0	0.458666	-3.072737	1.777869
34	0	-1.283394	-0.554531	-0.051146
17	0	-2.747979	1.070983	-0.090572

2b (O---Se–Br)
Symmetry C_1
energy MP2 = –5357.0908835 au
Standard orientation

6	0	1.884738	0.228566	-0.475082
6	0	0.581712	0.531755	-0.012982
6	0	0.283076	1.821201	0.462378
6	0	1.278533	2.812706	0.459622
6	0	2.575570	2.523114	0.004317
6	0	2.871922	1.228139	-0.450841
1	0	-0.718789	2.054320	0.823493
1	0	1.036121	3.812295	0.826279
1	0	3.348671	3.293375	0.011150
1	0	3.879554	0.986108	-0.799657
6	0	2.169055	-1.165275	-0.973536
1	0	1.674840	-1.342038	-1.941106
1	0	3.254394	-1.334069	-1.084326
8	0	1.600985	-2.134363	-0.090871
6	0	2.273846	-2.185372	1.166703
1	0	3.325012	-2.488250	1.022524
1	0	2.242035	-1.208284	1.675982
1	0	1.750892	-2.935306	1.771091
34	0	-0.689490	-0.910668	-0.015164
35	0	-2.647676	0.355156	-0.061325

2b (O---Se–I)
Symmetry C_1
energy MP2 = –9702.5365683 au
Standard orientation

6	0	2.214674	0.311031	-0.506306
6	0	0.914034	0.535321	0.007325
6	0	0.563205	1.800068	0.512752
6	0	1.496939	2.849172	0.483985
6	0	2.788538	2.640529	-0.027280
6	0	3.140160	1.369252	-0.508517
1	0	-0.434783	1.972230	0.917604
1	0	1.211307	3.828519	0.873460

1	0	3.515148	3.454696	-0.043378
1	0	4.145661	1.190010	-0.898938
6	0	2.579198	-1.058919	-1.021352
1	0	2.016546	-1.292404	-1.937984
1	0	3.661031	-1.118909	-1.235743
8	0	2.199617	-2.070869	-0.090054
6	0	2.965379	-2.018671	1.110412
1	0	4.036198	-2.172418	0.889832
1	0	2.837368	-1.052529	1.626207
1	0	2.600150	-2.829959	1.750693
34	0	-0.263679	-0.986637	0.044337
53	0	-2.494212	0.180504	-0.057262

2b (O---Se–SeMe)
Symmetry C_1
energy MP2 = –5224.2836861 au
Standard orientation

6	0	-1.928540	0.353135	0.521789
6	0	-0.672783	0.515714	-0.111531
6	0	-0.334306	1.745592	-0.704069
6	0	-1.233866	2.823151	-0.651360
6	0	-2.482195	2.676096	-0.023174
6	0	-2.822062	1.439977	0.549343
1	0	0.635637	1.861537	-1.191914
1	0	-0.959304	3.774188	-1.113341
1	0	-3.184982	3.510628	0.013671
1	0	-3.794795	1.310262	1.032178
6	0	-2.299465	-0.973119	1.141787
1	0	-1.623533	-1.212384	1.976743
1	0	-3.337481	-0.936060	1.520596
8	0	-2.146286	-2.050320	0.224323
6	0	-3.043118	-1.956095	-0.874312
1	0	-4.090720	-1.944479	-0.522816
1	0	-2.856106	-1.047781	-1.471653
1	0	-2.874716	-2.844071	-1.495010
34	0	0.510402	-1.009075	-0.155767
34	0	2.554872	0.056322	-0.276609
6	0	2.649776	0.690493	1.565371
1	0	2.593458	-0.163987	2.250209
1	0	3.615294	1.204742	1.675117
1	0	1.827554	1.393887	1.749360

2b (O---Se–C_{Me})
Symmetry C_1
energy MP2 = –2824.214722 au
Standard orientation

6	0	-1.205489	0.141736	-0.484500
6	0	-0.085280	-0.594652	-0.024058
6	0	-0.263156	-1.915325	0.435513
6	0	-1.536926	-2.508288	0.424819
6	0	-2.651025	-1.784333	-0.028836
6	0	-2.475234	-0.463009	-0.470623
1	0	0.584976	-2.490139	0.808169
1	0	-1.654347	-3.533608	0.782162
1	0	-3.643217	-2.239056	-0.032367
1	0	-3.335701	0.113473	-0.821395

6	0	-1.034320	1.556967	-0.984440
1	0	-0.364539	1.575716	-1.857373
1	0	-2.017465	1.970803	-1.276500
8	0	-0.411320	2.401612	-0.024874
6	0	-1.194130	2.553606	1.149440
1	0	-2.192476	2.961254	0.905761
1	0	-1.320810	1.593939	1.678766
1	0	-0.659314	3.259587	1.795963
34	0	1.626756	0.253150	-0.025286
6	0	2.730420	-1.346377	-0.106431
1	0	3.747817	-0.988912	-0.315401
1	0	2.731461	-1.885999	0.848405
1	0	2.395307	-1.998993	-0.922786

