Electronic Supplementary Information

Nature of S_2Se_2 σ(4c–6e) at naphthalene 1,8-positions and models, elucidated by QTAIM dual functional analysis

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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 $\rho_b(\boldsymbol{r}_c)$. While the chemical bonds or interactions between A and B are denoted by A–B, which correspond to BPs between A and B in QTAIM, A-∗-B emphasizes the presence of 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-S6] $H_b(\boldsymbol{r}_c)$ 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 Eq. (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] Eq. (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.

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

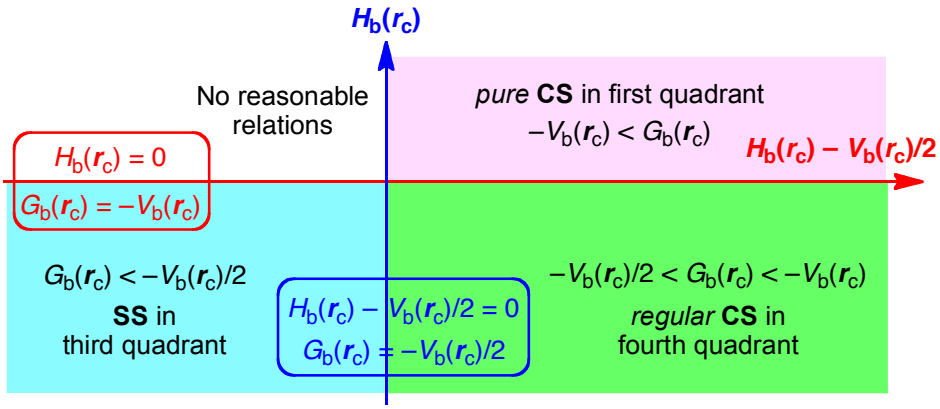
$$(\hbar^2/8m)\nabla^2\rho_b(\boldsymbol{r}_c) = H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2 \quad \text{(S2)}$$

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

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

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 can incorporate the classification of interactions by the signs of $\nabla^2\rho_b(\boldsymbol{r}_c)$ and $H_b(\boldsymbol{r}_c)$. Scheme S1 summarizes the QTAIM-DFA treatment. Interactions of *pure* CS appear in the first quadrant, those of *regular* CS in the forth quadrant and SS interactions do in the third quadrant. No interactions appear in the second one.



Scheme S1. 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-S6] 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,S6] Figure S1 explains the treatment. R in (R, θ) is defined by Eq. (S3) and given in the energy unit. R corresponds to the energy for an interaction at BCP. The plots show a spiral stream, as a whole. θ in (R, θ) defined by Eq. (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 Eq. (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 (Eq. (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 Eq. (S7), is a QTAIM function but it will be treated as if it were a QTAIM-DFA parameter, if suitable.

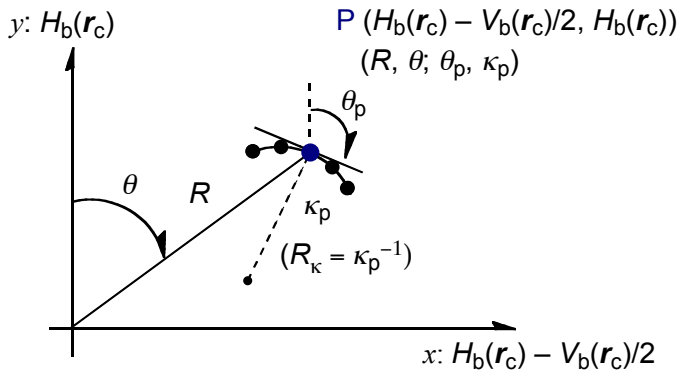


Figure S1. Polar (R, θ) coordinate representation of $H_b(\boldsymbol{r}_c)$ versus $H_b(\boldsymbol{r}_c) - V_b(\boldsymbol{r}_c)/2$, with ($\theta_p$, κ_p) parameters.

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

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

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

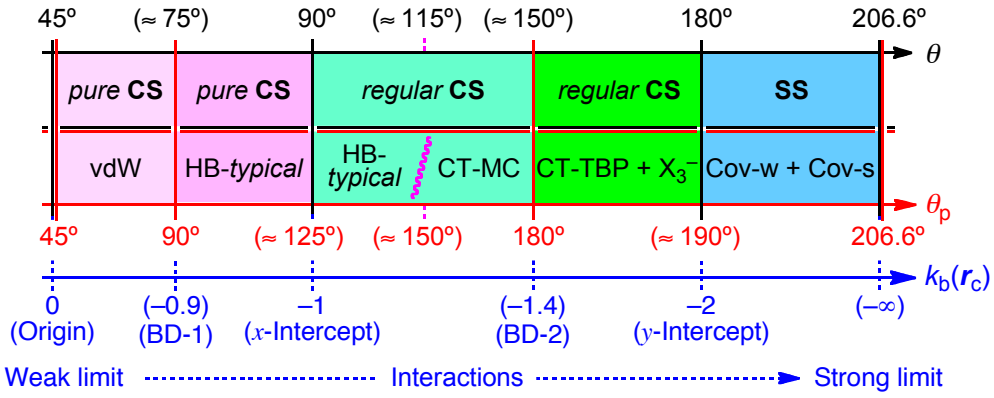
$$\kappa_p = \left|d^2y/dx^2\right| / [1 + (dy/dx)^2]^{3/2} \quad \text{(S6)}$$

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

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), HB (hydrogen bonds), CT-MC (molecular complexes through charge transfer), X_3^- (trihalide ions), CT-TBP (trigonal bipyramidal adducts through charge-transfer), Cov-w (weak covalent bonds) and Cov-s (strong covalent bonds).[S4-S6] Rough criteria are obtained, after the analysis of the plots for the typical interactions according to Eqs. (S3)–(S7), by applying QTAIM-DFA. Scheme S2 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 S2. Rough classification of interactions by θ and θ_p, together with $k_b(\boldsymbol{r}_c)$ (= $V_b(\boldsymbol{r}_c)/G_b(\boldsymbol{r}_c)$).

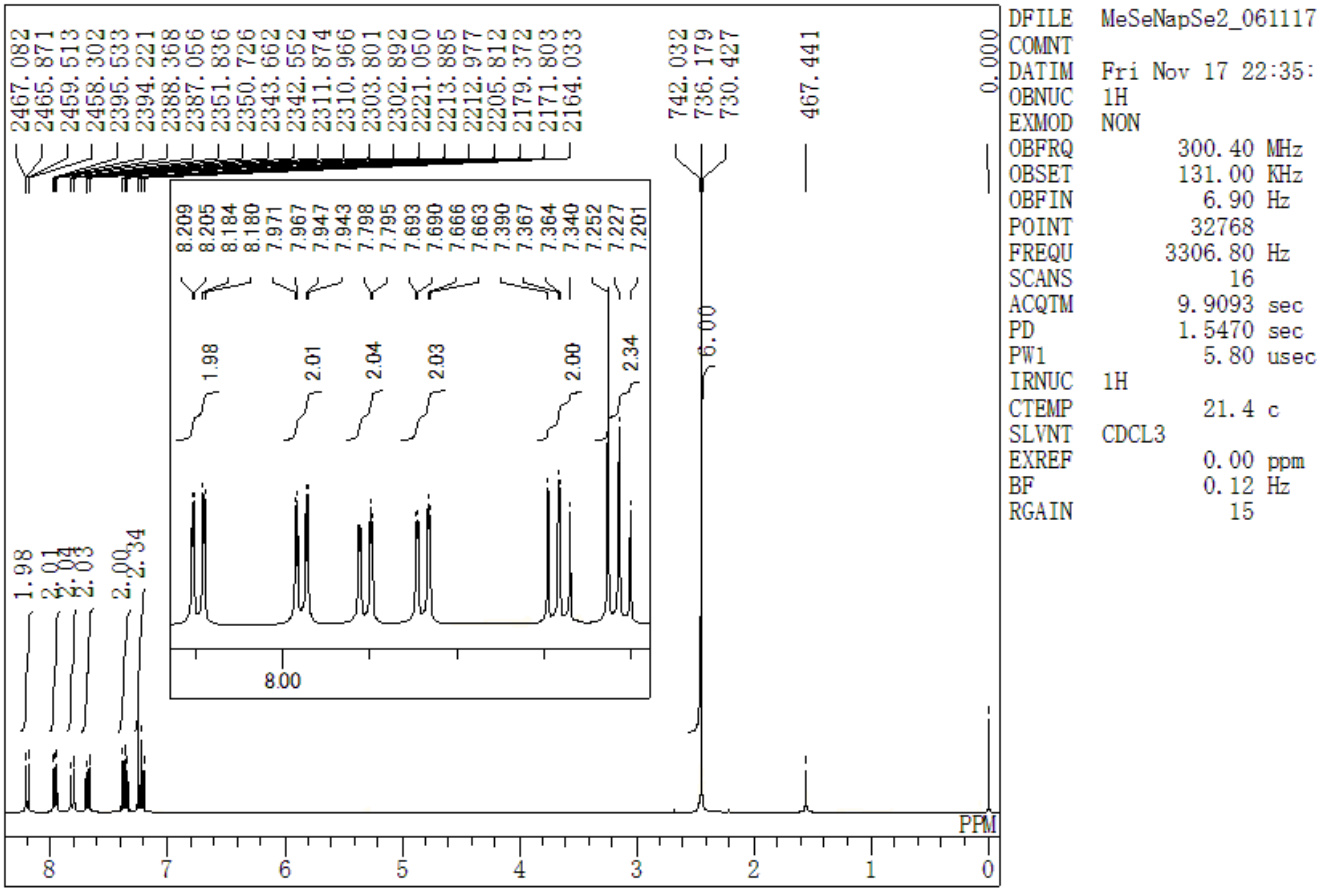


Figure S2. ^{1}H NMR spectrum of **4**.

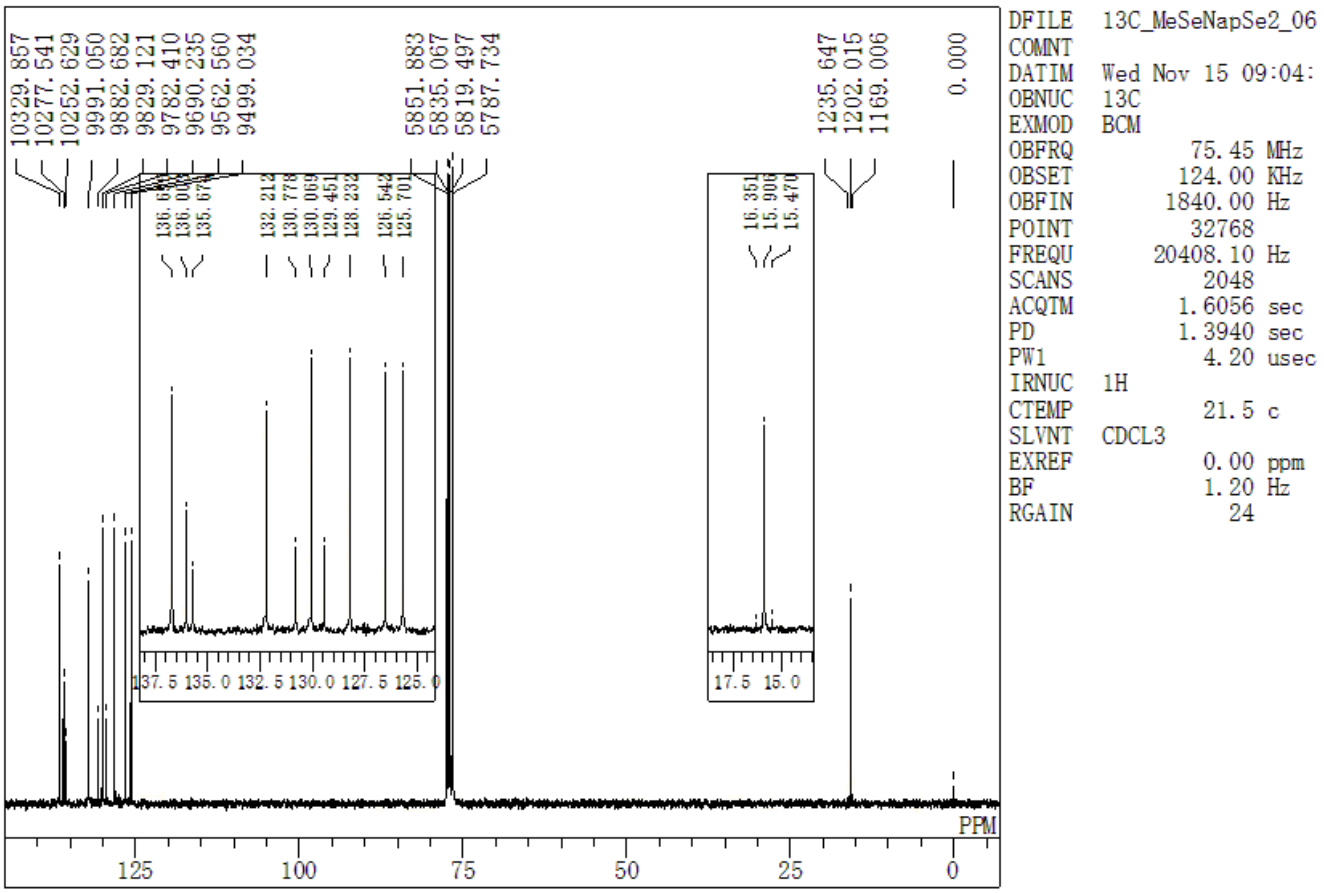


Figure S3. ^{13}C NMR spectrum of **4**.

