Electronic Supplementary Information

Behavior of Interactions Between Hydrogen Chalcogenides and Anthracene π-System, Elucidated by QTAIM Dual Functional Analysis with QC Calculations

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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 $\rho(r)$ reaches a minimum. It is donated by $\rho_b(r_c)$. 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 $\rho_b(r_c)$ ($\nabla^2\rho_b(r_c)$) indicates that $\rho_b(r_c)$ is depleted or concentrated with respect to its surrounding, since $\nabla^2\rho_b(r_c)$ is the second derivative of $\rho_b(r_c)$. $\rho_b(r_c)$ is locally depleted relative to the average distribution around r_c if $\nabla^2\rho_b(r_c) > 0$, but it is concentrated when $\nabla^2\rho_b(r_c) < 0$. Total electron energy densities at BCPs ($H_b(r_c)$) must be a more appropriate measure for weak interactions on the energy basis.[S1-S6] $H_b(r_c)$ are the sum of kinetic energy densities ($G_b(r_c)$) and potential energy densities ($V_b(r_c)$) at BCPs, as shown in eqn (S1). Electrons at BCPs are stabilized when $H_b(r_c) < 0$, therefore, interactions exhibit the covalent nature in this region, whereas they exhibit no covalency if $H_b(r_c) > 0$, due to the destabilization of electrons at BCPs under the conditions.[S1] Eqn (S2) represents the relation between $\nabla^2\rho_b(r_c)$ and $H_b(r_c)$, together with $G_b(r_c)$ and $V_b(r_c)$, which is closely related to the virial theorem.

$$H_b(r_c) = G_b(r_c) + V_b(r_c) \tag{S1}$$
$$(\hbar^2/8m)\nabla^2\rho_b(r_c) = H_b(r_c) - V_b(r_c)/2 \tag{S2}$$
$$= G_b(r_c) + V_b(r_c)/2 \tag{S2'}$$

Interactions are classified by the signs of $\nabla^2\rho_b(r_c)$ and $H_b(r_c)$. Interactions in the region of $\nabla^2\rho_b(r_c) < 0$ are called shared-shell (SS) interactions and they are closed-shell (CS) interactions for $\nabla^2\rho_b(r_c) > 0$. $H_b(r_c)$ must be negative when $\nabla^2\rho_b(r_c) < 0$, since $H_b(r_c)$ are larger than $(\hbar^2/8m)\nabla^2\rho_b(r_c)$ by $V_b(r_c)/2$ with negative $V_b(r_c)$ at all BCPs (eqn (S2)). Consequently, $\nabla^2\rho_b(r_c) < 0$ and $H_b(r_c) < 0$ for the SS interactions. The CS interactions are especially called *pure* CS interactions for $H_b(r_c) > 0$ and $\nabla^2\rho_b(r_c) > 0$, 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

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at BCPs, since $\nabla^2\rho_b(\mathbf{r}_c) > 0$ but $H_b(\mathbf{r}_c) < 0$.[S1a] We call the interactions in this region *regular* CS,[S4,S5] when it is necessary to distinguish from *pure* CS. The role of $\nabla^2\rho_b(\mathbf{r}_c)$ in the classification can be replaced by $H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2$, since $(\hbar^2/8m)\nabla^2\rho_b(\mathbf{r}_c) = H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2$ (eqn (S2)).