3a (S---S–F)
Symmetry C_1
energy MP2 = –1204.3534964 au
Standard orientation

6	0	0.319751	-0.874462	-0.566101
6	0	0.626482	0.410664	-0.055585
6	0	1.907784	0.665264	0.475306
6	0	2.872516	-0.354810	0.501573
6	0	2.568617	-1.637580	0.017506
6	0	1.289963	-1.889350	-0.506236
1	0	2.145678	1.656726	0.859137
1	0	3.859856	-0.144528	0.917582
1	0	3.313924	-2.433994	0.052004
1	0	1.040036	-2.883114	-0.886980
6	0	-1.046318	-1.131139	-1.141720
1	0	-1.176928	-0.611081	-2.104862
1	0	-1.233521	-2.204733	-1.289195
16	0	-2.311946	-0.402979	-0.070612
6	0	-1.956842	-1.279729	1.468383
1	0	-2.142855	-2.356210	1.348155
1	0	-0.916695	-1.103477	1.776671
1	0	-2.640087	-0.873087	2.225504
16	0	-0.590512	1.709880	-0.086391
9	0	0.522022	2.954437	-0.171637

3a (S---S–Cl)
Symmetry C_1
energy MP2 = –1564.3187378 au
Standard orientation

6	0	0.756233	0.654377	-0.640635
6	0	-0.478278	0.426975	0.019027
6	0	-1.176660	1.498603	0.608241
6	0	-0.660667	2.801596	0.529454
6	0	0.564663	3.040000	-0.114616
6	0	1.265619	1.965272	-0.685108
1	0	-2.124442	1.312324	1.114929
1	0	-1.212703	3.625640	0.985939
1	0	0.972951	4.050794	-0.169918
1	0	2.221776	2.141331	-1.185074
6	0	1.528433	-0.492481	-1.231471
1	0	0.932420	-1.028263	-1.986617
1	0	2.460888	-0.141101	-1.697059

16	0	1.899332	-1.752832	0.027360
6	0	2.764351	-0.718743	1.231063
1	0	3.669008	-0.279821	0.786298
1	0	2.104887	0.076041	1.607067
1	0	3.053091	-1.377633	2.060707
16	0	-1.077677	-1.246356	0.125524
17	0	-3.094501	-0.908582	-0.132832

3a (S---S–Br)
Symmetry C_1
energy MP2 = –3677.2916306 au
Standard orientation

6	0	-1.331495	0.542737	0.647897
6	0	-0.099717	0.551894	-0.055147
6	0	0.366179	1.737404	-0.655972
6	0	-0.376633	2.922674	-0.542693
6	0	-1.599286	2.927532	0.149227
6	0	-2.069364	1.738472	0.729475
1	0	1.312650	1.731530	-1.198499
1	0	-0.003193	3.836944	-1.008379
1	0	-2.183207	3.845906	0.233774
1	0	-3.022536	1.732555	1.264877
6	0	-1.865084	-0.731565	1.240936
1	0	-1.147354	-1.175431	1.947937
1	0	-2.816556	-0.553444	1.763244
16	0	-2.090939	-2.009240	-0.035935
6	0	-3.188165	-1.110857	-1.156427
1	0	-4.124407	-0.838561	-0.648139
1	0	-2.694562	-0.209525	-1.546214
1	0	-3.413974	-1.792242	-1.987458
16	0	0.781290	-0.987717	-0.210820
35	0	2.857969	-0.288462	0.085233

3a (S---S–I)
Symmetry C_1
energy MP2 = –8022.7392527 au
Standard orientation

6	0	-1.711388	0.497625	0.642806
6	0	-0.521782	0.575408	-0.125480
6	0	-0.142185	1.789850	-0.729512
6	0	-0.924333	2.940779	-0.551072
6	0	-2.102463	2.880512	0.212579
6	0	-2.488357	1.662607	0.794409
1	0	0.770894	1.832507	-1.326065
1	0	-0.617507	3.878270	-1.019225
1	0	-2.716610	3.772140	0.352117
1	0	-3.406834	1.608100	1.384924
6	0	-2.168433	-0.807201	1.233117
1	0	-1.373266	-1.277523	1.830670
1	0	-3.052561	-0.658093	1.870512
16	0	-2.549963	-2.030790	-0.061591
6	0	-3.806252	-1.103945	-0.972138
1	0	-4.663943	-0.869495	-0.324993
1	0	-3.384699	-0.178560	-1.389160
1	0	-4.141844	-1.752787	-1.792176
16	0	0.408079	-0.924201	-0.373641

