Assessing the effects of covalent, dative and halogen bond on the electronic structure of selenoamide

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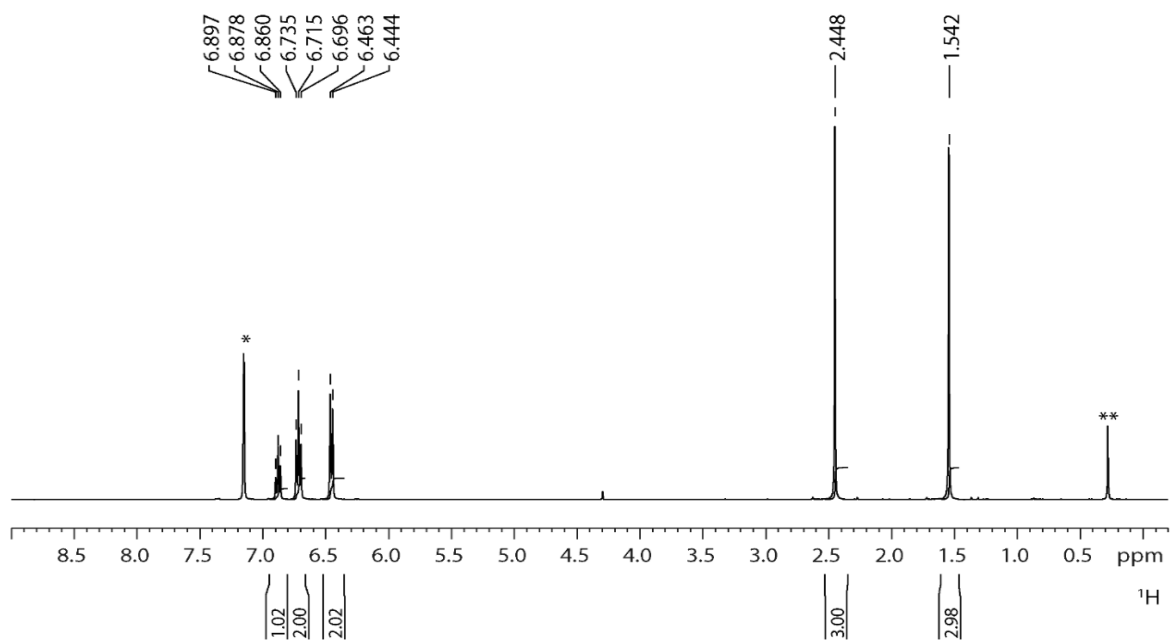
SUMMARY

Figure S1. ^{1}H NMR spectrum of **1-B** (solvent C_6D_6). * and ** denote the peaks relative to the residual non-deuterated solvent and silicon grease, respectively.

Figure S2. ^{77}Se, ^{13}C, ^{19}F and ^{11}B NMR spectra of **1-B** (solvent C_6D_6).THe