We proposed QTAIM-DFA by plotting $H_b(\mathbf{r}_c)$ versus $H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2$ $(= (\hbar^2/8m)\nabla^2\rho_b(\mathbf{r}_c))$,[S4a] after the proposal of $H_b(\mathbf{r}_c)$ versus $\nabla^2\rho_b(\mathbf{r}_c)$.[S4b] Both axes in the plot of the former are given in energy unit, therefore, distances on the (x, y) $(= (H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2, H_b(\mathbf{r}_c)))$ 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 $\nabla^2\rho_b(\mathbf{r}_c)$ and $H_b(\mathbf{r}_c)$. 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.
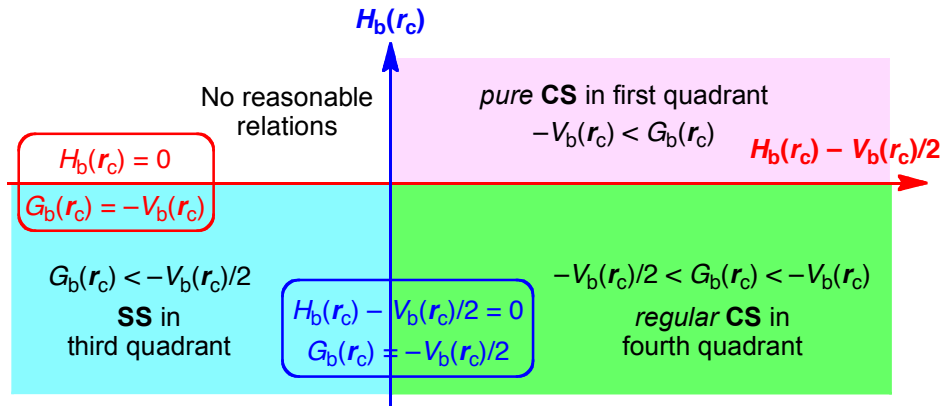
Scheme S1. QTAIM-DFA: Plot of $H_b(\mathbf{r}_c)$ versus $H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2$ for Weak to Strong Interactions

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 $H_b(\mathbf{r}_c)$ versus $H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2$ 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 eqn (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 eqn (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 eqn (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 (eqn (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 $\rho_b(\mathbf{r}_c)$, $\nabla^2\rho_b(\mathbf{r}_c)$, $G_b(\mathbf{r}_c)$, $V_b(\mathbf{r}_c)$, $H_b(\mathbf{r}_c)$ and $H_b(\mathbf{r}_c) - V_b(\mathbf{r}_c)/2$ belong to QTAIM functions. $k_b(\mathbf{r}_c)$, defined by eqn (S7), is an QTAIM function but it will be treated as if it were an QTAIM-DFA parameter, if suitable.
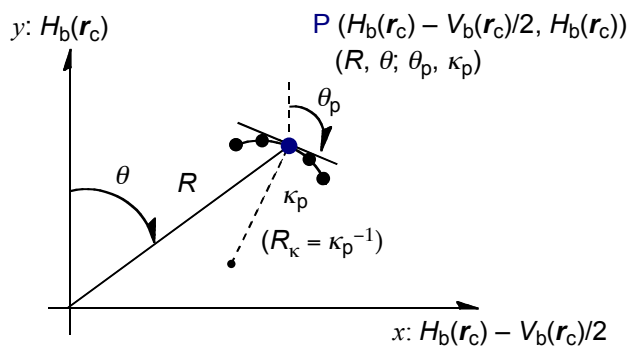
Figure S1. Polar (R, θ) coordinate representation of $H_b(r_c)$ versus $H_b(r_c) - V_b(r_c)/2$, with (θ_p, κ_p) parameters.

$$R = (x^2 + y^2)^{1/2} \tag{S3}$$
$$\theta = 90° - \tan^{-1}(y/x) \tag{S4}$$
$$\theta_p = 90° - \tan^{-1}(dy/dx) \tag{S5}$$
$$\kappa_p = |d^2y/dx^2| / [1 + (dy/dx)^2]^{3/2} \tag{S6}$$
$$k_b(r_c) = V_b(r_c)/G_b(r_c) \tag{S7}$$
$$\text{where } (x, y) = (H_b(r_c) - V_b(r_c)/2, H_b(r_c))$$

Criteria for Classification of Interactions: Behavior of Typical Interactions Elucidated by QTAIM-DFA