53	0	2.642409	-0.182802	0.082054

3a (S---S–SSMe)
Symmetry C_1
energy MP2 = –1542.1170063 au
Standard orientation

6	0	-0.898251	0.531006	0.596610
6	0	0.250973	0.473492	-0.232228
6	0	0.758304	1.645209	-0.825944
6	0	0.139334	2.882522	-0.590689
6	0	-0.999494	2.955775	0.229604
6	0	-1.508547	1.783652	0.810131
1	0	1.645031	1.582162	-1.459228
1	0	0.541809	3.784002	-1.057566
1	0	-1.486462	3.914929	0.415802
1	0	-2.392875	1.833866	1.451277
6	0	-1.487802	-0.708420	1.211939
1	0	-0.716051	-1.313147	1.711248
1	0	-2.260407	-0.442221	1.948806
16	0	-2.205569	-1.827799	-0.034304
6	0	-3.400775	-0.696210	-0.780353
1	0	-4.124252	-0.340757	-0.032118
1	0	-2.892872	0.158445	-1.248639
1	0	-3.934641	-1.267885	-1.551359
16	0	1.018024	-1.116995	-0.518739
16	0	3.013187	-0.658663	-0.436698
6	0	3.233839	-0.402887	1.344959
1	0	4.298207	-0.171247	1.499175
1	0	2.621442	0.446191	1.678985
1	0	2.965308	-1.313849	1.895304

3a (S---S–C_{Me})
Symmetry C_1
energy MP2 = –1144.4284973 au
Standard orientation

6	0	-0.275219	0.601095	0.600459
6	0	0.905613	0.053347	0.029415
6	0	1.890790	0.917466	-0.492497
6	0	1.720530	2.310748	-0.445541
6	0	0.557371	2.860058	0.115679
6	0	-0.426208	2.000902	0.631067
1	0	2.794957	0.509221	-0.944457
1	0	2.496660	2.960524	-0.855492
1	0	0.418694	3.941953	0.157208
1	0	-1.331175	2.418780	1.080592
6	0	-1.358821	-0.278028	1.160462
1	0	-0.936210	-1.078856	1.785832
1	0	-2.055995	0.315399	1.770918
16	0	-2.303826	-1.154872	-0.129478
6	0	-2.926206	0.272672	-1.045301
1	0	-3.538245	0.918060	-0.398037
1	0	-2.099867	0.851872	-1.480359
1	0	-3.555895	-0.122862	-1.853715
16	0	1.075061	-1.707604	-0.015926
6	0	2.873800	-1.903326	-0.030043
1	0	3.050605	-2.974406	0.138315

1	0	3.310233	-1.624565	-0.997819
1	0	3.336574	-1.325096	0.781273

3b (S---Se–F)
Symmetry C_1
energy MP2 = –3206.7392001 au
Standard orientation

6	0	0.966377	-0.880269	-0.505855
6	0	0.626665	0.414445	-0.051013
6	0	1.632311	1.275485	0.430477
6	0	2.966515	0.837946	0.471939
6	0	3.309120	-0.455200	0.043035
6	0	2.304396	-1.308309	-0.441027
1	0	1.368294	2.277769	0.765957
1	0	3.736927	1.510788	0.854209
1	0	4.344304	-0.797962	0.087550
1	0	2.558155	-2.315230	-0.783271
6	0	-0.106211	-1.776341	-1.066875
1	0	-0.391676	-1.468848	-2.086706
1	0	0.202447	-2.831665	-1.087887
16	0	-1.630441	-1.590976	-0.109486
6	0	-1.049363	-2.110324	1.520238
1	0	-0.800706	-3.180573	1.508801
1	0	-0.176566	-1.511480	1.815341
1	0	-1.876792	-1.929948	2.218770
34	0	-1.197449	1.024087	-0.090366
9	0	-0.673658	2.766580	-0.097119

3b (S---Se–Cl)
Symmetry C_1
energy MP2 = –3566.7031958 au
Standard orientation

6	0	1.309477	0.523497	-0.598309
6	0	0.029791	0.703322	-0.020658
6	0	-0.317996	1.943054	0.546862
6	0	0.603294	3.003696	0.534546
6	0	1.877655	2.834059	-0.030611
6	0	2.224215	1.591885	-0.586379
1	0	-1.304131	2.080275	0.990682
1	0	0.322538	3.959958	0.980625
1	0	2.596643	3.655149	-0.032945
1	0	3.214788	1.446135	-1.025466
6	0	1.687733	-0.807510	-1.189117
1	0	1.113895	-1.019067	-2.106242
1	0	2.761614	-0.859723	-1.420085
16	0	1.225670	-2.151767	-0.060920
6	0	2.126157	-1.643768	1.421338
1	0	3.208946	-1.665321	1.234126
1	0	1.811071	-0.638604	1.734210
1	0	1.874864	-2.371677	2.203888
34	0	-1.195324	-0.786481	0.003628
17	0	-3.047759	0.452475	-0.127849

3b (S---Se–Br)

Symmetry C_1
energy MP2 = –5679.675519 au
Standard orientation

6	0	1.633371	0.643851	-0.621869
6	0	0.361395	0.683570	-0.001299
6	0	-0.095945	1.874965	0.591113
6	0	0.704524	3.028896	0.557436
6	0	1.968520	3.000437	-0.053913
6	0	2.426801	1.805469	-0.631859
1	0	-1.074795	1.903130	1.070514
1	0	0.338718	3.946722	1.022260
1	0	2.594301	3.894387	-0.074699
1	0	3.411708	1.769516	-1.105091
6	0	2.138926	-0.637669	-1.225928
1	0	1.542293	-0.932586	-2.104481
1	0	3.194818	-0.556149	-1.522218
16	0	1.923213	-2.015881	-0.062865
6	0	2.822900	-1.365763	1.363473
1	0	3.884424	-1.227803	1.113886
1	0	2.381567	-0.415532	1.694915
1	0	2.728870	-2.115723	2.159828
34	0	-0.681607	-0.937765	0.055514
35	0	-2.810333	0.104846	-0.085699