Figure S3. ^1H, ^{77}Se and $^{13}C\{^1H\}$ NMR spectra of **1-Me$^+$I$^-$** (solvent CDCl$_3$). * and ** denote the peaks relative to the residual non-deuterated solvent and water, respectively.
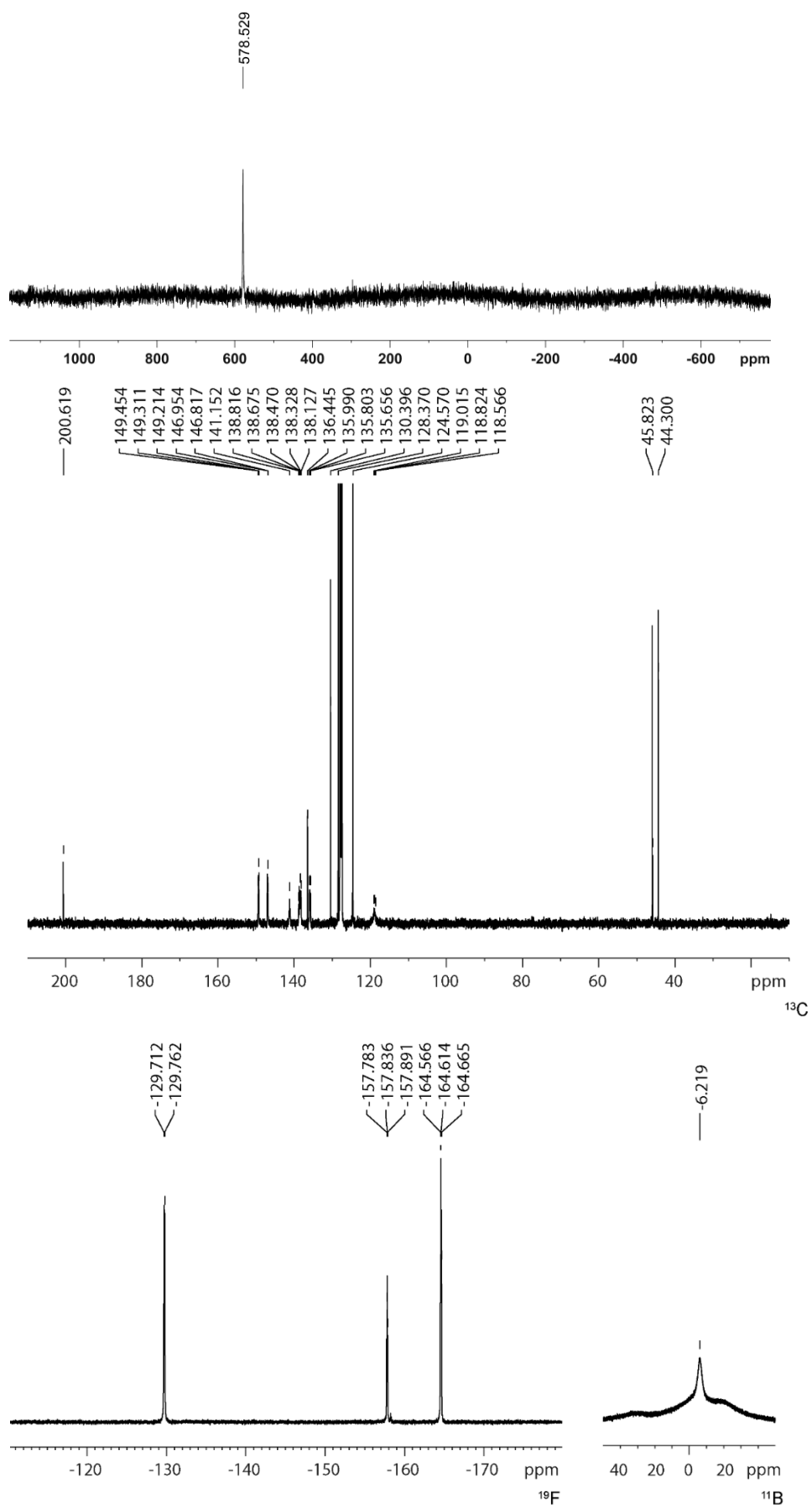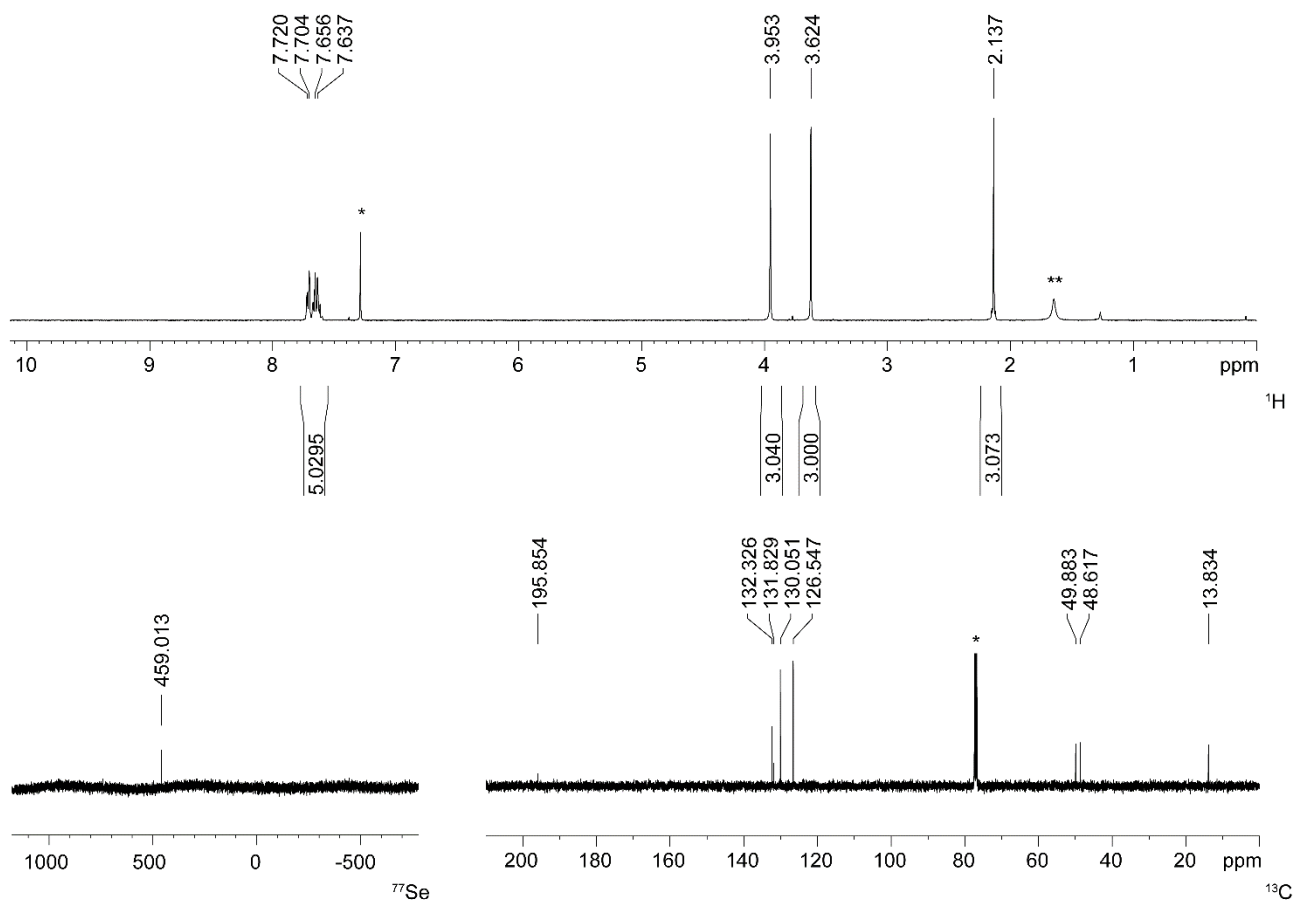
2   NMR Titrations.