$H_b(r_c)$ are plotted versus $H_b(r_c) - V_b(r_c)/2$ 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 eqns (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 $k_b(r_c)$. The criteria will be employed to discuss the nature of interactions in question, as a reference.
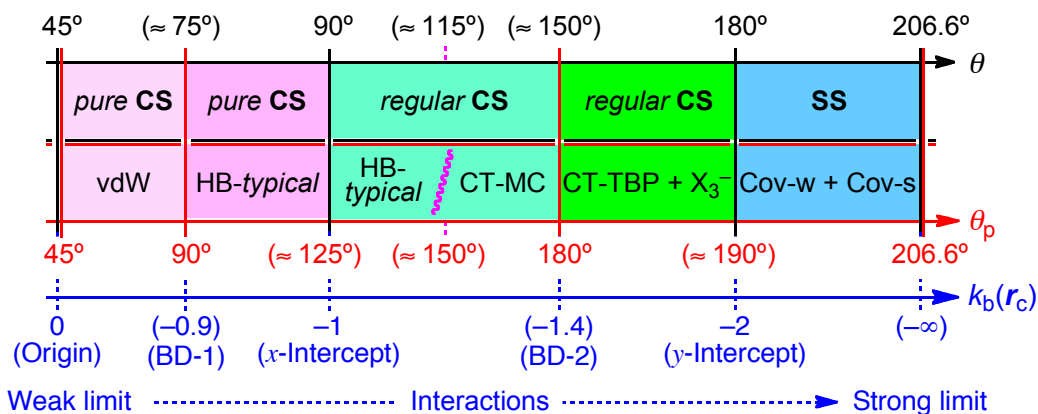
Scheme S2. Rough classification of interactions by θ and θ_p, together with $k_b(r_c)$ ($= V_b(r_c)/G_b(r_c)$).

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Table S1. Optimization processes starting from type II_{Atc} of (EH_2)---$\pi(C_{14}H_{10})$ (E = O, S, Se and Te).