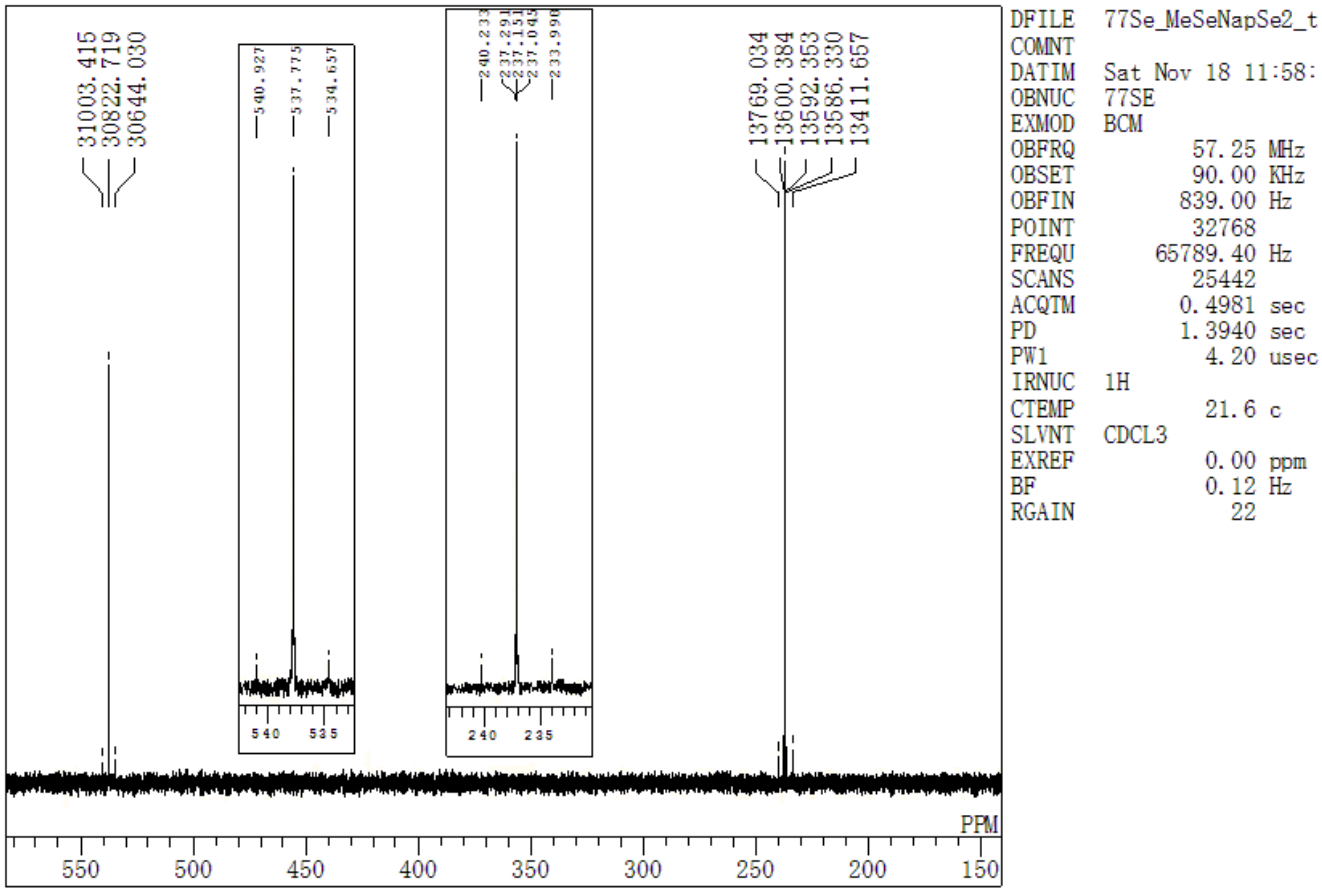


Figure S4. ^{77}Se NMR spectrum of **4**.

Table S1. Structural parameters evaluated for **1**–**4** with MP2/BSS-A and MP2/BS-B, together with the observed values for **4** and **I**.[a,b]

Species (^{A}E, ^{B}E) (symmetry)	r_o(^{A}E, ^{A}E) (Å)	r_o(^{A}E, ^{B}E) (Å)	Δr_o(^{A}E, ^{B}E)[c] (Å)	∠C$_1$^{A}E^{A}E (°)	∠C$_8$^{B}EC$_{11}$ (°)	∠^{B}E^{A}E^{A}E (°)	ϕ_1[d] (°)	ϕ_2[e] (°)
MP2/BSS-A								
1 (S, S) (C_1)	2.0559	2.9418	–0.66	104.9	99.6	171.4	83.7	75.5
2 (S, Se) (C_2)	2.0603	3.0255	–0.67	104.6	97.0	170.2	85.7	69.9
3 (Se, S) (C_2)	2.3440	2.9556	–0.74	101.9	99.4	177.8	83.3	73.7
4 (Se, Se) (C_2)	2.3532	3.0353	–0.76	101.6	96.6	176.9	85.1	68.3
MP2/BSS-B								
1 (S, S) (C_1)	2.0937	2.9419	–0.66	104.7	99.5	171.7	83.9	74.9
2 (S, Se) (C_2)	2.0990	3.0293	–0.67	104.3	96.8	170.5	86.0	69.5
3 (Se, S) (C_2)	2.3744	2.9682	–0.73	101.9	99.3	178.0	83.4	73.3
4 (Se, Se) (C_2)	2.3839	3.0540	–0.75	101.6	96.5	177.1	84.9	67.9
Observed Value								
4 (Se, Se)[f]	2.3864(4)	3.030	–0.77	102.64(6)	96.98(9)[g]	173.3	79.1	78.7[h]
I (S, S)	2.055(2)	2.988(2)	–0.61	104.9[i]	102.8[g,h]	167.3[i]	–89.0	76.4[h,i]
I (S, Se)	2.0706	3.0560[i]	–0.64	104.2[i]	99.2[g,h]	168.1[i]	–81.3	70.8[h,i]
I (Se, S)	2.3561	2.9809[i]	–0.72	101.8[i]	102.3[g,h]	174.4[i]	–91.5	76.6[h,i]
I (Se, Se)	2.365(1)	3.053(1)[i]	–0.75	102.4[i]	100.3[g,h]	173.8[i]	91.4(4)	73.1[h,i]

[a] BSS-A: the 6-311+G(3df) basis sets being employed for S and Se with the 6-311G(d) basis sets for C and H. [b] BSS-B: the 6-311+G(3d) basis sets being employed for S and Se with the 6-311G(d) basis sets for C and H. [c] Δr_o(^{A}E, ^{B}E) = r_o(^{A}E, ^{B}E) – Σr_{vdW}(^{A}E, ^{B}E), where r_{vdW}(S) = 1.80 Å and r_{vdW}(Se) = 1.90 Å (ref. 37 in the text). [d] ϕ_1 = ϕ(C$_1$^{A}E^{A}EC$_{1'}$). [e] ϕ_2 = ϕ(C$_9$C$_8$^{B}EC$_{11}$). [f] Prepared and measured in this work. [g] ∠C$_8$^{B}EC$_i$. [h] ϕ_2 = ϕ(C$_9$C$_8$^{B}EC$_i$). [g] Averaged value.

Table S2. Structural parameters evaluated for models **A**–**D** with MP2/BSS-C.[a]

Species (^{A}E, ^{B}E)	r_o(^{A}E, ^{A}E) (Å)	r_o(^{A}E, ^{B}E) (Å)	Δr_o(^{A}E, ^{B}E)[b] (Å)	∠A^{B}E^{A}E[c] (º)	∠^{B}E^{A}E^{A}E (º)	ϕ_1[d] (º)	ϕ_2[e] (º)	ΔE_{ES} (kJ mol^{-1})	ΔE_{ZP} (kJ mol^{-1})
model **A** (C_2)									
(S, S)	2.0590	3.5251	–0.07	74.2	167.9	–90.5	–128.8	–21.7	–15.9
(S, Se)	2.0601	3.6334	–0.07	74.1	167.9	–90.5	–129.4	–21.3	–16.1
(Se, S)	2.3408	3.5791	–0.12	80.7	169.2	–90.3	–131.3	–21.6	–16.4
(Se, Se)	2.3425	3.6894	–0.11	80.7	169.0	–90.3	–131.8	–21.3	–16.6
model **B** (C_2)									
(S, S)	2.0332	3.6907	0.09	55.1	171.0	–84.7	–116.9	–24.2	–18.4
(S, Se)	2.0336	3.7981	0.10	54.7	170.6	–84.8	–116.5	–24.4	–19.4
(Se, S)	2.3004	3.7302	0.03	60.6	176.1	–85.4	–122.1	–25.0	–19.2
(Se, Se)	2.3011	3.8281	0.03	58.5	175.7	–85.4	–120.9	–25.5	–20.6
model **C** (C_2)									
(S, S)	2.0695	3.2537	–0.35	85.4	173.7	–90.5	–118.3	–41.4	–36.7
(S, Se)	2.0720	3.3302	–0.37	83.7	175.5	–90.4	–130.8	–43.2	–39.0
(Se, S)	2.3412	3.2707	–0.43	87.9	174.4	–90.4	–120.4	–45.0	–41.0
(Se, Se)	2.3444	3.3654	–0.43	86.9	172.0	–90.4	–103.6	–46.2	–42.4
model **D** (C_2)									
(S, S)	2.0407	3.4434	–0.16	83.6	167.0	–84.4	–107.4	–41.6	–37.8
(S, Se)	2.0416	3.5215	–0.18	80.2	167.0	–84.4	–114.7	–43.4	–39.9
(Se, S)	2.3123	3.4081	–0.29	87.0	169.5	–84.9	–94.7	–46.5	–42.9
(Se, Se)	2.3127	3.5190	–0.28	82.5	164.4	–84.6	–82.6	–48.2	–45.0

[a] BSS-C: the 6-311+G(3df) basis sets being employed for S and Se with the 6-311G(d,p) basis sets for C and H. [b] $\Delta r_o(^{A}E, ^{B}E) = r_o(^{A}E, ^{B}E) - \Sigma r_{vdW}(^{A}E, ^{B}E)$, where r_{vdW}(S) = 1.80 Å and r_{vdW}(Se) = 1.90 Å (ref. 37 in the text). [c] A = H or C_{Me}. [c] $\phi_1 = \phi$(H^{A}E^{A}EH or C_{Me}^{A}E^{A}EC_{Me}). [d] $\phi_2 = \phi$(H^{B}E^{A}EH, H^{B}E^{A}EC_{Me}, C_{Me}^{B}E^{A}EH, or C_{Me}^{B}E^{A}EC_{Me}).