In all the cases, the data have been fitting using the equations described in the literature.[1]
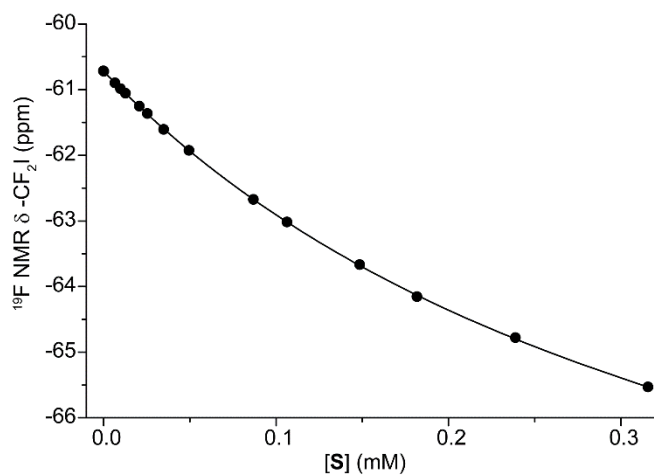
Figure S4. Trend of the chemical shift of the α-fluorine nuclei (-CF$_2$I) of **I** (C = 5.8 mM) with [**1**] T = 297.2 K. The limit value of δ (fitted) is -71.44 ± 0.08 ppm, the value of K_f is 2.60 ± 0.03 M^{-1}.
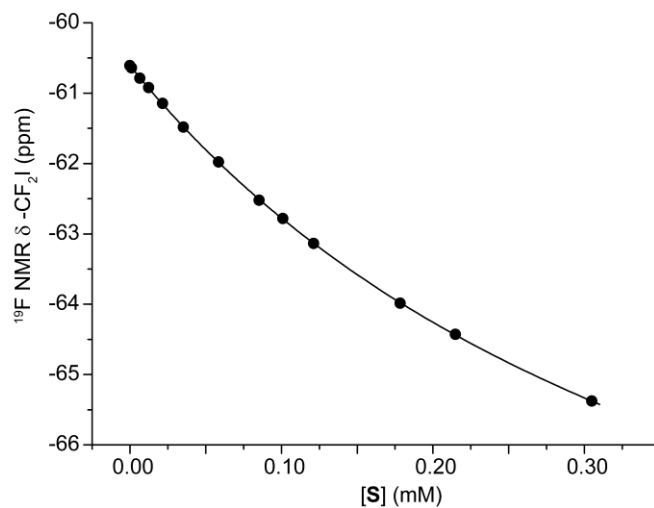
Figure S5. Trend of the chemical shift of the α-fluorine nuclei (-CF$_2$I) of **I** (C = 5.6 mM) with [**1**]; T = 303.0 K. The limit value of δ (fitted) is -72.05 ± 0.07 ppm, the value of K_f is 2.36 ± 0.02 M^{-1}.