E	Stating → Converged	Stating → Converged	Stating → Converged
O	type IIA_{Atc} → type IIA_{Atc}	type IIB_{Atc} → type IIB_{Atc}	type IIC_{Atc} → type IIB_{Atc}
S	type IIA_{Atc} → type IIA_{Atc}	type IIB_{Atc} → type IIB_{Atc}	type IIC_{Atc} → type IIB_{Atc}
Se	type IIA_{Atc} → type IIB_{Atc}	type IIB_{Atc} → type IIB_{Atc}	type IIC_{Atc} → type IIB_{Atc}
Te	type IIA_{Atc} → type IIB_{Atc}	type IIB_{Atc} → type IIB_{Atc}	type IIC_{Atc} → type IIB_{Atc}
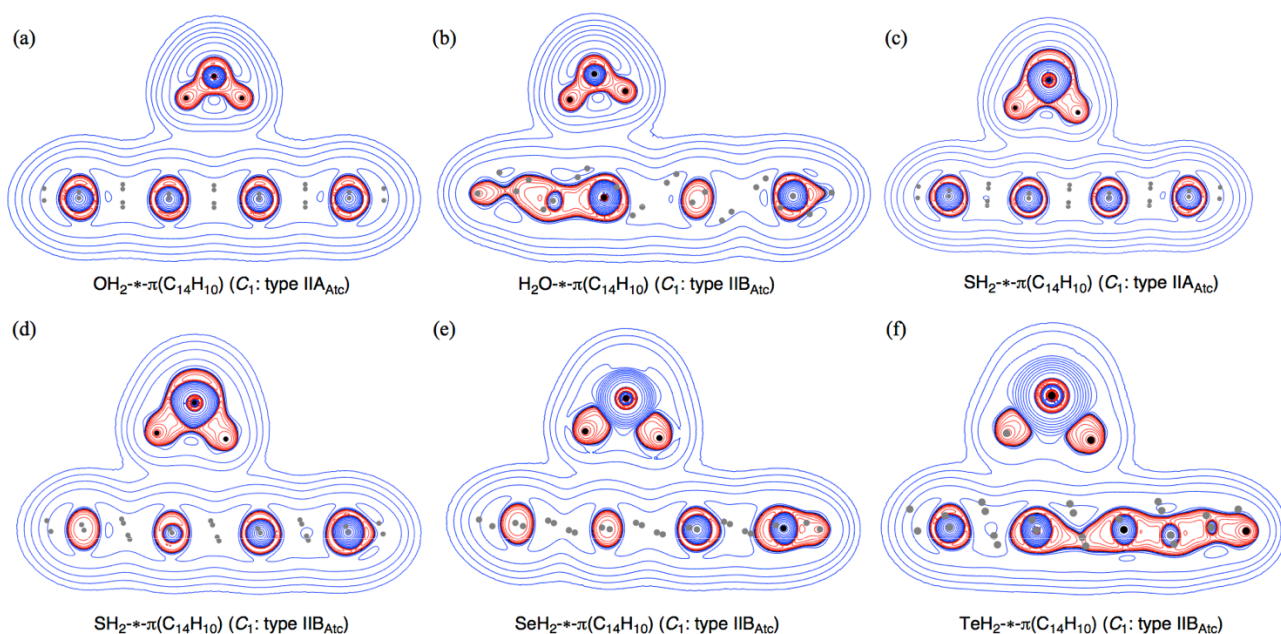
Figure S2. Negative Laplacian for OH_2-*-$\pi(C_{14}H_{10})$ (C_1: type IIA_{Atc}) (a), H_2O-*-$\pi(C_{14}H_{10})$ (C_1: type IIB_{Atc}) (b), SH_2-*-$\pi(C_{14}H_{10})$ (C_1: type IIA_{Atc}) (c), SH_2-*-$\pi(C_{14}H_{10})$ (C_1: type IIB_{Atc}) (d), SeH_2-*-$\pi(C_{14}H_{10})$ (C_1: type IIB_{Atc}) (e) and TeH_2-*-$\pi(C_{14}H_{10})$ (C_1: type IIB_{Atc}), calculated with MP2/BSS-F. Positive and negative areas are shown by blue and red lines, respectively.
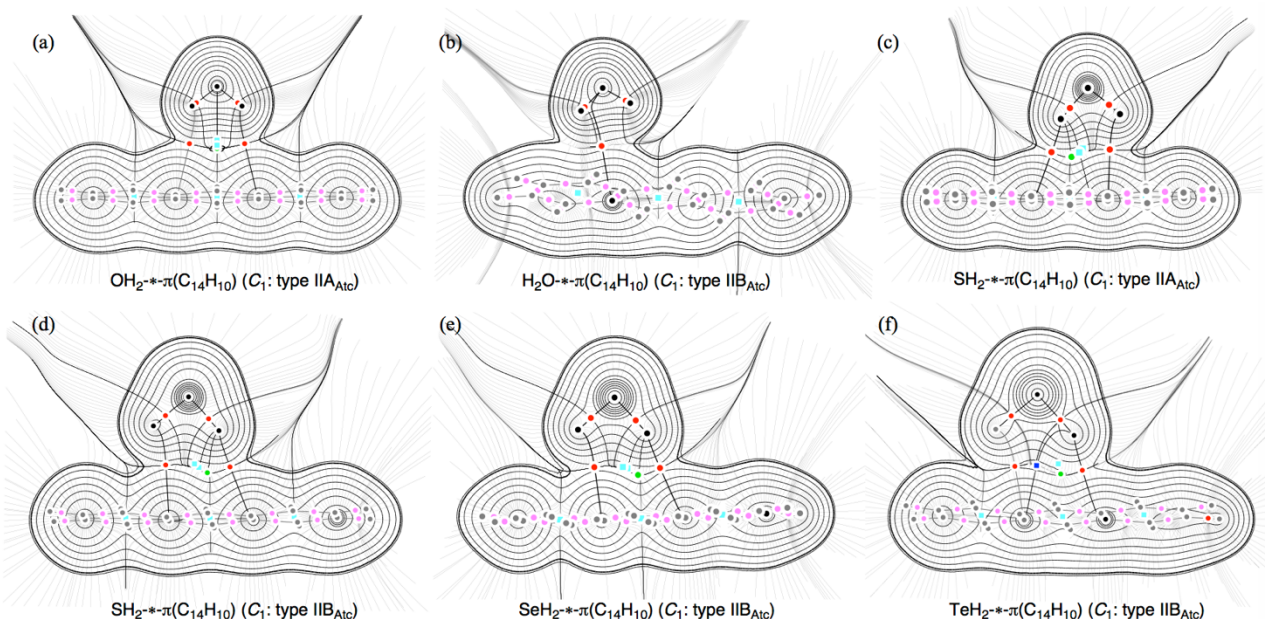
Figure S3. Trajectory plots for OH$_2$-*-π(C$_{14}$H$_{10}$) (C$_1$: type IIA$_{Atc}$) (a), H$_2$O-*-π(C$_{14}$H$_{10}$) (C$_1$: type IIB$_{Atc}$) (b), SH$_2$-*-π(C$_{14}$H$_{10}$) (C$_1$: type IIA$_{Atc}$) (c), SH$_2$-*-π(C$_{14}$H$_{10}$) (C$_1$: type IIB$_{Atc}$) (d), SeH$_2$-*-π(C$_{14}$H$_{10}$) (C$_1$: type IIB$_{Atc}$) (e) and TeH$_2$-*-π(C$_{14}$H$_{10}$) (C$_1$: type IIB$_{Atc}$), calculated with MP2/BSS-F. Colors are the same as those in Figure 3.