Table S3. Results of NBO analysis for the ^{A}E---^{B}E interactions in **1**–**4** with M06-2X/BSS-A//MP2/BSS-A and models **A**–**D** with MP2/BSS-C//MP2/BSS-C.[a]

Compound (^{A}E, ^{B}E)	$E(2)$[b,c] ([f])	$E(2)$[b,c] ([g])	$[E(i) - E(j)]$[d] (au)	$F(i,j)$[e] (au)	Compound (^{A}E, ^{B}E)	$E(2)$[b,c] ([f])	$E(2)$[b,c] ([g])	$[E(i) - E(j)]$[d] (au)	$F(i,j)$[e] (au)
1 (S, S)	8.83	36.9	0.40	0.053	**2** (S, Se)	9.40	39.3	0.38	0.054
3 (Se, S)	15.19	63.6	0.35	0.066	**4** (Se, Se)	16.97	71.0	0.33	0.067
A (S, S)	1.88	7.9	0.43	0.025	**A** (S, Se)	1.96	8.2	0.41	0.025
A (Se, S)	2.99	12.5	0.37	0.030	**A** (Se, Se)	3.12	13.1	0.36	0.030
B (S, S)	0.52	2.2	0.45	0.014	**B** (Se, S)	0.51	2.1	0.44	0.013
B (Se, S)	1.02	4.3	0.40	0.018	**B** (Se, Se)	1.01	4.2	0.39	0.018
C (S, S)	4.30	18.0	0.39	0.037	**C** (Se, S)	5.01	21.0	0.38	0.039
C (Se, S)	6.73	28.2	0.34	0.043	**C** (Se, Se)	7.32	30.6	0.33	0.044
D (S, S)	1.88	7.9	0.41	0.025	**D** (Se, S)	2.15	9.0	0.39	0.026
D (Se, S)	3.68	15.4	0.36	0.032	**D** (Se, Se)	3.61	15.1	0.34	0.031

[a] M06-2X/BSS-A//MP2/BSS-A was applied to **1**–**4**, since the calculations stopped before the end of the evaluations, if MP/BSS-A//MP2/BSS-A was employed. [b] Second-order perturbation energy. [c] Only one side of energy is shown. [d] Donor orbital of NBO(i) is n_p(^{A}E) and acceptor orbital of NBO (j) corresponds to σ*(^{A}E–^{A}E). [e] Fock matrix. [f] In kcal mol^{-1}. [g] In kJ mol^{-1}.

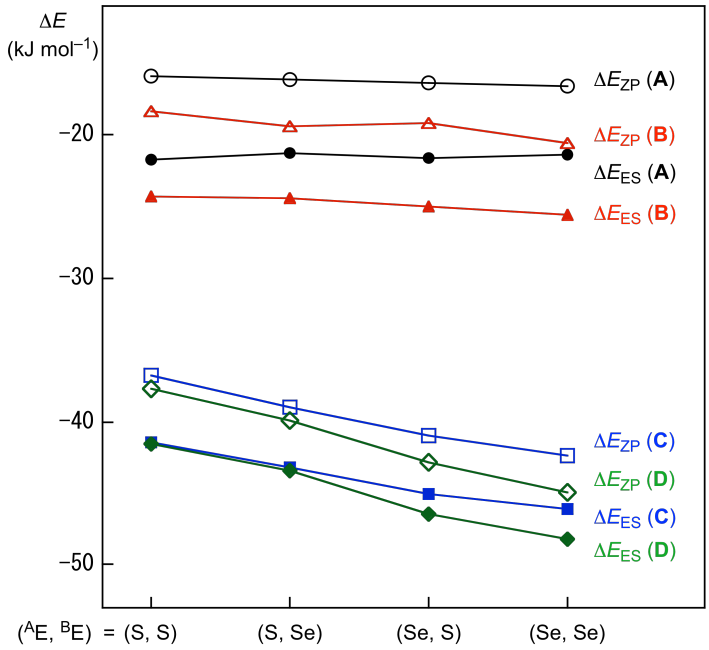


Figure S5. Plots of ΔE_{ES} and ΔE_{ZP} for models **A**–**D**.

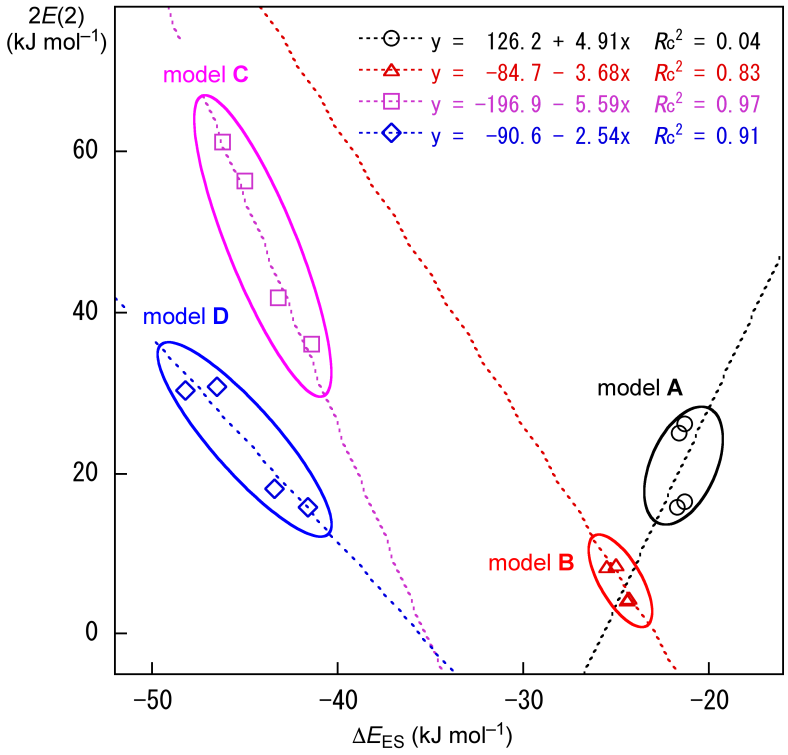


Figure S6. Plot of $2E(2)$ versus ΔE_{ES} for models **A**–**D**.

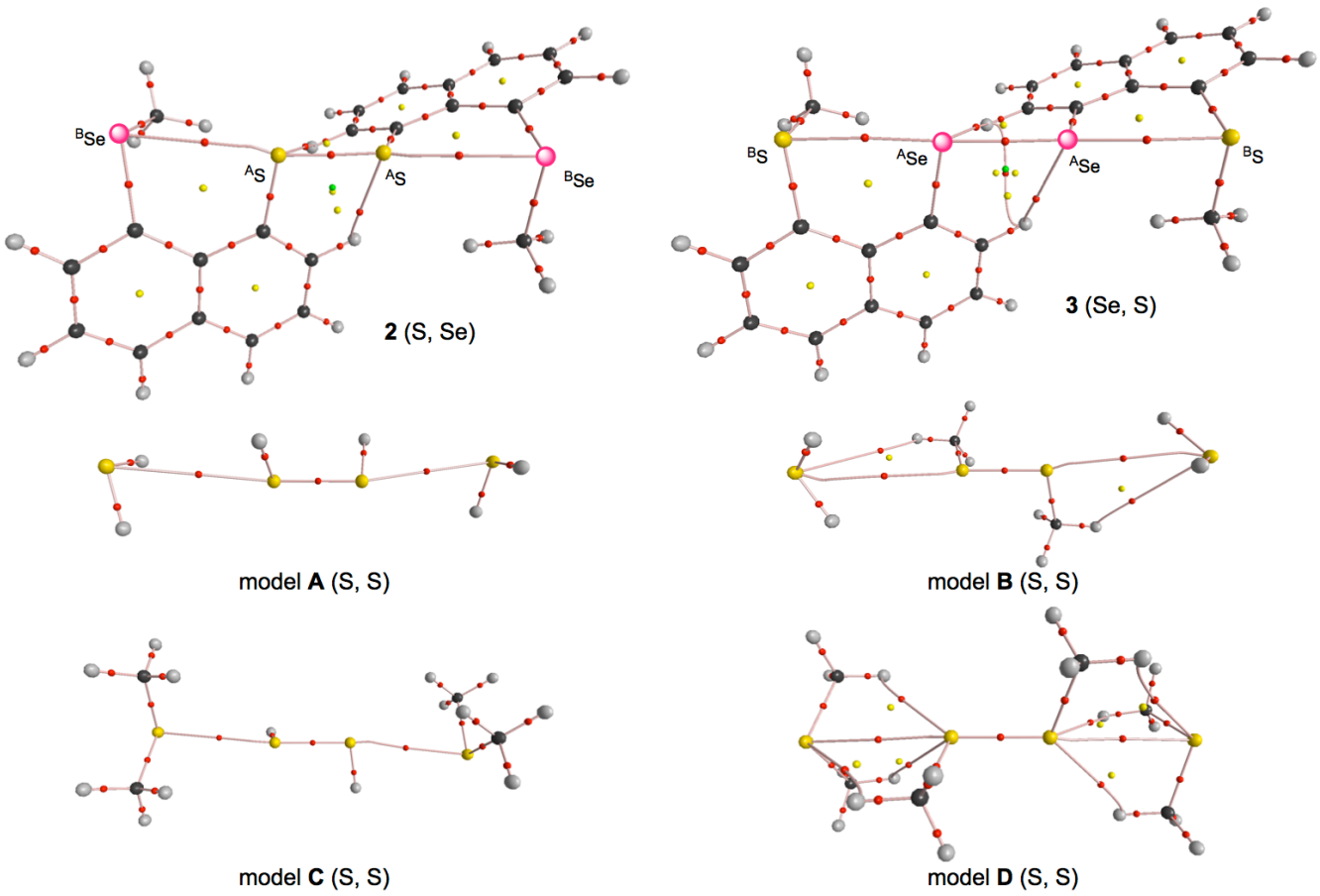


Figure S7. Molecular graphs for **2**, **3** and models **A** (S, S)–**D** (S, S), evaluated with MP2/6-311G(3d). BCPs are shown by red dots (●), RCPs by yellow dots (●) and CCPs by green dots (●), together with BPs by pink lines (-●-). Carbon atoms are drawn in black (●), hydrogen atoms in gray (●), sulfur atoms in yellow (●).and selenium atoms in pink (●).