Figure S6. Trend of the chemical shift of the α-fluorine nuclei (-CF$_2$I) of **I** (C = 9.2 mM) with [**1**]; T = 309 K. The limit value of δ (fitted) is -71.4 ± 0.2 ppm, the value of K_f is 2.16 ± 0.05 M^{-1}.

Figure S7. Trend of the chemical shift of the α-fluorine nuclei (-CF$_2$I) of **I** (C = 3.2 mM) with [**1**]; T = 317.2 K. The limit value of δ (fitted) is -72.2 ± 0.15 ppm, the value of K_f is 1.94 ± 0.04 M^{-1}.

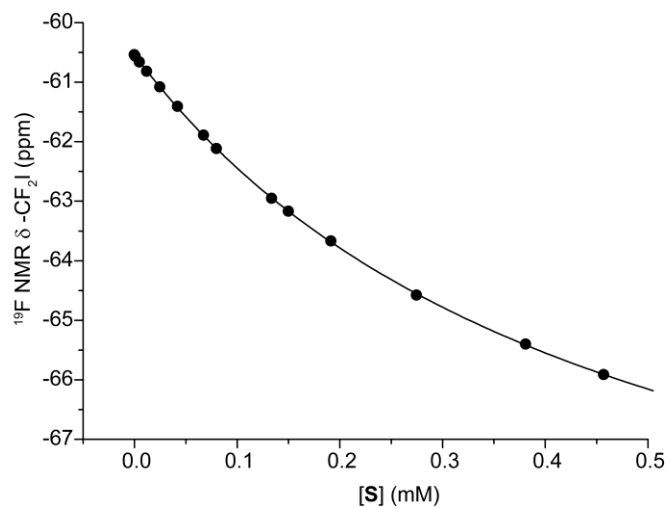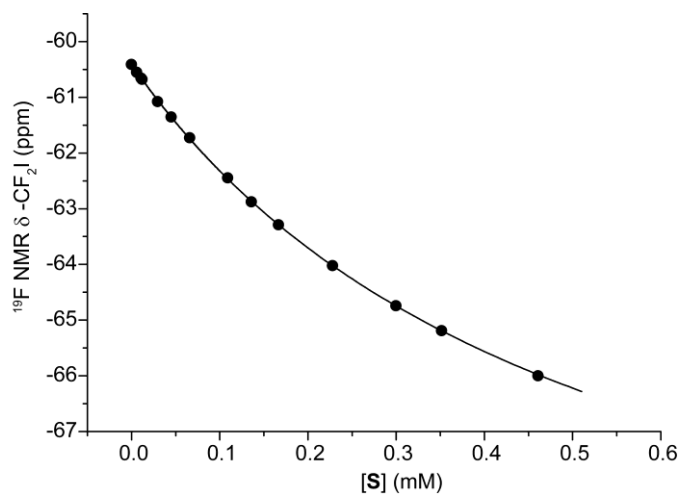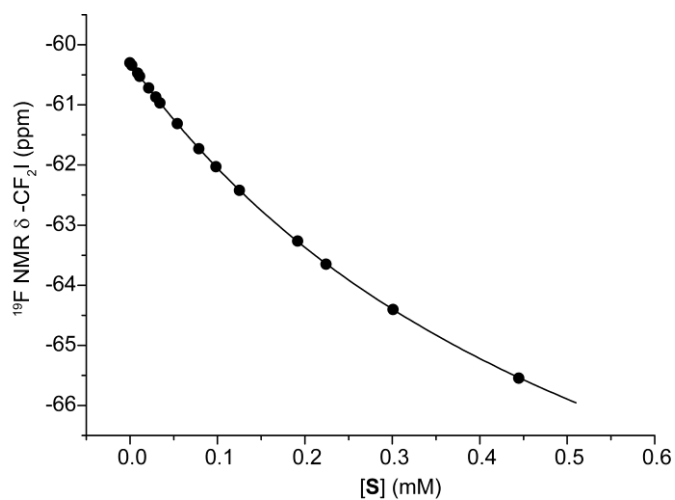**Figure S8**. Trend of the chemical shift of the α-fluorine nuclei (-CF_2I) of **I** (C = 1.8 mM) with [**1**]; T = 325 K. The limit value of δ (fitted) is -72.7 ± 0.1 ppm, the value of K_f is 1.65 ± 0.02 M^{-1}.
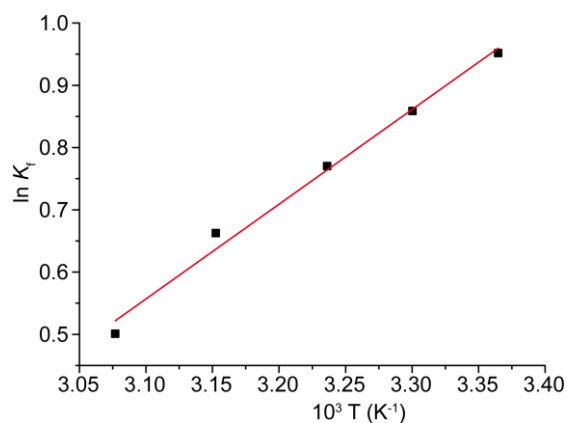
Figure S9. van't Hoff plot for the formation of XB **1**···**I** adduct. The slope of the fitting line is 1521 ± 90, the intercept -4.2 ± 0.3 (r^2 = 0.9868).