Table S2. Lengths of Bond Paths (r_{BP}) with Components (r_{BP-1} and r_{BP-2}) and Corresponding Straight line Distances (R_{SL}) in (EH$_2$)-*-π(C$_{14}$H$_{10}$) (E = O, S, Se and Te), Evaluated at the MP2 with BSS-F[a,b]

Interaction (X-*-Y)[d]	type[c]	r_{BP-1} (Å)	r_{BP-2} (Å)	r_{BP} (Å)	R_{SL} (Å)
OHH-*-$^{11(13)}$**C**(π)	IIA$_{Atc}$[e]	1.1374	1.7356	2.8730	2.7869
H$_2$O-*-^{11}**C**(π)	IIB$_{Atc}$	1.8589	1.6483	3.5072	3.3373
S^{o}H^i**H**-*-^{11}**C**(π)	IIA$_{Atc}$	1.2260	1.6786	2.7938	2.7938
S^{i}H^o**H**-*-^{13}**C**(π)	IIA$_{Atc}$	1.1154	1.7056	2.8210	2.7925
S^{o}H^i**H**-*-^{11}**C**(π)	IIB$_{Atc}$	1.1139	1.7046	2.8185	2.7902
S^{i}H^o**H**-*-^{13}**C**(π)	IIB$_{Atc}$	1.2392	1.7399	2.9791	2.8165
Se^{o}H^i**H**-*-^{11}**C**(π)	IIB$_{Atc}$	1.1114	1.6842	2.7956	2.7696
Se^{i}H^o**H**-*-^{13}**C**(π)	IIB$_{Atc}$	1.2697	2.0024	3.2721	2.8572
Te^{o}H^i**H**-*-^{11}**C**(π)	IIB$_{Atc}$	1.0787	1.6973	2.7760	2.6707
Te^{i}H^o**H***-^{13}**C**(π)	IIB$_{Atc}$	1.3129	1.6501	2.9630	2.8409

[a] See "Methodological details in calculations" for BSSs. [b] See text for r_{BP-1} and r_{BP-2}, where $r_{BP} = r_{BP-1} + r_{BP-2}$.
[c] See Scheme 1 and Figures 1 and 2. [d] The optimized structure has the C$_1$ symmetry and atoms taking part in the interaction are shown by bold with BCP denoted by *. [e] Very close to the C$_s$ symmetry.