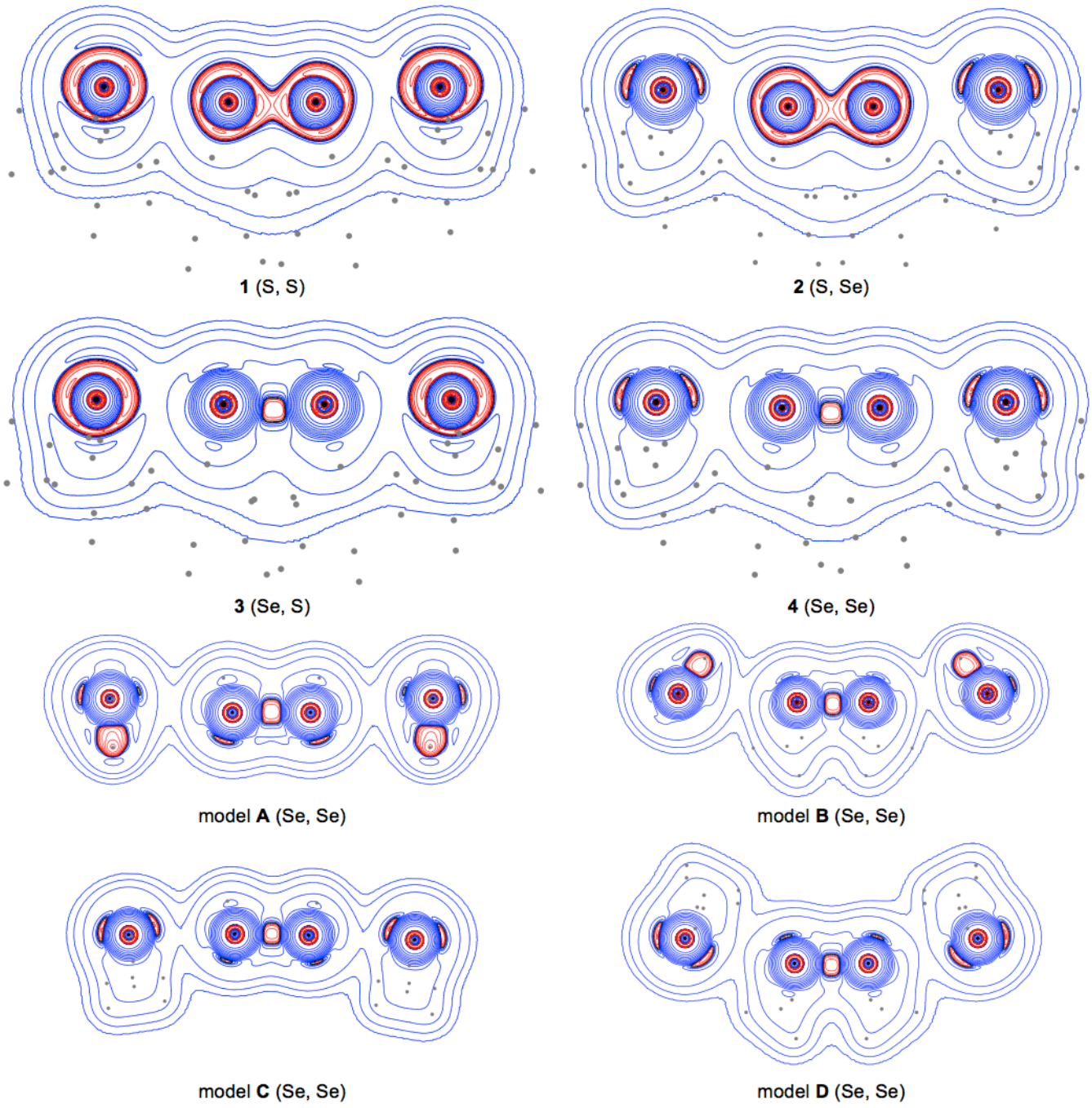


Figure S8. Negative Laplacians for **1**–**4** and models **A** (Se, Se)–**D** (Se, Se) drawn with MP2/6-311G(d), similarly to the case of Figure 4 in the text. Blue and red lines correspond to the positive and negative values, respectively.

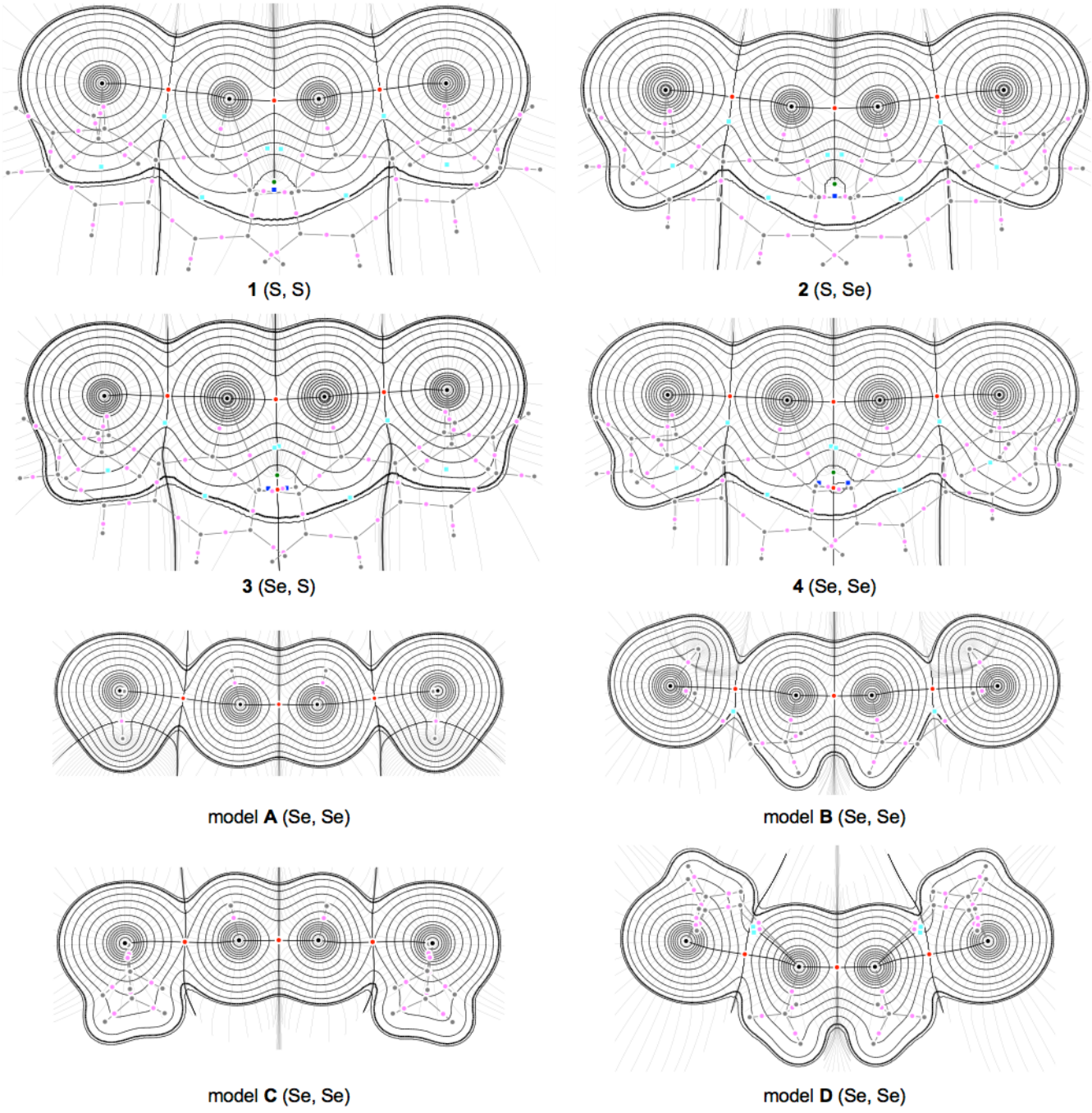


Figure S9. Trajectory plots for **1**–**4** and models **A**–**D** (Se, Se) drawn with MP2/6-311G(d), similarly to the case of Figure 4 in the text. Colors and marks are the same as those in Figure 4.

Table S4. r_{BP} and R_{SL} values for the ^{B}E ---^{A}E–^{A}E---^{B}E interactions in compounds **1**–**4** with MP2/BSS-A and models of **A**–**D** with MP2/BSS-C.[a]

species ^{B}E ---^{A}E–^{A}E---^{B}E	R_{SL}(^{B}E, ^{A}E) (Å)	R_{SL}(^{A}E, ^{A}E) (Å)	r_{BP}(^{B}E, ^{A}E) (Å)	r_{BP}(^{A}E, ^{A}E) (Å)	Δr_{BP}(^{B}E, ^{A}E)[b] (Å)	Δr_{BP}(^{A}E, ^{A}E)[c] (Å)
compounds **1**–**4**						
^{B}S-∗-^{A}S-∗-^{A}S-∗-^{B}S in **1**	2.9418	2.0559	2.9577	2.0576	0.0159	0.0017
^{B}Se-∗-^{A}S-∗-^{A}S-∗-^{B}Se in **2**	3.0255	2.0603	3.0396	2.0621	0.0141	0.0018
^{B}S-∗-^{A}Se-∗-^{A}Se-∗-^{B}S in **3**	2.9556	2.3440	2.9625	2.3457	0.0069	0.0017
^{B}Se-∗-^{A}Se-∗-^{A}Se-∗-^{B}Se in **4**	3.0353	2.3532	3.0408	2.3549	0.0055	0.0017
model **A**						
^{B}S-∗-^{A}S-∗-^{A}S-∗-^{B}S	3.5251	2.0590	3.5357	2.0607	0.0106	0.0017
^{B}Se-∗-^{A}S-∗-^{A}S-∗-^{B}Se	3.6334	2.0601	3.6404	2.0618	0.0070	0.0017
^{B}S-∗-^{A}Se-∗-^{A}Se-∗-^{B}S	3.5791	2.3408	3.5880	2.3415	0.0089	0.0007
^{B}Se-∗-^{A}Se-∗-^{A}Se-∗-^{B}Se	3.6894	2.3425	3.6949	2.3432	0.0055	0.0007
model **B**						
^{B}S-∗-^{A}S-∗-^{A}S-∗-^{B}S	3.6907	2.0332	3.7386	2.0342	0.0479	0.0010
^{B}Se-∗-^{A}S-∗-^{A}S-∗-^{B}Se	3.7981	2.0336	3.8191	2.0347	0.0210	0.0011
^{B}S-∗-^{A}Se-∗-^{A}Se-∗-^{B}S	3.7302	2.3004	3.7388	2.3009	0.0086	0.0005
^{B}Se-∗-^{A}Se-∗-^{A}Se-∗-^{B}Se	3.8281	2.3011	3.8356	2.3015	0.0075	0.0004
model **C**						
^{B}S-∗-^{A}S-∗-^{A}S-∗-^{B}S	3.2537	2.0695	3.2705	2.0712	0.0168	0.0017
^{B}Se-∗-^{A}S-∗-^{A}S-∗-^{B}Se	3.3302	2.0720	3.3448	2.0737	0.0146	0.0017
^{B}S-∗-^{A}Se-∗-^{A}Se-∗-^{B}S	3.2707	2.3412	3.2788	2.3418	0.0081	0.0006
^{B}Se-∗-^{A}Se-∗-^{A}Se-∗-^{B}Se	3.3654	2.3444	3.3719	2.3450	0.0065	0.0006
model **D**						
^{B}S-∗-^{A}S-∗-^{A}S-∗-^{B}S	3.4434	2.0407	3.4649	2.0418	0.0215	0.0011
^{B}Se-∗-^{A}S-∗-^{A}S-∗-^{B}Se	3.5215	2.0416	3.5391	2.0427	0.0176	0.0011
^{B}S-∗-^{A}Se-∗-^{A}Se-∗-^{B}S	3.4081	2.3123	3.4192	2.3127	0.0111	0.0004
^{B}Se-∗-^{A}Se-∗-^{A}Se-∗-^{B}Se	3.5190	2.3127	3.5286	2.3132	0.0096	0.0005

[a] BSS-A: the 6-311+G(3df) basis sets being employed for S and Se with the 6-311G(d) basis sets for C and H. BSS-C: the 6-311+G(3df) basis sets being employed for S and Se with the 6-311G(d,p) basis sets for C and H. [b] $\Delta r_{BP}(^{B}E, ^{A}E) = \Delta r_{BP}(^{B}E, ^{A}E) - R_{SL}(^{B}E, ^{A}E)$. [c] $\Delta r_{BP}(^{A}E, ^{A}E) = \Delta r_{BP}(^{A}E, ^{A}E) - R_{SL}(^{A}E, ^{A}E)$.