3b (S---Se–I)
Symmetry C_1
energy MP2 = –10025.1209058 au
Standard orientation

6	0	-1.935663	0.650104	0.655474
6	0	-0.696766	0.680371	-0.030223
6	0	-0.263754	1.864033	-0.655356
6	0	-1.048260	3.026737	-0.582230
6	0	-2.276155	3.011316	0.099378
6	0	-2.713564	1.822079	0.704451
1	0	0.687144	1.881477	-1.189689
1	0	-0.700039	3.939454	-1.070041
1	0	-2.890545	3.911774	0.153938
1	0	-3.671916	1.797593	1.230050
6	0	-2.435613	-0.625798	1.275004
1	0	-1.757382	-0.983041	2.066254
1	0	-3.441493	-0.494323	1.699836
16	0	-2.450645	-1.975684	0.055606
6	0	-3.460834	-1.209502	-1.232837
1	0	-4.465833	-0.982260	-0.849494
1	0	-2.981628	-0.294211	-1.607415
1	0	-3.539407	-1.943514	-2.045694
34	0	0.312072	-0.958315	-0.142402
53	0	2.648012	0.038579	0.078533

3b (S---Se–SeMe)
Symmetry C_1
energy MP2 = –5546.8668862 au
Standard orientation

6	0	-1.580757	0.661693	0.625820
6	0	-0.409496	0.651574	-0.170532
6	0	0.001836	1.817069	-0.843118

6	0	-0.737879	3.004027	-0.717612
6	0	-1.900659	3.029910	0.070969
6	0	-2.313254	1.861328	0.730465
1	0	0.908385	1.796051	-1.450897
1	0	-0.409874	3.901735	-1.246303
1	0	-2.481674	3.948833	0.170598
1	0	-3.218153	1.873353	1.344371
6	0	-2.068919	-0.581085	1.318860
1	0	-1.282379	-1.023970	1.949360
1	0	-2.942239	-0.356111	1.949092
16	0	-2.496686	-1.898840	0.136351
6	0	-3.692743	-0.999151	-0.877121
1	0	-4.543294	-0.659316	-0.268510
1	0	-3.217450	-0.141126	-1.372783
1	0	-4.053509	-1.705334	-1.636911
34	0	0.589878	-0.990635	-0.330982
34	0	2.731519	-0.114564	-0.213614
6	0	2.715774	0.374006	1.673648
1	0	3.702206	0.803504	1.900022
1	0	1.932920	1.124559	1.844264
1	0	2.541144	-0.520201	2.284045

3b (S---Se–C_{Me})
Symmetry C_1
energy MP2 = –3146.7971124 au
Standard orientation

6	0	-0.820364	0.647523	0.616898
6	0	0.457602	0.633900	0.002750
6	0	0.978983	1.819097	-0.553619
6	0	0.252371	3.019537	-0.490966
6	0	-1.013945	3.042812	0.115076
6	0	-1.538206	1.859286	0.658722
1	0	1.952988	1.809772	-1.045119
1	0	0.672855	3.927974	-0.927748
1	0	-1.587626	3.970285	0.164603
1	0	-2.522316	1.869934	1.135371
6	0	-1.423983	-0.598340	1.204521
1	0	-0.713354	-1.103163	1.876705
1	0	-2.335983	-0.355154	1.770017
16	0	-1.818450	-1.848599	-0.060505
6	0	-2.913987	-0.861683	-1.105199
1	0	-3.788037	-0.511827	-0.536554
1	0	-2.377649	-0.004340	-1.535342
1	0	-3.253857	-1.520999	-1.915203
34	0	1.446468	-1.001362	-0.076888
6	0	3.221335	-0.241547	0.192696
1	0	3.880881	-1.095034	0.400594
1	0	3.578298	0.276199	-0.705514
1	0	3.210242	0.436733	1.055190

4a (Se---S–F)
Symmetry C_1
energy MP2 = –3206.7220837 au
Standard orientation

6	0	0.5947	-0.83213	-0.63332
6	0	1.056	0.37195	-0.04555

6	0	2.34103	0.42585	0.53103
6	0	3.16056	-0.71465	0.52974
6	0	2.70221	-1.91924	-0.02769
6	0	1.41917	-1.97038	-0.59754
1	0	2.69467	1.35762	0.97211
1	0	4.15296	-0.6606	0.98173
1	0	3.33181	-2.8106	-0.01472
1	0	1.05299	-2.90202	-1.03677
6	0	-0.77101	-0.88305	-1.25349
1	0	-0.83776	-0.23905	-2.14457
1	0	-1.06794	-1.90657	-1.51873
34	0	-2.06159	-0.10328	-0.01808
6	0	-1.63717	-1.22409	1.50818
1	0	-1.87258	-2.2721	1.28196
1	0	-0.57518	-1.10994	1.76292
1	0	-2.2636	-0.87292	2.33821
16	0	0.03287	1.82832	-0.03797
9	0	1.30664	2.90546	-0.16313