3   EXSY NMR.

VT ^{1}H-EXSY NMR experiments have been carried out through the noesygpph pulse sequence,[2,3] using a mixing time (τ_m) between 0.1 and 0.8 s, depending on the rate of the process.

Table S1. k_r values for **1**, **1···I** and **1-B** derived from VT-^{1}H EXSY NMR experiments at different temperature (T) and mixing time (τ_m) values

Compound	I_{AA}	I_{BB}	I_{AB}	I_{BA}	τ_m	T (K)	k_r (s^{-1})
1	1.000	0.9846	0.0524	0.0594	0.80	298	0.141
	1.000	0.9934	0.0240	0.0250	0.20	303	0.246
	1.000	0.9964	0.0425	0.0410	0.35	303	0.239
	1.000	1.002	0.0799	0.0682	0.50	303	0.296
	1.000	0.9693	0.081	0.0674	0.30	309	0.579
	1.000	0.9789	0.1428	0.1418	0.50	309	0.503
	1.000	0.9564	0.2779	0.2842	0.5	317	1.18
	1.000	0.9624	0.3153	0.3208	0.30	325	2.24
	1.000	0.9638	0.1655	0.1794	0.15	325	2.37
1···I	1.000	0.9855	0.0498	0.0516	0.50	303	0.204
([**1**] = 3.6 mM; [**I**] = 411 mM)	1.000	0.9790	0.0358	0.0389	0.40	303	0.189
	1.000	0.9669	0.1214	0.1206	0.53	309	0.467
	1.000	0.9572	0.0825	0.0840	0.35	309	0.487
	1.000	0.9584	0.0394	0.0548	0.22	309	0.437
	1.000	0.9340	0.0624	0.0763	0.15	317	0.958
	1.000	0.9399	0.1292	0.1074	0.25	317	0.981
	1.000	0.9283	0.1031	0.1078	0.10	325	2.20
	1.000	0.9449	0.2495	0.2890	0.25	325	2.27