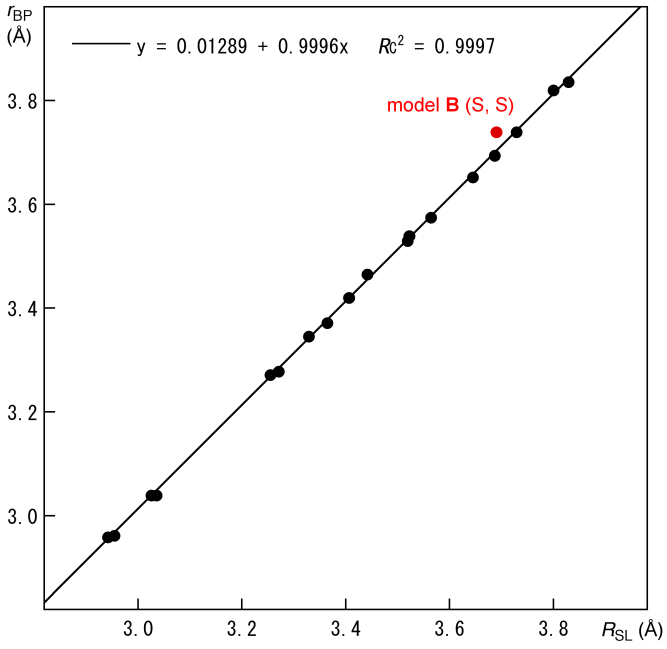


Figure S10. Plots of r_{BP} versus R_{SL} for the interactions in models **A**–**D**. Correlation is very good, which are shown in the figure.

Table S5. AIM functions and parameters evaluated for ^{A}E-∗-^{A}E and ^{A}E-∗-^{B}E at BCPs of models **A**–**D** with MP2/BSS-C.[a]

Model (^{A}E, ^{B}E)	Interaction (^{A}E-∗-^{B}E)	$\rho_b(\boldsymbol{r}_c)$ (au)	$c\nabla^2\rho_b(\boldsymbol{r}_c)$[b] (au)	$H_b(\boldsymbol{r}_c)$ (au)	$k_b(\boldsymbol{r}_c)$[c]	ν (n)[d] (cm^{-1})	k_f[e] ([f])	R (au)	θ (º)	θ_p (º)	κ_p (au^{-1})
model **A**: $H_2{}^{B}E$---$^{A}E(H)$-$(H)^{A}E$---$^{B}EH_2$ (C_2)											
(S, S)	(^{A}S-∗-^{A}S)	0.1480	-0.0178	-0.0890	-2.6636	527.5 (14)	4.3230	0.0910	191.3	197.7	0.4
(S, Se)	(^{A}S-∗-^{A}Se)	0.1476	-0.0176	-0.0886	-2.6568	525.2 (14)	4.2905	0.0906	191.2	197.7	0.4
(Se, S)	(^{A}Se-∗-^{A}S)	0.1044	-0.0068	-0.0494	-2.3831	296.6 (13)	3.3845	0.0498	187.9	191.4	0.3
(Se, Se)	(^{A}Se-∗-^{A}Se)	0.1041	-0.0067	-0.0491	-2.3783	295.0 (13)	3.3969	0.0496	187.8	191.4	0.2
(S, S)	(^{A}S-∗-^{B}S)	0.0081	0.0031	0.0009	-0.839	75.4 (7)	0.032	0.0032	74.5	92.7	163
(S, Se)	(^{A}S-∗-^{B}Se)	0.0077	0.0028	0.0008	-0.831	61.2 (6)	0.016	0.0029	73.9	87.8	134
(Se, S)	(^{A}Se-∗-^{B}S)	0.0085	0.0030	0.0009	-0.829	59.6 (7)	0.062	0.0031	73.7	91.2	238
(Se, Se)	(^{A}Se-∗-^{B}Se)	0.0082	0.0027	0.0008	-0.823	45.5 (7)	0.053	0.0028	73.2	86.9	214
model **B**: $H_2{}^{B}E$---$^{A}E(Me)$-$(Me)^{A}E$---$^{B}EH_2$ (C_2)											
(S, S)	(^{A}S-∗-^{A}S)	0.1558	-0.0199	-0.0986	-2.6752	532.5 (18)	2.7540	0.1006	191.4	197.6	0.3
(S, Se)	(^{A}S-∗-^{A}Se)	0.1557	-0.0197	-0.0984	-2.6696	531.7 (18)	2.7526	0.1003	191.3	197.6	0.4
(Se, S)	(^{A}Se-∗-^{A}S)	0.1110	-0.0066	-0.0546	-2.3203	310.7 (18)	2.6416	0.0550	186.9	190.1	0.2
(Se, Se)	(^{A}Se-∗-^{A}Se)	0.1108	-0.0066	-0.0544	-2.3176	310.1 (18)	2.7050	0.0548	186.9	190.2	0.2
(S, S)	(^{A}S-∗-^{B}S)	0.0064	0.0027	0.0010	-0.766	73.0 (8)	0.033	0.0029	69.2	83.1	61.6
(S, Se)	(^{A}S-∗-^{B}Se)	0.0060	0.0025	0.0010	-0.754	30.6 (3)	0.006	0.0026	68.4	80.1	735
(Se, S)	(^{A}Se-∗-^{B}S)	0.0065	0.0025	0.0009	-0.777	64.8 (6)	0.044	0.0027	70.0	86.9	228
(Se, Se)	(^{A}Se-∗-^{B}Se)	0.0063	0.0023	0.0009	-0.770	50.6 (6)	0.021	0.0025	69.5	88.0	115
model **C**: $Me_2{}^{B}E$---$^{A}E(H)$-$(H)^{A}E$---$^{B}EMe_2$ (C_2)											
(S, S)	(^{A}S-∗-^{A}S)	0.1455	-0.0166	-0.0858	-2.6304	509.0 (20)	3.5641	0.0873	190.9	197.7	0.4
(S, Se)	(^{A}S-∗-^{A}Se)	0.1449	-0.0163	-0.0850	-2.6201	503.3 (20)	3.5247	0.0865	190.8	197.7	0.4
(Se, S)	(^{A}Se-∗-^{A}S)	0.1038	-0.0057	-0.0481	-2.3069	288.5 (19)	2.8836	0.0485	186.7	190.8	0.3
(Se, Se)	(^{A}Se-∗-^{A}Se)	0.1032	-0.0055	-0.0476	-2.2976	284.7 (19)	3.1112	0.0479	186.5	190.9	0.3
(S, S)	(^{A}S-∗-^{B}S)	0.0145	0.0047	0.0003	-0.971	90.5 (8)	0.042	0.0047	86.7	114.5	148
(S, Se)	(^{A}S-∗-^{B}Se)	0.0144	0.0044	0.0003	-0.963	76.0 (8)	0.037	0.0044	86.0	113.8	207
(Se, S)	(^{A}Se-∗-^{B}S)	0.0161	0.0048	0.0001	-0.985	70.9 (8)	0.038	0.0048	88.3	121.8	175
(Se, Se)	(^{A}Se-∗-^{B}Se)	0.0155	0.0043	0.0002	-0.974	55.5 (7)	0.049	0.0043	87.1	121.2	311
model **D**: $Me_2{}^{B}E$---$^{A}E(Me)$-$(Me)^{A}E$---$^{B}EMe_2$ (C_2)											
(S, S)	(^{A}S-∗-^{B}S)	0.1539	-0.0190	-0.0959	-2.6534	521.9 (24)	2.7080	0.0978	191.2	197.6	0.4
(S, Se)	(^{A}S-∗-^{B}Se)	0.1536	-0.0188	-0.0955	-2.6485	519.8 (24)	2.6946	0.0974	191.1	197.6	0.4
(Se, S)	(^{A}Se-∗-^{B}S)	0.1091	-0.0061	-0.0527	-2.3036	301.4 (24)	2.6443	0.0531	186.6	190.3	0.2
(Se, Se)	(^{A}Se-∗-^{B}Se)	0.1089	-0.0060	-0.0525	-2.2983	300.7 (24)	2.6416	0.0528	186.6	190.4	0.3
(S, S)	(^{A}S-∗-^{B}S)	0.0106	0.0036	0.0006	-0.909	81.9 (10)	0.020	0.0037	80.5	103.4	170
(S, Se)	(^{A}S-∗-^{B}Se)	0.0105	0.0034	0.0006	-0.906	58.9 (7)	0.030	0.0035	80.2	100.0	247
(Se, S)	(^{A}Se-∗-^{B}S)	0.0128	0.0040	0.0005	-0.935	69.1 (8)	0.017	0.0040	83.0	111.7	256
(Se, Se)	(^{A}Se-∗-^{B}Se)	0.0121	0.0036	0.0005	-0.925	49.5 (7)	0.024	0.0036	82.1	106.0	249

[a] BSS-C: the 6-311+G(3df) basis sets being employed for S and Se with the 6-311G(d,p) basis sets for C and H. [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] Corresponding to the interaction in question. [e] Force constant for ν. [f] mdyn $Å^{-1}$.

Table S6. Classification and characterization of the chalcogen-chalcogen interactions in models **A**–**D** by θ, θ_p and R values, evaluated with MP2/BSS-C.[a,b]

models (^{A}E-∗-^{B}E)	θ (º)	θ_p (º)	R (au)	classification /character	models (^{A}E-∗-^{B}E)	θ (º)	θ_p (º)	R (au)	classification /character
A (^{A}S-∗-^{B}S)	74.5	92.7	0.0032	*p*-CS/*t*-HB	**A** (^{A}S-∗-^{B}Se)	73.9	87.8	0.0029	*p*-CS/vdW
A (^{A}Se-∗-^{B}S)	73.7	91.2	0.0031	*p*-CS/*t*-HB	**A** (^{A}Se-∗-^{B}Se)	73.2	86.9	0.0028	*p*-CS/vdW
B (^{A}S-∗-^{B}S)	69.2	83.1	0.0029	*p*-CS/vdW	**B** (^{A}S-∗-^{B}Se)	68.4	80.1	0.0026	*p*-CS/vdW
B (^{A}Se-∗-^{B}S)	70.0	86.9	0.0027	*p*-CS/vdW	**B** (^{A}Se-∗-^{B}Se)	69.5	88.0	0.0025	*p*-CS/vdW
C (^{A}S-∗-^{B}S)	86.7	114.5	0.0047	*p*-CS/*t*-HB	**C** (^{A}S-∗-^{B}Se)	86.0	113.8	0.0044	*p*-CS/*t*-HB
C (^{A}Se-∗-^{B}S)	88.3	121.8	0.0048	*p*-CS/*t*-HB	**C** (^{A}Se-∗-^{B}Se)	87.1	121.2	0.0043	*p*-CS/*t*-HB[c]
D (^{A}S-∗-^{B}S)	80.5	103.4	0.0037	*p*-CS/*t*-HB	**D** (^{A}S-∗-^{B}Se)	80.2	100.0	0.0035	*p*-CS/*t*-HB[c]
D (^{A}Se-∗-^{B}S)	83.0	111.7	0.0040	*p*-CS/*t*-HB	**D** (^{A}Se-∗-^{B}Se)	82.1	106.0	0.0036	*p*-CS/*t*-HB[c]

[a] 0.045 au < R < 0.090 au for ^{A}E-∗-^{A}E and 0.007 au < R < 0.008 au for ^{A}E-∗-^{B}E. The values are much less than 0.15 au for BSS-A; the 6-311+G(3df) basis set for O, S and Se with the 6-311+G(d,p) basis set for C and H. [b] Data are given at BCP of the interaction in question. [c] *Typical*-HB nature with covalency.

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Optimized structures given by Cartesian coordinates

The structures were optimized employing the Gaussian 09 programs. Several types of basis sets were examined to search the suitable methods for the purpose. The Møller-Plesset second order energy correlation (MP2) level is applied to the calculations. The DFT level of M06-2X is also employed to examine the suitable methods.