4a (Se---S–Cl)
Symmetry C_1
energy MP2 = –3566.6878454 au
Standard orientation

6	0	-0.061177	1.002565	0.694984
6	0	0.969929	0.341306	-0.019970
6	0	1.987401	1.082370	-0.650820
6	0	1.995524	2.483244	-0.561031
6	0	0.975951	3.152294	0.136131
6	0	-0.045845	2.409137	0.749083
1	0	2.773598	0.560878	-1.198606
1	0	2.791360	3.048381	-1.050316
1	0	0.973471	4.241963	0.200732
1	0	-0.843784	2.923461	1.291253
6	0	-1.174555	0.223722	1.328242
1	0	-0.796229	-0.538638	2.025539
1	0	-1.880695	0.882120	1.851666
34	0	-2.130964	-0.810421	-0.032800
6	0	-2.474218	0.670769	-1.240598
1	0	-3.091581	1.430072	-0.742826
1	0	-1.524677	1.105878	-1.578880
1	0	-3.021034	0.254533	-2.096673
16	0	0.908020	-1.434229	-0.144126
17	0	2.912116	-1.858772	0.123718

4a (Se---S–Br)
Symmetry C_1
energy MP2 = –5679.6608911 au
Standard orientation

6	0	-0.820472	1.010822	0.700997
6	0	0.351546	0.745098	-0.052671
6	0	1.037615	1.793511	-0.695109
6	0	0.577050	3.113870	-0.574938
6	0	-0.583898	3.391783	0.165794
6	0	-1.275732	2.340313	0.788307
1	0	1.935163	1.573960	-1.275371
1	0	1.119329	3.919912	-1.073343

1	0	-0.949858	4.416224	0.256371
1	0	-2.182420	2.549103	1.362362
6	0	-1.593185	-0.105495	1.336014
1	0	-0.960745	-0.722178	1.991617
1	0	-2.453641	0.272295	1.904419
34	0	-2.218757	-1.356863	-0.036183
6	0	-3.078537	-0.034985	-1.169428
1	0	-3.885165	0.468287	-0.620204
1	0	-2.337918	0.694510	-1.522563
1	0	-3.499869	-0.582820	-2.022391
16	0	0.873533	-0.949595	-0.220355
35	0	3.056858	-0.708341	0.078892

4a (Se---S–I)
Symmetry C_1
energy MP2 = –10025.1085851 au
Standard orientation

6	0	-1.248535	0.945789	0.692440
6	0	-0.092341	0.826951	-0.120720
6	0	0.446065	1.956909	-0.765850
6	0	-0.141151	3.218377	-0.585288
6	0	-1.283789	3.353387	0.221555
6	0	-1.830078	2.220164	0.844642
1	0	1.330632	1.846041	-1.395801
1	0	0.287622	4.089178	-1.085314
1	0	-1.747365	4.331512	0.363321
1	0	-2.721901	2.319472	1.469180
6	0	-1.877716	-0.257875	1.325357
1	0	-1.144680	-0.863784	1.876986
1	0	-2.699252	0.026201	1.996851
34	0	-2.567566	-1.473855	-0.050320
6	0	-3.668191	-0.163833	-0.968977
1	0	-4.433176	0.234515	-0.289289
1	0	-3.040248	0.646804	-1.361176
1	0	-4.154678	-0.692835	-1.798961
16	0	0.587013	-0.801027	-0.373749
53	0	2.913255	-0.407713	0.076531

4a (Se---S–SMe)
Symmetry C_1
energy MP2 = –3544.4861371 au
Standard orientation

6	0	-0.353461	0.882309	0.631929
6	0	0.725525	0.574179	-0.235681
6	0	1.456525	1.604263	-0.857591
6	0	1.133657	2.947891	-0.612888
6	0	0.068012	3.270050	0.245120
6	0	-0.665357	2.239813	0.853796
1	0	2.284553	1.345903	-1.520196
1	0	1.707366	3.738398	-1.101270
1	0	-0.189549	4.312992	0.439539
1	0	-1.492779	2.485039	1.525236
6	0	-1.175089	-0.191330	1.279410
1	0	-0.547343	-0.978629	1.720741
1	0	-1.833098	0.226697	2.053533
34	0	-2.280018	-1.141200	-0.035272

6	0	-3.163223	0.431962	-0.753613
1	0	-3.726730	0.948142	0.035078
1	0	-2.424390	1.106957	-1.204700
1	0	-3.858191	0.073974	-1.524627
16	0	1.115325	-1.144770	-0.537841
16	0	3.163051	-1.141049	-0.441062
6	0	3.419936	-0.951101	1.343805
1	0	4.507928	-0.957722	1.506821
1	0	3.004500	0.009025	1.680348
1	0	2.955170	-1.785086	1.885450

4a (Se---S–C_{Me})
Symmetry C_1
energy MP2 = –3146.7975832 au
Standard orientation