References

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

Optimized structures given by Cartesian coordinates

The structures were optimized employing the Gaussian 09 programs.

MP2/BSS-F   C, H: 6-311++G(d,p), O: 6-311+G(3df)
Adduct $OH_2---\pi(C_{14}H_{10})$
Symmetry $(C_1: IIA_{Atc})$
energy $E = -614.3482466$ au
Standard orientation

6	0	-0.000009	-1.397290	-0.363121
6	0	0.000006	1.418544	-0.285819
1	0	-0.000013	-2.487335	-0.369673
1	0	0.000012	2.508425	-0.273680
6	0	-1.226148	-0.712974	-0.308868
6	0	-1.226144	0.733639	-0.326399
6	0	1.226132	-0.712992	-0.308865
6	0	1.226147	0.733618	-0.326397
6	0	-2.478809	-1.400560	-0.341765
6	0	-2.477685	1.420756	-0.261479
1	0	-2.477642	-2.488808	-0.357179
1	0	-2.476430	2.508977	-0.245013
6	0	2.478799	-1.400565	-0.341773
6	0	2.477681	1.420748	-0.261482
1	0	2.477649	-2.488813	-0.357188
1	0	2.476408	2.508969	-0.245015
6	0	-3.666706	-0.702509	-0.293096
6	0	-3.666520	0.722691	-0.272160
1	0	-4.611657	-1.239496	-0.304196
1	0	-4.610704	1.259548	-0.230784
6	0	3.666696	-0.702510	-0.293110
6	0	3.666518	0.722690	-0.272172
1	0	4.611648	-1.239494	-0.304221
1	0	4.610700	1.259551	-0.230801
8	0	0.000029	-0.095328	2.964906
1	0	-0.756121	-0.099464	2.368767
1	0	0.756184	-0.099156	2.368771

MP2/BSS-F   C, H: 6-311++G(d,p), O: 6-311+G(3df)
Adduct $OH_2---\pi(C_{14}H_{10})$
Symmetry $(C_1: IIB_{Atc})$
energy $E = -614.347928$ au
Standard orientation

6	0	-0.178929	-1.379624	-0.388904
6	0	-0.188318	1.431633	-0.215095
1	0	-0.171940	-2.468808	-0.430676
1	0	-0.193269	2.520651	-0.167808
6	0	-1.399992	-0.707952	-0.210575
6	0	-1.409671	0.737792	-0.173803
6	0	1.042372	-0.686116	-0.422961
6	0	1.033340	0.759974	-0.391048
6	0	-2.646853	-1.404716	-0.167363
6	0	-2.655855	1.411831	0.012612
1	0	-2.640531	-2.491753	-0.219761
1	0	-2.659848	2.498895	0.065376
6	0	2.292615	-1.362027	-0.573807
6	0	2.280753	1.456491	-0.417065
1	0	2.297192	-2.449308	-0.624517
1	0	2.274109	2.543539	-0.364833
6	0	-3.831360	-0.718974	-0.003106
6	0	-3.838029	0.704654	0.064954
1	0	-4.771355	-1.263068	0.039007

1	0	-4.779537	1.231693	0.196199
6	0	3.477104	-0.654920	-0.603295
6	0	3.469979	0.769559	-0.540176
1	0	4.421533	-1.183949	-0.702714
1	0	4.410928	1.313039	-0.562551
8	0	1.740932	-0.246231	2.810603
1	0	0.892072	-0.023805	2.415520
1	0	2.310255	-0.402922	2.049721

MP2/BSS-F   C, H: 6-311++G(d,p), S: 6-311+G(3df)
Adduct SH_2---$\pi(C_{14}H_{10})$
Symmetry $(C_1$: $IIA_{Atc})$
energy E = -936.9261462 au
Standard orientation