MP2/BSS-A
Compound **1**
Symmetry C_1
energy MP2 = -2437.5263943 au
Standard orientation

6	0	-4.127475	-0.446699	-0.562813
6	0	-3.261563	0.446210	0.155653
6	0	-3.894628	1.330759	1.112384
6	0	-5.311114	1.426871	1.165641
6	0	-6.112460	0.619079	0.385951
6	0	-5.512524	-0.324238	-0.472418
6	0	-1.823280	0.490105	0.064571
6	0	-1.100721	1.295331	0.943123
6	0	-1.738701	2.119346	1.891473
6	0	-3.114891	2.172528	1.946843
1	0	-5.754795	2.128941	1.869386
1	0	-7.195462	0.703132	0.430296
1	0	-6.127132	-1.015142	-1.044505
1	0	-0.017575	1.314405	0.877338
1	0	-1.133277	2.739876	2.548236
1	0	-3.620936	2.829691	2.651281
16	0	-3.529789	-1.761690	-1.587177
16	0	-0.947338	-0.399005	-1.229531
6	0	4.127482	0.446680	-0.562810
6	0	3.261557	-0.446211	0.155663
6	0	3.894608	-1.330768	1.112394
6	0	5.311093	-1.426907	1.165646
6	0	6.112450	-0.619132	0.385949
6	0	5.512529	0.324193	-0.472420
6	0	1.823273	-0.490080	0.064584
6	0	1.100701	-1.295285	0.943144
6	0	1.738669	-2.119308	1.891496
6	0	3.114858	-2.172518	1.946861
1	0	5.754763	-2.128982	1.869392
1	0	7.195451	-0.703206	0.430291
1	0	6.127147	1.015085	-1.044511
1	0	0.017554	-1.314337	0.877366
1	0	1.133234	-2.739821	2.548266
1	0	3.620892	-2.829688	2.651299
16	0	3.529813	1.761682	-1.587169
16	0	0.947344	0.399033	-1.229525
6	0	3.030908	2.940211	-0.306038
1	0	3.879919	3.176951	0.338013
1	0	2.702306	3.841524	-0.829624
1	0	2.199389	2.543565	0.280301
6	0	-3.030856	-2.940213	-0.306052
1	0	-3.879857	-3.176960	0.338009
1	0	-2.702255	-3.841524	-0.829643
1	0	-2.199332	-2.543562	0.280275

MP2/BSS-A
Compound **2**
Symmetry C_2
energy MP2 = -6442.3460668 au

Standard orientation

6	0	0.126941	-4.164389	-0.351975
6	0	- 0.697788	-3.234203	0.364700
6	0	-1.672051	-3.804343	1.274606
6	0	-1.914267	-5.203915	1.275344
6	0	-1.171891	-6.057344	0.486266
6	0	-0.137009	-5.531687	-0.314072
6	0	-0.609363	-1.795813	0.313016
6	0	-1.348743	-1.025454	1.209164
6	0	-2.249348	-1.607716	2.123131
6	0	-2.443492	-2.972184	2.126453
1	0	-2.678935	-5.595419	1.943949
1	0	-1.366383	-7.127033	0.489605
1	0	0.510712	-6.201711	-0.873748
1	0	-1.263351	0.056006	1.177151
1	0	-2.813365	-0.965451	2.795691
1	0	-3.166359	-3.432628	2.797039
34	0	1.672051	-3.661354	-1.358040
16	0	0.349979	-0.968885	-0.962588
6	0	-0.126941	4.164389	-0.351975
6	0	0.697788	3.234203	0.364700
6	0	1.672051	3.804343	1.274606
6	0	1.914267	5.203915	1.275344
6	0	1.171891	6.057344	0.486266
6	0	0.137009	5.531687	-0.314072
6	0	0.609363	1.795813	0.313016
6	0	1.348743	1.025454	1.209164
6	0	2.249348	1.607716	2.123131
6	0	2.443492	2.972184	2.126453
1	0	2.678935	5.595419	1.943949
1	0	1.366383	7.127033	0.489605
1	0	-0.510712	6.201711	-0.873748
1	0	1.263351	-0.056006	1.177151
1	0	2.813365	0.965451	2.795691
1	0	3.166359	3.432628	2.797039
34	0	-1.672051	3.661354	-1.358040
16	0	-0.349979	0.968885	-0.962588
6	0	-2.796800	3.185257	0.158275
1	0	-2.811486	4.007468	0.874369
1	0	-3.800724	3.018916	-0.238574
1	0	-2.429248	2.267462	0.619844
6	0	2.796800	-3.185257	0.158275
1	0	2.811486	-4.007468	0.874369
1	0	3.800724	-3.018916	-0.238574
1	0	2.429248	-2.267462	0.619844

MP2/BSS-A
Compound **3**
Symmetry C_2
energy MP2 = -6442.365514 au
Standard orientation

6	0	0.429659	-4.291382	-0.326390
6	0	-0.429659	-3.390705	0.386115
6	0	-1.386456	-3.985993	1.295875
6	0	-1.480019	-5.398974	1.409014
6	0	-0.694050	-6.232007	0.638948
6	0	0.289889	-5.671331	-0.200974
6	0	-0.470152	-1.962233	0.223861
6	0	-1.246280	-1.196267	1.090196
6	0	-2.108660	-1.792365	2.033644
6	0	-2.183127	-3.165369	2.135521
1	0	-2.214554	-5.814778	2.096590
1	0	-0.786215	-7.312116	0.721350

1	0	0.969056	-6.312283	-0.758020
1	0	-1.257929	-0.115078	0.986066
1	0	-2.702065	-1.156604	2.687175
1	0	-2.879096	-3.637147	2.826593
16	0	1.787137	-3.718326	-1.306263
34	0	0.501059	-1.059483	-1.196055
6	0	-0.429659	4.291382	-0.326390
6	0	0.429659	3.390705	0.386115
6	0	1.386456	3.985993	1.295875
6	0	1.480019	5.398974	1.409014
6	0	0.694050	6.232007	0.638948
6	0	-0.289889	5.671331	-0.200974
6	0	0.470152	1.962233	0.223861
6	0	1.246280	1.196267	1.090196
6	0	2.108660	1.792365	2.033644
6	0	2.183127	3.165369	2.135521
1	0	2.214554	5.814778	2.096590
1	0	0.786215	7.312116	0.721350
1	0	-0.969056	6.312283	-0.758020
1	0	1.257929	0.115078	0.986066
1	0	2.702065	1.156604	2.687175
1	0	2.879096	3.637147	2.826593
16	0	-1.787137	3.718326	-1.306263
34	0	-0.501059	1.059483	-1.196055
6	0	-2.931228	3.247483	0.017527
1	0	-3.157988	4.114562	0.640829
1	0	-3.841730	2.893820	-0.472754
1	0	-2.507935	2.439476	0.618205
6	0	2.931228	-3.247483	0.017527
1	0	3.157988	-4.114562	0.640829
1	0	3.841730	-2.893820	-0.472754
1	0	2.507935	-2.439476	0.618205

MP2/BSS-A
Compound **4**
Symmetry C_2
energy MP2 = -10447.1847475 au
Standard orientation

6	0	-3.248055	-2.869481	-0.181003
6	0	-3.020466	-1.641928	0.522197
6	0	-4.084632	-1.189889	1.396779
6	0	-5.306127	-1.910984	1.468600
6	0	-5.518374	-3.036030	0.698463
6	0	-4.465464	-3.539424	-0.093529
6	0	-1.867653	-0.790382	0.394176
6	0	-1.705569	0.280462	1.270316
6	0	-2.713680	0.647774	2.185563
6	0	-3.889855	-0.068871	2.244532
1	0	-6.088528	-1.537703	2.127147
1	0	-6.462880	-3.572136	0.749630
1	0	-4.588377	-4.474993	-0.633501
1	0	-0.821983	0.907468	1.193774
1	0	-2.547906	1.494821	2.847741
1	0	-4.696868	0.235418	2.908392
34	0	-1.867653	-3.771376	-1.142979
34	0	-0.546161	-1.042148	-1.008053
6	0	3.248055	2.869481	-0.181003
6	0	3.020466	1.641928	0.522197
6	0	4.084632	1.189889	1.396779
6	0	5.306127	1.910984	1.468600
6	0	5.518374	3.036030	0.698463
6	0	4.465464	3.539424	-0.093529
6	0	1.867653	0.790382	0.394176

6	0	1.705569	-0.280462	1.270316
6	0	2.713680	-0.647774	2.185563
6	0	3.889855	0.068871	2.244532
1	0	6.088528	1.537703	2.127147
1	0	6.462880	3.572136	0.749630
1	0	4.588377	4.474993	-0.633501
1	0	0.821983	-0.907468	1.193774
1	0	2.547906	-1.494821	2.847741
1	0	4.696868	-0.235418	2.908392
34	0	1.867653	3.771376	-1.142979
34	0	0.546161	1.042148	-1.008053
6	0	0.816166	4.291959	0.411441
1	0	1.447193	4.846122	1.107106
1	0	0.010275	4.931707	0.045080
1	0	0.394716	3.403547	0.884513
6	0	-0.816166	-4.291959	0.411441
1	0	-1.447193	-4.846122	1.107106
1	0	-0.010275	-4.931707	0.045080
1	0	-0.394716	-3.403547	0.884513

MP2/BSS-B
Compound **1**
Symmetry C_1
energy MP2 = -2437.411118 au
Standard orientation

6	0	-4.142271	-0.451780	-0.566009
6	0	-3.276362	0.441418	0.151545
6	0	-3.911418	1.338755	1.094532
6	0	-5.327558	1.444036	1.135962
6	0	-6.127599	0.637149	0.354133
6	0	-5.526676	-0.318728	-0.489370
6	0	-1.837263	0.480192	0.065808
6	0	-1.117464	1.282826	0.949173
6	0	-1.757436	2.115444	1.888402
6	0	-3.133484	2.177594	1.933463
1	0	-5.772163	2.154366	1.830747
1	0	-7.210340	0.728906	0.388400
1	0	-6.141515	-1.011088	-1.059424
1	0	-0.034103	1.299638	0.888693
1	0	-1.153047	2.733060	2.548876
1	0	-3.641142	2.843351	2.628562
16	0	-3.541260	-1.786889	-1.565836
16	0	-0.963292	-0.410581	-1.226929
6	0	4.142110	0.451435	-0.567426
6	0	3.276410	-0.441320	0.150932
6	0	3.911736	-1.338035	1.094330
6	0	5.327889	-1.443253	1.135457
6	0	6.127706	-0.636850	0.352900
6	0	5.526538	0.318468	-0.491063
6	0	1.837288	-0.480181	0.065604
6	0	1.117744	-1.282271	0.949669
6	0	1.757984	-2.114272	1.889262
6	0	3.134046	-2.176357	1.934001
1	0	5.772694	-2.153126	1.830582
1	0	7.210458	-0.728556	0.386943
1	0	6.141209	1.010472	-1.061727
1	0	0.034367	-1.299148	0.889484
1	0	1.153784	-2.731483	2.550288
1	0	3.641903	-2.841654	2.629394
16	0	3.540808	1.785877	-1.567967
16	0	0.962952	0.409756	-1.227462
6	0	3.053892	2.944447	-0.261137
1	0	3.906686	3.165257	0.383215

1	0	2.727364	3.857287	-0.765187
1	0	2.223426	2.542002	0.322371
6	0	-3.054017	-2.944608	-0.258375
1	0	-3.906646	-3.164985	0.386346
1	0	-2.727634	-3.857782	-0.761912
1	0	-2.223394	-2.541791	0.324653

MP2/BSS-B
Compound **2**
Symmetry C_2
energy MP2 = -6442.2132526 au
Standard orientation