6	0	0.292135	0.721954	0.647131
6	0	1.326973	-0.053745	0.055354
6	0	2.446989	0.592460	-0.507341
6	0	2.554475	1.992755	-0.481098
6	0	1.539065	2.766876	0.101309
6	0	0.421880	2.124739	0.658474
1	0	3.241314	0.009684	-0.973769
1	0	3.431004	2.471928	-0.922359
1	0	1.617596	3.855248	0.128889
1	0	-0.367900	2.717995	1.127504
6	0	-0.920199	0.082831	1.252029
1	0	-0.662214	-0.815491	1.831547
1	0	-1.455298	0.789139	1.901678
34	0	-2.181873	-0.559047	-0.110149
6	0	-2.468031	1.162852	-0.959996
1	0	-2.882155	1.880973	-0.239357
1	0	-1.526480	1.538442	-1.381075
1	0	-3.193822	0.996694	-1.767079
16	0	1.137130	-1.811503	0.041578
6	0	2.847112	-2.373947	-0.126756
1	0	2.811964	-3.459819	0.035270
1	0	3.244390	-2.181924	-1.131852
1	0	3.488789	-1.911880	0.635788

4b (Se---Se–F)
Symmetry C_1
energy MP2 = –5209.10778 au
Standard orientation

6	0	0.734396	-1.125632	-0.558871
6	0	1.052313	0.156795	-0.053383
6	0	2.338402	0.409883	0.462317
6	0	3.296803	-0.616801	0.491776
6	0	2.982458	-1.900133	0.015322
6	0	1.701533	-2.146302	-0.504719
1	0	2.582492	1.404384	0.834555
1	0	4.287461	-0.411152	0.902483
1	0	3.722498	-2.701547	0.050264
1	0	1.447482	-3.138983	-0.886022
6	0	-0.618698	-1.388375	-1.157510
1	0	-0.734664	-0.897531	-2.137472
1	0	-0.830924	-2.461107	-1.260784

34	0	-1.983362	-0.543945	-0.057070
6	0	-1.527529	-1.406520	1.619766
1	0	-1.752168	-2.479174	1.559577
1	0	-0.463654	-1.236777	1.831850
1	0	-2.147873	-0.934135	2.392040
34	0	-0.240015	1.584415	-0.063075
9	0	1.080680	2.842506	-0.121086

4b (Se---Se–Cl)
Symmetry C_1
energy MP2 = –5569.0723486 au
Standard orientation

6	0	0.397126	1.316716	-0.654888
6	0	-0.703219	0.692289	-0.019189
6	0	-1.703183	1.473236	0.588453
6	0	-1.612754	2.875151	0.561790
6	0	-0.522388	3.505529	-0.059288
6	0	0.478223	2.721559	-0.656428
1	0	-2.549608	0.988066	1.075129
1	0	-2.393037	3.470552	1.040221
1	0	-0.446153	4.594204	-0.073459
1	0	1.332548	3.202045	-1.140689
6	0	1.477813	0.488530	-1.286191
1	0	1.106061	-0.088015	-2.147990
1	0	2.338839	1.096432	-1.594691
34	0	2.056323	-0.886222	-0.025675
6	0	2.419114	0.289784	1.475464
1	0	3.241935	0.971339	1.223710
1	0	1.509991	0.850804	1.728655
1	0	2.711565	-0.356379	2.313055
34	0	-0.787975	-1.234856	0.034299
17	0	-3.021197	-1.340537	-0.142088

4b (Se---Se–Br)
Symmetry C_1
energy MP2 = –7682.0448723 au
Standard orientation

6	0	1.121366	1.183390	-0.675502
6	0	-0.092011	0.909935	0.001585
6	0	-0.798309	1.950167	0.632271
6	0	-0.305806	3.265048	0.583435
6	0	0.897566	3.548350	-0.082727
6	0	1.605883	2.504524	-0.700037
1	0	-1.731440	1.734533	1.153688
1	0	-0.861787	4.063470	1.079100
1	0	1.285737	4.567898	-0.116045
1	0	2.545993	2.713719	-1.217430
6	0	1.899420	0.073030	-1.317908
1	0	1.341625	-0.401055	-2.140702
1	0	2.877609	0.412473	-1.683960
34	0	2.144843	-1.375759	-0.029073
6	0	2.871557	-0.300276	1.414606
1	0	3.827590	0.141646	1.105168
1	0	2.150884	0.481144	1.689086
1	0	3.031414	-0.982121	2.259724
34	0	-0.715301	-0.914087	0.088066

35	0	-3.036287	-0.390913	-0.093392

4b (Se---Se–I)
Symmetry C_1
energy MP2 = –12027.4903324 au
Standard orientation

6	0	-1.487871	1.109808	0.704167
6	0	-0.290465	0.932895	-0.031724
6	0	0.303525	2.024096	-0.691237
6	0	-0.277274	3.300204	-0.605276
6	0	-1.461734	3.490707	0.125010
6	0	-2.061467	2.394304	0.765475
1	0	1.221476	1.879901	-1.262903
1	0	0.193748	4.139666	-1.120739
1	0	-1.918883	4.479699	0.190321
1	0	-2.987384	2.532334	1.330200
6	0	-2.165097	-0.057414	1.358078
1	0	-1.515933	-0.552758	2.096288
1	0	-3.109819	0.234503	1.835986
34	0	-2.510458	-1.450526	0.026042
6	0	-3.388354	-0.314834	-1.281923
1	0	-4.303492	0.113808	-0.852907
1	0	-2.701856	0.478863	-1.604473
1	0	-3.643929	-0.960787	-2.131845
34	0	0.439568	-0.846714	-0.168881
53	0	2.908467	-0.217315	0.081532