6	0	-0.140977	-0.609500	-1.395343
6	0	-0.140592	-0.550848	1.421086
1	0	-0.141934	-0.645774	-2.484781
1	0	-0.137794	-0.502771	2.510153
6	0	1.079789	-0.709030	-0.707586
6	0	1.083801	-0.621540	0.735964
6	0	-1.364743	-0.517796	-0.711217
6	0	-1.360141	-0.434650	0.733113
6	0	2.330416	-0.752894	-1.396351
6	0	2.333105	-0.691343	1.425186
1	0	2.327439	-0.788454	-2.484174
1	0	2.333276	-0.653081	2.513002
6	0	-2.609166	-0.390585	-1.402411
6	0	-2.609272	-0.329638	1.419515
1	0	-2.609047	-0.427039	-2.490249
1	0	-2.606606	-0.293231	2.507339
6	0	3.519173	-0.790253	-0.698133
6	0	3.521290	-0.740629	0.726356
1	0	4.463093	-0.827428	-1.235948
1	0	4.465493	-0.775086	1.263986
6	0	-3.793002	-0.269793	-0.706274
6	0	-3.791491	-0.222785	0.718394
1	0	-4.732560	-0.181848	-1.245771
1	0	-4.732917	-0.130027	1.253798
16	0	0.722724	2.936815	-0.069643
1	0	1.691968	2.025522	0.081455
1	0	-0.233136	1.997889	-0.048319

MP2/BSS-F   C, H: 6-311++G(d,p), S: 6-311+G(3df)
Adduct SH_2---$\pi(C_{14}H_{10})$
Symmetry $(C_1$: $IIB_{Atc})$
energy E = -936.9261451 au
Standard orientation

6	0	0.139670	-0.570426	1.408587
6	0	0.141309	-0.590421	-1.408364
1	0	0.139753	-0.576137	2.498618
1	0	0.139343	-0.572531	-2.498335
6	0	-1.080601	-0.688838	0.722889
6	0	-1.083623	-0.641870	-0.722554
6	0	1.363938	-0.498127	0.723136
6	0	1.360382	-0.455152	-0.722954
6	0	-2.331800	-0.712822	1.411735
6	0	-2.332373	-0.731482	-1.410428
1	0	-2.329630	-0.717501	2.500154
1	0	-2.331712	-0.723477	-2.498855
6	0	2.607867	-0.351885	1.411420
6	0	2.610040	-0.369533	-1.411121
1	0	2.606932	-0.357959	2.499844

1	0	2.608192	-0.363552	-2.499544
6	0	-3.520092	-0.769243	0.713888
6	0	-3.521085	-0.760690	-0.711469
1	0	-4.464404	-0.791187	1.251893
1	0	-4.464895	-0.810221	-1.248572
6	0	3.792225	-0.250635	0.713050
6	0	3.791762	-0.243357	-0.712374
1	0	4.731401	-0.147720	1.250554
1	0	4.733597	-0.165755	-1.249473
16	0	-0.720748	2.938337	0.001265
1	0	-1.695816	2.021823	-0.042407
1	0	0.233509	1.997721	-0.016767

MP2/BSS-F   C, H: 6-311++G(d,p), Se: 6-311+G(3df)
Adduct SeH_2---$\pi(C_{14}H_{10})$
Symmetry   (C_1: IIB_{Atc})
energy E = -2939.3326286 au
Standard orientation

6	0	0.401446	-0.931680	1.413971
6	0	0.411757	-0.986420	-1.402520
1	0	0.399670	-0.922838	2.504033
1	0	0.409406	-0.981661	-2.492659
6	0	-0.790188	-1.221655	0.729163
6	0	-0.796553	-1.193303	-0.716738
6	0	1.605579	-0.700263	0.728198
6	0	1.599435	-0.677121	-0.718348
6	0	-2.028470	-1.401344	1.417968
6	0	-2.021080	-1.454140	-1.403896
1	0	-2.028228	-1.390027	2.506415
1	0	-2.019231	-1.459582	-2.492356
6	0	2.815594	-0.374550	1.415213
6	0	2.826399	-0.426658	-1.407007
1	0	2.812792	-0.366639	2.503622
1	0	2.826300	-0.435289	-2.495418
6	0	-3.198939	-1.615625	0.720175
6	0	-3.197505	-1.628367	-0.705141
1	0	-4.133618	-1.752969	1.258063
1	0	-4.126167	-1.804816	-1.241957
6	0	3.975743	-0.117494	0.716158
6	0	3.977686	-0.129295	-0.709248
1	0	4.890386	0.121362	1.252758
1	0	4.900691	0.072376	-1.246811
34	0	-1.046596	2.447013	-0.015536
1	0	-1.950524	1.303187	0.057552
1	0	0.117373	1.565937	-0.052690