6	0	0.119114	-4.179909	-0.361441
6	0	-0.703344	-3.248259	0.355270
6	0	-1.690195	-3.817386	1.251663
6	0	-1.945716	-5.214455	1.237520
6	0	-1.206877	-6.067283	0.444552
6	0	-0.159021	-5.544276	-0.340341
6	0	-0.603971	-1.810024	0.312405
6	0	-1.339831	-1.042074	1.213660
6	0	-2.249863	-1.624069	2.118221
6	0	-2.457030	-2.986470	2.108732
1	0	-2.718990	-5.604626	1.896921
1	0	-1.412161	-7.134924	0.435649
1	0	0.488140	-6.215502	-0.899194
1	0	-1.249088	0.039009	1.188733
1	0	-2.809909	-0.982661	2.794929
1	0	-3.189154	-3.446131	2.769706
34	0	1.690195	-3.681039	-1.338946
16	0	0.359844	-0.985901	-0.960503
6	0	-0.119114	4.179909	-0.361441
6	0	0.703344	3.248259	0.355270
6	0	1.690195	3.817386	1.251663
6	0	1.945716	5.214455	1.237520
6	0	1.206877	6.067283	0.444552
6	0	0.159021	5.544276	-0.340341
6	0	0.603971	1.810024	0.312405
6	0	1.339831	1.042074	1.213660
6	0	2.249863	1.624069	2.118221
6	0	2.457030	2.986470	2.108732
1	0	2.718990	5.604626	1.896921
1	0	1.412161	7.134924	0.435649
1	0	-0.488140	6.215502	-0.899194
1	0	1.249088	-0.039009	1.188733
1	0	2.809909	0.982661	2.794929
1	0	3.189154	3.446131	2.769706
34	0	-1.690195	3.681039	-1.338946
16	0	-0.359844	0.985901	-0.960503
6	0	-2.791932	3.226800	0.207275
1	0	-2.783431	4.052873	0.918640
1	0	-3.805880	3.068997	-0.166307
1	0	-2.425811	2.308236	0.668059
6	0	2.791932	-3.226800	0.207275
1	0	2.783431	-4.052873	0.918640
1	0	3.805880	-3.068997	-0.166307
1	0	2.425811	-2.308236	0.668059

MP2/BSS-B
Compound **3**
Symmetry C_2
energy MP2 = -6442.2348538 au

Standard orientation

6	0	0.429345	-4.312938	-0.331104
6	0	-0.429345	-3.410838	0.380322
6	0	-1.391588	-4.005540	1.284614
6	0	-1.499670	-5.418481	1.383830
6	0	-0.717254	-6.251653	0.610591
6	0	0.275550	-5.692131	-0.219470
6	0	-0.457904	-1.980561	0.229966
6	0	-1.232402	-1.216536	1.099317
6	0	-2.100550	-1.813028	2.036905
6	0	-2.185793	-3.186046	2.127628
1	0	-2.239734	-5.833396	2.065953
1	0	-0.820340	-7.331566	0.681828
1	0	0.953285	-6.334687	-0.776397
1	0	-1.238809	-0.134835	1.001506
1	0	-2.691624	-1.177740	2.692989
1	0	-2.887302	-3.658478	2.812581
16	0	1.802410	-3.742138	-1.294858
34	0	0.512415	-1.070916	-1.192868
6	0	-0.429345	4.312938	-0.331104
6	0	0.429345	3.410838	0.380322
6	0	1.391588	4.005540	1.284614
6	0	1.499670	5.418481	1.383830
6	0	0.717254	6.251653	0.610591
6	0	-0.275550	5.692131	-0.219470
6	0	0.457904	1.980561	0.229966
6	0	1.232402	1.216536	1.099317
6	0	2.100550	1.813028	2.036905
6	0	2.185793	3.186046	2.127628
1	0	2.239734	5.833396	2.065953
1	0	0.820340	7.331566	0.681828
1	0	-0.953285	6.334687	-0.776397
1	0	1.238809	0.134835	1.001506
1	0	2.691624	1.177740	2.692989
1	0	2.887302	3.658478	2.812581
16	0	-1.802410	3.742138	-1.294858
34	0	-0.512415	1.070916	-1.192868
6	0	-2.932074	3.282024	0.048277
1	0	-3.146839	4.152265	0.671052
1	0	-3.851041	2.930253	-0.426803
1	0	-2.505312	2.474960	0.647267
6	0	2.932074	-3.282024	0.048277
1	0	3.146839	-4.152265	0.671052
1	0	3.851041	-2.930253	-0.426803
1	0	2.505312	-2.474960	0.647267

MP2/BSS-B
Compound **4**
Symmetry C_2
energy MP2 = -10447.0363764 au
Standard orientation

6	0	-3.257675	-2.890539	-0.181318
6	0	-3.029032	-1.661182	0.518673
6	0	-4.093758	-1.207095	1.391672
6	0	-5.318522	-1.922976	1.459127
6	0	-5.532306	-3.047509	0.689016
6	0	-4.477718	-3.555427	-0.097573
6	0	-1.873375	-0.812346	0.394746
6	0	-1.713494	0.259234	1.270187
6	0	-2.722251	0.628187	2.183672
6	0	-3.899887	-0.085949	2.239401
1	0	-6.101250	-1.546550	2.115457
1	0	-6.479137	-3.579833	0.736459

1	0	-4.601694	-4.491534	-0.636316
1	0	-0.830360	0.886646	1.193670
1	0	-2.556649	1.475614	2.845388
1	0	-4.708517	0.219679	2.900631
34	0	-1.873375	-3.807143	-1.135219
34	0	-0.549343	-1.057799	-1.013506
6	0	3.257675	2.890539	-0.181318
6	0	3.029032	1.661182	0.518673
6	0	4.093758	1.207095	1.391672
6	0	5.318522	1.922976	1.459127
6	0	5.532306	3.047509	0.689016
6	0	4.477718	3.555427	-0.097573
6	0	1.873375	0.812346	0.394746
6	0	1.713494	-0.259234	1.270187
6	0	2.722251	-0.628187	2.183672
6	0	3.899887	0.085949	2.239401
1	0	6.101250	1.546550	2.115457
1	0	6.479137	3.579833	0.736459
1	0	4.601694	4.491534	-0.636316
1	0	0.830360	-0.886646	1.193670
1	0	2.556649	-1.475614	2.845388
1	0	4.708517	-0.219679	2.900631
34	0	1.873375	3.807143	-1.135219
34	0	0.549343	1.057799	-1.013506
6	0	0.826052	4.317365	0.431718
1	0	1.461721	4.857334	1.133923
1	0	0.024594	4.968619	0.076727
1	0	0.397695	3.427319	0.894762
6	0	-0.826052	-4.317365	0.431718
1	0	-1.461721	-4.857334	1.133923
1	0	-0.024594	-4.968619	0.076727
1	0	-0.397695	-3.427319	0.894762

MP2/BSS-C
Compound Model **A** (S, S)
Symmetry C_2
energy MP2 = -1594.3864296 au
Standard orientation

16	0	-0.182058	4.515400	-0.205900
1	0	-1.468017	4.148897	-0.199415
1	0	-0.047725	4.277458	1.103112
16	0	-0.182058	1.013261	0.195466
1	0	0.706861	1.383101	-0.736758
16	0	0.182058	-1.013261	0.195466
1	0	-0.706861	-1.383101	-0.736758
16	0	0.182058	-4.515400	-0.205900
1	0	1.468017	-4.148897	-0.199415
1	0	0.047725	-4.277458	1.103112

MP2/BSS-C
Compound Model **A** (S, Se)
Symmetry C_2
energy MP2 = -5598.867083 au
Standard orientation

34	0	-0.181650	4.622826	-0.144853
1	0	-1.588748	4.221117	-0.128045
1	0	-0.050681	4.363083	1.289371
16	0	-0.181650	1.013911	0.276232
1	0	0.708042	1.382131	-0.656020
16	0	0.181650	-1.013911	0.276232
1	0	-0.708042	-1.382131	-0.656020
34	0	0.181650	-4.622826	-0.144853
1	0	1.588748	-4.221117	-0.128045

1	0	0.050681	-4.363083	1.289371

MP2/BSS-C
Compound Model **A** (Se, S)
Symmetry C_2
energy MP2 = -5598.8873202 au
Standard orientation

16	0	-0.178113	4.713482	-0.269990
1	0	-1.497904	4.497647	-0.263533
1	0	-0.099774	4.642358	1.063186
34	0	-0.178113	1.156788	0.129932
1	0	0.816430	1.483883	-0.897504
34	0	0.178113	-1.156788	0.129932
1	0	-0.816430	-1.483883	-0.897504
16	0	0.178113	-4.713482	-0.269990
1	0	1.497904	-4.497647	-0.263533
1	0	0.099774	-4.642358	1.063186

MP2/BSS-C
Compound Model **A** (Se, Se)
Symmetry C_2
energy MP2 = -9603.3680377 au
Standard orientation

34	0	-0.182597	4.822859	-0.211016
1	0	-1.626869	4.587078	-0.191482
1	0	-0.108816	4.736923	1.248127
34	0	-0.182597	1.156943	0.204148
1	0	0.811632	1.485903	-0.823132
34	0	0.182597	-1.156943	0.204148
1	0	-0.811632	-1.485903	-0.823132
34	0	0.182597	-4.822859	-0.211016
1	0	1.626869	-4.587078	-0.191482
1	0	0.108816	-4.736923	1.248127

MP2/BSS-C
Compound Model **B** (S, S)
Symmetry C_2
energy MP2 = -1672.7825301 au
Standard orientation

16	0	0.033052	4.665330	-0.594195
1	0	1.102213	3.916868	-0.301069
1	0	-0.384677	3.792796	-1.518075
16	0	-0.033052	1.016046	-0.046834
6	0	-1.236521	1.378588	1.259139
1	0	-1.345657	2.467242	1.267210
1	0	-0.865966	1.038081	2.228135
1	0	-2.191585	0.904919	1.025423
16	0	0.033052	-1.016046	-0.046834
6	0	1.236521	-1.378588	1.259139
1	0	1.345657	-2.467242	1.267210
1	0	0.865966	-1.038081	2.228135
1	0	2.191585	-0.904919	1.025423
16	0	-0.033052	- 4.665330	-0.594195
1	0	-1.102213	-3.916868	-0.301069
1	0	0.384677	-3.792796	-1.518075

MP2/BSS-C
Compound Model **B** (S, Se)
Symmetry C_2
energy MP2 = -5677.5934432 au
Standard orientation

34	0	-1.639103	4.476296	-0.439268
1	0	-0.269776	4.116144	-0.091607

1	0	-1.713461	3.380979	-1.398721
16	0	-0.384516	0.941301	0.157116
6	0	-1.639103	0.861442	1.463103
1	0	-2.121271	1.843712	1.471331
1	0	-1.173262	0.671626	2.432260
1	0	-2.369160	0.084525	1.229363
16	0	0.384516	-0.941301	0.157116
6	0	1.639103	-0.861442	1.463103
1	0	2.121271	-1.843712	1.471331
1	0	1.173262	-0.671626	2.432260
1	0	2.369160	-0.084525	1.229363
34	0	1.639103	-4.476296	-0.439268
1	0	0.269776	-4.116144	-0.091607
1	0	1.713461	-3.380979	-1.398721

MP2/BSS-C
Compound Model **B** (Se, S)
Symmetry C_2
energy MP2 = -5677.6170425 au
Standard orientation

16	0	0.006526	4.871876	-0.383168
1	0	1.162178	4.221800	-0.205497
1	0	-0.306535	4.132058	-1.453042
34	0	-0.006526	1.150201	-0.131536
6	0	-1.311374	1.473206	1.280728
1	0	-1.420013	2.559149	1.342596
1	0	-0.938873	1.076158	2.225612
1	0	-2.258298	1.006515	1.008879
34	0	0.006526	-1.150201	-0.131536
6	0	1.311374	-1.473206	1.280728
1	0	1.420013	-2.559149	1.342596
1	0	0.938873	-1.076158	2.225612
1	0	2.258298	-1.006515	1.008879
16	0	-0.006526	-4.871876	-0.383168
1	0	-1.162178	-4.221800	-0.205497
1	0	0.306535	-4.132058	-1.453042

MP2/BSS-C
Compound Model **B** (Se, Se)
Symmetry C_2
energy MP2 = -9682.4281348 au
Standard orientation