4b (Se---Se–SeMe)
Symmetry C_1
energy MP2 = –7549.2359593 au
Standard orientation

6	0	-1.095479	1.068016	0.654958
6	0	0.031766	0.861438	-0.178016
6	0	0.618282	1.941299	-0.863084
6	0	0.099651	3.237877	-0.715242
6	0	-1.016742	3.459505	0.109001
6	0	-1.604980	2.376862	0.781592
1	0	1.488596	1.766166	-1.498363
1	0	0.561513	4.068211	-1.253892
1	0	-1.426575	4.464522	0.227186
1	0	-2.473940	2.543123	1.424315
6	0	-1.770200	-0.069820	1.360746
1	0	-1.055175	-0.683890	1.928149
1	0	-2.557112	0.291447	2.036759
34	0	-2.562073	-1.323632	0.076605
6	0	-3.560747	-0.000494	-0.935488
1	0	-4.285488	0.508983	-0.286692
1	0	-2.871806	0.724402	-1.388262
1	0	-4.094719	-0.549313	-1.722344
34	0	0.730401	-0.925421	-0.373087
34	0	2.988504	-0.425014	-0.203335
6	0	3.013251	0.030463	1.691911
1	0	4.051669	0.288500	1.944660
1	0	2.360763	0.897102	1.861392
1	0	2.681172	-0.831850	2.282625

4b (Se---Se–C_{Me})
Symmetry C_1
energy MP2 = –5149.1659943 au
Standard orientation

6	0	-0.067598	1.039242	0.663939
6	0	1.048717	0.464423	0.004305
6	0	2.017428	1.296872	-0.590442
6	0	1.899753	2.694885	-0.521806
6	0	0.798514	3.274316	0.128778
6	0	-0.172646	2.444474	0.710874
1	0	2.865953	0.856648	-1.116639
1	0	2.660400	3.324442	-0.988565
1	0	0.696056	4.359803	0.184222
1	0	-1.029877	2.889498	1.223562
6	0	-1.132308	0.193420	1.294120
1	0	-0.701052	-0.613021	1.905067
1	0	-1.805874	0.801197	1.913599
34	0	-2.204748	-0.747270	-0.053025
6	0	-2.697114	0.827867	-1.076507
1	0	-3.259235	1.532063	-0.448637
1	0	-1.798485	1.308398	-1.484575
1	0	-3.337094	0.478984	-1.897684
34	0	1.211572	-1.439280	-0.088647
6	0	3.139609	-1.541478	0.185954
1	0	3.356861	-2.600488	0.380846
1	0	3.689858	-1.220996	-0.706623
1	0	3.424337	-0.937965	1.056948

5c (Te---Te–F)
Symmetry C_1
energy MP2 = –13632.7611676 au
Standard orientation

6	0	-0.717989	1.466770	-0.612290
6	0	-1.320145	0.308449	-0.063753
6	0	-2.619667	0.391377	0.477705
6	0	-3.300942	1.620023	0.507496
6	0	-2.695335	2.778447	-0.004901
6	0	-1.409945	2.693184	-0.563413
1	0	-3.094510	-0.506347	0.874637
1	0	-4.300392	1.668863	0.944854
1	0	-3.215061	3.737840	0.026704
1	0	-0.937832	3.586442	-0.981661
6	0	0.631389	1.414226	-1.275637
1	0	0.606290	0.841899	-2.217662
1	0	1.040592	2.414743	-1.468823
52	0	1.986338	0.301751	-0.039515
6	0	1.519618	1.384912	1.739083
1	0	1.920335	2.404308	1.673024
1	0	0.426567	1.394051	1.848611
1	0	1.981427	0.849623	2.578838
52	0	-0.358973	-1.593571	-0.031766
9	0	-2.174698	-2.395681	-0.088626

5c (Te---Te–Cl)

Symmetry C_1
energy MP2 = –13992.7214604 au
Standard orientation

6	0	0.211505	1.613911	-0.695669
6	0	-0.851456	0.947987	-0.036640
6	0	-1.861237	1.700833	0.593759
6	0	-1.813052	3.105507	0.583094
6	0	-0.755925	3.772006	-0.056297
6	0	0.249009	3.022188	-0.688659
1	0	-2.686465	1.191415	1.093127
1	0	-2.598295	3.673025	1.086829
1	0	-0.709353	4.862585	-0.061700
1	0	1.072144	3.533364	-1.195396
6	0	1.303640	0.850899	-1.389911
1	0	0.924488	0.250773	-2.232853
1	0	2.112521	1.506339	-1.738358
52	0	2.093097	-0.616388	-0.028219
6	0	2.247552	0.743599	1.610629
1	0	3.012741	1.499669	1.393903
1	0	1.264890	1.209519	1.763847
1	0	2.535193	0.158790	2.494020
52	0	-0.941410	-1.184997	0.035194
17	0	-3.364459	-1.103238	-0.146352