MP2/BSS-F   C, H: 6-311++G(d,p), Te: 7433111/743111/7411/2 + 1s1p1d1f
Adduct TeH_2---$\pi(C_{14}H_{10})$
Symmetry   (C_1: IIB_{Atc})
energy E = -7151.0717911 au
Standard orientation

6	0	-0.770553	1.069753	1.431082
6	0	-0.824912	1.223579	-1.381140
1	0	-0.753568	1.021268	2.520016
1	0	-0.835940	1.261392	-2.470791
6	0	0.336274	1.605117	0.752193
6	0	0.330505	1.630828	-0.693755
6	0	-1.915861	0.636627	0.743054
6	0	-1.922340	0.665670	-0.703271
6	0	1.527457	1.985381	1.441317
6	0	1.477227	2.138438	-1.376562
1	0	1.541825	1.934028	2.528516

1	0	1.461145	2.185128	-2.464100
6	0	-3.028958	0.053272	1.422849
6	0	-3.085282	0.206069	-1.394962
1	0	-3.011025	0.006225	2.510175
1	0	-3.100519	0.254650	-2.482298
6	0	2.630217	2.437174	0.746665
6	0	2.610223	2.500208	-0.676992
1	0	3.530333	2.723835	1.284704
1	0	3.484219	2.864257	-1.211400
6	0	-4.124953	-0.401148	0.720426
6	0	-4.146784	-0.338171	-0.703423
1	0	-4.967661	-0.835766	1.251997
1	0	-5.019004	-0.697204	-1.243806
52	0	1.366729	-1.950372	-0.029304
1	0	2.150236	-0.515541	-0.303458
1	0	-0.103492	-1.259703	-0.360648

MP2/BSS-F'   C, H: 6-311+G(d,p), S: 6-311+G(3df)
Adduct SH_2---$\pi(C_{14}H_{10})$
Symmetry   (C_1: IIA_{Atc})
energy E = -936.925122 au
Standard orientation

6	0	0.045237	-0.539578	1.423183
6	0	0.046200	-0.643211	-1.391883
1	0	0.045037	-0.507749	2.512850
1	0	0.045802	-0.662222	-2.481953
6	0	-1.179412	-0.615314	0.739368
6	0	-1.180036	-0.611205	-0.707082
6	0	1.271472	-0.552718	0.737928
6	0	1.270379	-0.550581	-0.708740
6	0	-2.430826	-0.555434	1.426141
6	0	-2.431650	-0.673722	-1.393365
1	0	-2.429094	-0.522242	2.514122
1	0	-2.430461	-0.703870	-2.481472
6	0	2.519881	-0.434982	1.423121
6	0	2.523021	-0.554065	-1.396496
1	0	2.517879	-0.401485	2.511094
1	0	2.522020	-0.585213	-2.484558
6	0	-3.620139	-0.587921	0.728909
6	0	-3.620474	-0.630996	-0.695785
1	0	-4.564615	-0.548930	1.265660
1	0	-4.565322	-0.661706	-1.232435
6	0	3.708442	-0.414000	0.724585
6	0	3.709205	-0.458749	-0.700095
1	0	4.650817	-0.332668	1.260255
1	0	4.653922	-0.446212	-1.237674
16	0	-0.234083	3.009250	-0.073922
1	0	-1.207728	2.090764	-0.114978
1	0	0.719266	2.068388	-0.106903