34	0	0.009020	4.968138	-0.312082
1	0	1.238022	4.215643	-0.089448
1	0	-0.349244	4.112067	-1.436923
34	0	-0.009020	1.150500	-0.030465
6	0	-1.315106	1.469237	1.381989
1	0	-1.427252	2.554902	1.444264
1	0	-0.941505	1.073163	2.326892
1	0	-2.260626	0.999768	1.109897
34	0	0.009020	-1.150500	-0.030465
6	0	1.315106	-1.469237	1.381989
1	0	1.427252	-2.554902	1.444264
1	0	0.941505	-1.073163	2.326892
1	0	2.260626	-0.999768	1.109897
34	0	-0.009020	-4.968138	-0.312082
1	0	-1.238022	-4.215643	-0.089448
1	0	0.349244	-4.112067	-1.436923

MP2/BSS-C
Compound Model **C** (S, S)
Symmetry C_2
energy MP2 = -1751.1629564 au

Standard orientation

16	0	0.068525	4.283003	-0.366693
6	0	-1.713850	4.216418	-0.108397
1	0	-2.183028	4.231555	-1.094789
1	0	-1.989082	3.290847	0.405005
1	0	-2.050458	5.083558	0.466593
6	0	0.599512	4.210148	1.354313
1	0	1.691480	4.242634	1.356065
1	0	0.211717	5.067542	1.911405
1	0	0.267343	3.275344	1.814360
16	0	-0.068525	1.032498	-0.325574
1	0	0.855657	1.297836	-1.257850
16	0	0.068525	-1.032498	-0.325574
1	0	-0.855657	-1.297836	-1.257850
16	0	-0.068525	-4.283003	-0.366693
6	0	1.713850	-4.216418	-0.108397
1	0	2.183028	-4.231555	-1.094789
1	0	1.989082	-3.290847	0.405005
1	0	2.050458	-5.083558	0.466593
6	0	-0.599512	-4.210148	1.354313
1	0	-1.691480	-4.242634	1.356065
1	0	-0.211717	-5.067542	1.911405
1	0	-0.267343	-3.275344	1.814360

MP2/BSS-C
Compound Model **C** (S, Se)
Symmetry C_2
energy MP2 = -5755.9852957 au
Standard orientation

34	0	0.045975	4.362268	-0.265867
6	0	-1.883660	4.198464	-0.354575
1	0	-2.162261	4.252724	-1.408766
1	0	-2.187155	3.233051	0.055410
1	0	-2.351755	5.018650	0.193152
6	0	0.183513	4.201277	1.661149
1	0	1.244141	4.259890	1.913132
1	0	-0.355443	5.020114	2.141633
1	0	-0.214814	3.234662	1.976065
16	0	-0.045975	1.034960	-0.161053
1	0	0.883346	1.279754	-1.093760
16	0	0.045975	-1.034960	-0.161053
1	0	-0.883346	-1.279754	-1.093760
34	0	-0.045975	-4.362268	-0.265867
6	0	1.883660	-4.198464	-0.354575
1	0	2.162261	-4.252724	-1.408766
1	0	2.187155	-3.233051	0.055410
1	0	2.351755	-5.018650	0.193152
6	0	-0.183513	-4.201277	1.661149
1	0	-1.244141	-4.259890	1.913132
1	0	0.355443	-5.020114	2.141633
1	0	0.214814	-3.234662	1.976065

MP2/BSS-C
Compound Model **C** (Se, S)
Symmetry C_2
energy MP2 = -5755.9953278 au
Standard orientation

16	0	0.065085	4.435988	-0.292079
6	0	-1.727373	4.444886	-0.103780
1	0	-2.156787	4.420840	-1.107888
1	0	-2.056586	3.559461	0.447890
1	0	-2.053690	5.353663	0.409386
6	0	0.526849	4.445599	1.450379

1	0	1.618291	4.432289	1.494093
1	0	0.155483	5.350291	1.939641
1	0	0.137317	3.554704	1.951214
34	0	-0.065085	1.168794	-0.214822
1	0	0.953300	1.393605	-1.236719
34	0	0.065085	-1.168794	-0.214822
1	0	-0.953300	-1.393605	-1.236719
16	0	-0.065085	-4.435988	-0.292079
6	0	1.727373	-4.444886	-0.103780
1	0	2.156787	-4.420840	-1.107888
1	0	2.056586	-3.559461	0.447890
1	0	2.053690	-5.353663	0.409386
6	0	-0.526849	-4.445599	1.450379
1	0	-1.618291	-4.432289	1.494093
1	0	-0.155483	-5.350291	1.939641
1	0	-0.137317	-3.554704	1.951214

MP2/BSS-C
Compound Model **C** (Se, Se)
Symmetry C_2
energy MP2 = -9760.8173984 au
Standard orientation

34	0	0.095084	4.527300	-0.223212
6	0	-1.650779	4.367457	0.604231
1	0	-2.392255	4.424428	-0.194976
1	0	-1.729597	3.402197	1.109425
1	0	-1.803663	5.186119	1.310110
6	0	1.120007	4.323935	1.410399
1	0	2.175246	4.385461	1.137071
1	0	0.872707	5.127976	2.106348
1	0	0.910989	3.347040	1.851217
34	0	-0.095084	1.168347	-0.308439
1	0	0.917470	1.416624	-1.330830
34	0	0.095084	-1.168347	-0.308439
1	0	-0.917470	-1.416624	-1.330830
34	0	-0.095084	-4.527300	-0.223212
6	0	1.650779	-4.367457	0.604231
1	0	2.392255	-4.424428	-0.194976
1	0	1.729597	-3.402197	1.109425
1	0	1.803663	-5.186119	1.310110
6	0	-1.120007	-4.323935	1.410399
1	0	-2.175246	-4.385461	1.137071
1	0	-0.872707	-5.127976	2.106348
1	0	-0.910989	-3.347040	1.851217

MP2/BSS-C
Compound Model **D** (S, S)
Symmetry C_2
energy MP2 = -1829.5581602 au
Standard orientation

16	0	-0.004779	4.375512	-0.215236
6	0	1.648002	3.936488	-0.783142
1	0	2.344018	4.197981	0.017303
1	0	1.709069	2.861735	-0.975127
1	0	1.904904	4.499661	-1.684758
6	0	-0.942748	3.834623	-1.656668
1	0	-1.995367	4.048161	-1.455672
1	0	-0.627992	4.386121	-2.547133
1	0	-0.814268	2.759198	-1.807674
16	0	0.004779	1.020351	0.559049
6	0	-1.182950	1.411477	1.871349
1	0	-1.246563	2.502854	1.895125
1	0	-0.824545	1.040149	2.833891

1	0	-2.155977	0.977199	1.633816
16	0	-0.004779	-1.020351	0.559049
6	0	1.182950	-1.411477	1.871349
1	0	1.246563	-2.502854	1.895125
1	0	0.824545	-1.040149	2.833891
1	0	2.155977	-0.977199	1.633816
16	0	0.004779	-4.375512	-0.215236
6	0	-1.648002	-3.936488	-0.783142
1	0	-2.344018	-4.197981	0.017303
1	0	-1.709069	-2.861735	-0.975127
1	0	-1.904904	-4.499661	-1.684758
6	0	0.942748	-3.834623	-1.656668
1	0	1.995367	-4.048161	-1.455672
1	0	0.627992	-4.386121	-2.547133
1	0	0.814268	-2.759198	-1.807674

MP2/BSS-C
Compound Model **D** (S, Se)
Symmetry C_2
energy MP2 = -5834.3805116 au
Standard orientation

34	0	0.026018	4.454379	-0.166032
6	0	1.846485	3.915411	-0.555540
1	0	2.461657	4.223944	0.292068
1	0	1.889133	2.829848	-0.664001
1	0	2.193861	4.412553	-1.463399
6	0	-0.751942	3.757500	-1.799680
1	0	-1.821504	3.974721	-1.765179
1	0	-0.304777	4.252891	-2.663808
1	0	-0.595870	2.677715	-1.842872
16	0	-0.026018	1.020475	0.612828
6	0	-1.225147	1.374405	1.925519
1	0	-1.324326	2.463198	1.949019
1	0	-0.854287	1.015207	2.887956
1	0	-2.183666	0.908873	1.688231
16	0	0.026018	-1.020475	0.612828
6	0	1.225147	-1.374405	1.925519
1	0	1.324326	-2.463198	1.949019
1	0	0.854287	-1.015207	2.887956
1	0	2.183666	-0.908873	1.688231
34	0	-0.026018	-4.454379	-0.166032
6	0	-1.846485	-3.915411	-0.555540
1	0	-2.461657	-4.223944	0.292068
1	0	-1.889133	-2.829848	-0.664001
1	0	-2.193861	-4.412553	-1.463399
6	0	0.751942	-3.757500	-1.799680
1	0	1.821504	-3.974721	-1.765179
1	0	0.304777	-4.252891	-2.663808
1	0	0.595870	-2.677715	-1.842872

MP2/BSS-C
Compound Model **D** (Se, S)
Symmetry C_2
energy MP2 = -5834.3942751 au
Standard orientation

16	0	-0.051484	4.513532	-0.217264
6	0	1.421781	4.157784	-1.191826
1	0	2.284740	4.304354	-0.538203
1	0	1.404826	3.120512	-1.539314
1	0	1.490906	4.840778	-2.043099
6	0	-1.299916	4.166189	-1.471107
1	0	-2.276252	4.339404	-1.011855
1	0	-1.180864	4.837359	-2.326351

1	0	-1.230579	3.122623	-1.791398
34	0	0.051484	1.154987	0.352646
6	0	-1.233825	1.515930	1.774179
1	0	-1.272987	2.603409	1.873400
1	0	-0.887706	1.063974	2.704715
1	0	-2.207997	1.116150	1.490886
34	0	-0.051484	-1.154987	0.352646
6	0	1.233825	-1.515930	1.774179
1	0	1.272987	-2.603409	1.873400
1	0	0.887706	-1.063974	2.704715
1	0	2.207997	-1.116150	1.490886
16	0	0.051484	-4.513532	-0.217264
6	0	-1.421781	-4.157784	-1.191826
1	0	-2.284740	-4.304354	-0.538203
1	0	-1.404826	-3.120512	-1.539314
1	0	-1.490906	-4.840778	-2.043099
6	0	1.299916	-4.166189	-1.471107
1	0	2.276252	-4.339404	-1.011855
1	0	1.180864	-4.837359	-2.326351
1	0	1.230579	-3.122623	-1.791398

MP2/BSS-C
Compound Model **D** (Se, Se)
Symmetry C_2
energy MP2 = - 9839.2165615 au
Standard orientation

34	0	-0.103719	4.575692	-0.267441
6	0	1.152174	3.974659	-1.615846
1	0	2.155075	4.187088	-1.240267
1	0	1.034330	2.899428	-1.767916
1	0	0.983833	4.518219	-2.547614
6	0	-1.702226	4.001260	-1.203950
1	0	-2.556127	4.256668	-0.572784
1	0	-1.782813	4.526435	-2.157839
1	0	-1.661889	2.920233	-1.355797
34	0	0.110131	1.151097	0.513562
6	0	-1.152174	1.576996	1.938136
1	0	-1.129678	2.664473	2.044170
1	0	-0.831358	1.100736	2.865664
1	0	-2.148048	1.234909	1.654220
34	0	-0.110131	-1.151097	0.513562
6	0	1.152174	-1.576996	1.938136
1	0	1.129678	-2.664473	2.044170
1	0	0.831358	-1.100736	2.865664
1	0	2.148048	-1.234909	1.654220
34	0	0.103719	-4.575692	-0.267441
6	0	-1.152174	-3.974659	-1.615846
1	0	-2.155075	-4.187088	-1.240267
1	0	-1.034330	-2.899428	-1.767916
1	0	-0.983833	-4.518219	-2.547614
6	0	1.702226	-4.001260	-1.203950
1	0	2.556127	-4.256668	-0.572784
1	0	1.782813	-4.526435	-2.157839
1	0	1.661889	-2.920233	-1.355797