5c (Te---Te–Br)
Symmetry C_1
energy MP2 = –16105.6921829 au
Standard orientation

6	0	0.827885	1.573788	-0.713881
6	0	-0.322809	1.127639	-0.017652
6	0	-1.147628	2.062223	0.637567
6	0	-0.832397	3.431601	0.610848
6	0	0.310556	3.880492	-0.069453
6	0	1.133056	2.949205	-0.723820
1	0	-2.038041	1.722840	1.168745
1	0	-1.477453	4.141032	1.133407
1	0	0.563868	4.942107	-0.089112
1	0	2.022447	3.291011	-1.260288
6	0	1.737539	0.610814	-1.421172
1	0	1.225260	0.066661	-2.230858
1	0	2.636200	1.101918	-1.816705
52	0	2.307869	-0.938595	-0.038277
6	0	2.737165	0.414555	1.557167
1	0	3.602144	1.035882	1.292750
1	0	1.847208	1.033222	1.734013
1	0	2.965223	-0.189933	2.444727
52	0	-0.802713	-0.952062	0.079568
35	0	-3.322149	-0.432356	-0.105184

5c (Te---Te–I)
Symmetry C_1
energy MP2 = –20451.1342904 au
Standard orientation

6	0	1.201464	1.515400	-0.743037
6	0	0.053425	1.155634	0.005951
6	0	-0.668786	2.147055	0.697408

6	0	-0.262265	3.491319	0.645269
6	0	0.873935	3.856333	-0.094128
6	0	1.598509	2.867017	-0.778322
1	0	-1.552910	1.873300	1.275524
1	0	-0.830052	4.245840	1.193701
1	0	1.197718	4.897984	-0.135936
1	0	2.484161	3.143685	-1.356884
6	0	2.020150	0.485392	-1.464531
1	0	1.433546	-0.071467	-2.212315
1	0	2.908728	0.921060	-1.939587
52	0	2.627508	-1.024157	-0.047745
6	0	3.168501	0.384794	1.464495
1	0	4.013001	0.993675	1.117770
1	0	2.295642	1.013616	1.684656
1	0	3.460083	-0.189064	2.353880
52	0	-0.546314	-0.890520	0.137203
53	0	-3.236634	-0.239304	-0.094929

5c (Te---Te–TeMe)
Symmetry C_1
energy MP2 = –20184.6924597 au
Standard orientation

6	0	-1.203091	1.385370	0.709090
6	0	-0.119879	1.093925	-0.158471
6	0	0.477732	2.125799	-0.908596
6	0	0.017517	3.448400	-0.799115
6	0	-1.051640	3.749278	0.061054
6	0	-1.651618	2.720388	0.803206
1	0	1.315088	1.897844	-1.571628
1	0	0.488872	4.235147	-1.392329
1	0	-1.416293	4.774248	0.154461
1	0	-2.484040	2.949745	1.474538
6	0	-1.912358	0.319564	1.486678
1	0	-1.215737	-0.343172	2.022254
1	0	-2.632075	0.748160	2.195923
52	0	-2.971941	-0.994870	0.125447
6	0	-3.601049	0.595445	-1.159988
1	0	-4.247845	1.292188	-0.612314
1	0	-2.716539	1.113604	-1.552929
1	0	-4.165081	0.136601	-1.983169
52	0	0.599896	-0.908089	-0.342269
52	0	3.204918	-0.245487	-0.123674
6	0	3.116866	0.226967	1.972091
1	0	4.127102	0.515418	2.294678
1	0	2.423305	1.065566	2.114048
1	0	2.778978	-0.657018	2.526563

5c (Te---Te–C_{Me})
Symmetry C_1
energy MP2 = –13572.7942334 au
Standard orientation

6	0	-0.054241	1.342573	0.752843
6	0	1.062007	0.849434	0.029015
6	0	1.919908	1.755494	-0.629237
6	0	1.694151	3.140775	-0.565276
6	0	0.592067	3.635187	0.150558

6	0	-0.270954	2.736225	0.796165
1	0	2.768862	1.381291	-1.205027
1	0	2.369648	3.824413	-1.083875
1	0	0.402728	4.709033	0.204395
1	0	-1.129705	3.117486	1.355658
6	0	-1.021868	0.432744	1.443975
1	0	-0.510488	-0.346169	2.029463
1	0	-1.707521	0.993063	2.092333
52	0	-2.193392	-0.667097	-0.013255
6	0	-2.392482	1.001475	-1.337713
1	0	-2.933597	1.817900	-0.843369
1	0	-1.395470	1.333386	-1.655263
1	0	-2.965953	0.652599	-2.207133
52	0	1.475123	-1.225952	-0.083341
6	0	3.580481	-0.943425	0.255400
1	0	4.005135	-1.935847	0.461005
1	0	4.070281	-0.517453	-0.628387
1	0	3.721651	-0.294089	1.128781