1-B	1.000	0.9458	0.0392	0.0390	0.30	343	0.268
	1.000	0.9765	0.0725	0.0715	0.30	348	0.487
	1.000	0.9585	0.1004	0.1071	0.30	353	0.709
	1.000	0.9864	0.2856	0.2829	0.30	363	1.96

In the case of the **1-I** adducts, as the formation and disruption of the adduct is kinetically fast, the observed value k_r is the average value
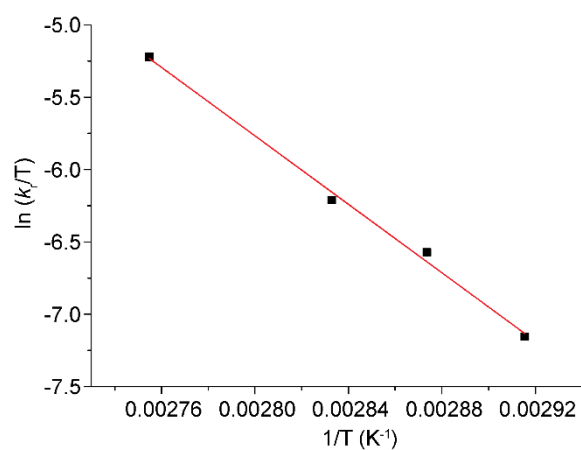
Figure S10. Eyring plot of the -NMe2 rotation for **1-B**.

4 PGSE NMR.

^{1}H PGSE NMR measurements were performed by using the double-stimulated echo sequence with longitudinal eddy current delay[4] at 298 K without spinning. The dependence of the resonance intensity (I) on a constant waiting time and on a varied gradient strength G is described by the following equation (3):

$$ln\frac{I}{I_0} = (\gamma\delta)^2 D_t \left(\Delta - \frac{\delta}{3}\right) G^2 \tag{3}$$

where I is the intensity of the observed spin echo, I_0 the intensity of the spin echo in the absence of gradient, D_t the self-diffusion coefficient, Δ the delay between the midpoints of the gradients (0.2 s), δ the length of the gradient pulse (4 ms), and γ the magnetogyric ratio. The shape of the gradients was rectangular, their length δ was 4–5 ms, and their strength G was varied during the experiments.

The self-diffusion coefficient D_t, was estimated by evaluating the proportionality constant for a sample of HDO (5%) in D_2O [known diffusion coefficients in the range 274–318 K[5]] under the exact same conditions as the sample of interest. The solvent or TMS was taken as internal standard.

Since the aromatic protons of **S** overlap with the residual solvent peak of C_6D_6, the latter cannot be used as internal reference, as usually done.[6] For this reason, the hydrodynamic properties of dichloromethane in C_6D_6 has been determined (Figure SX), in order to use CH_2Cl_2 as internal standard for all the other measurements.
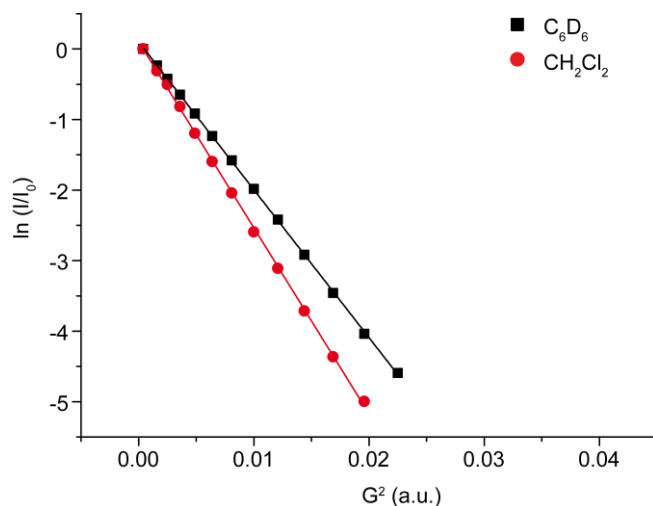
Figure S11. Plot of $\ln(I/I_0)$ *vs.* G^2 for a solution containing one drop of CH_2Cl_2 in C_6D_6 at 25°C.
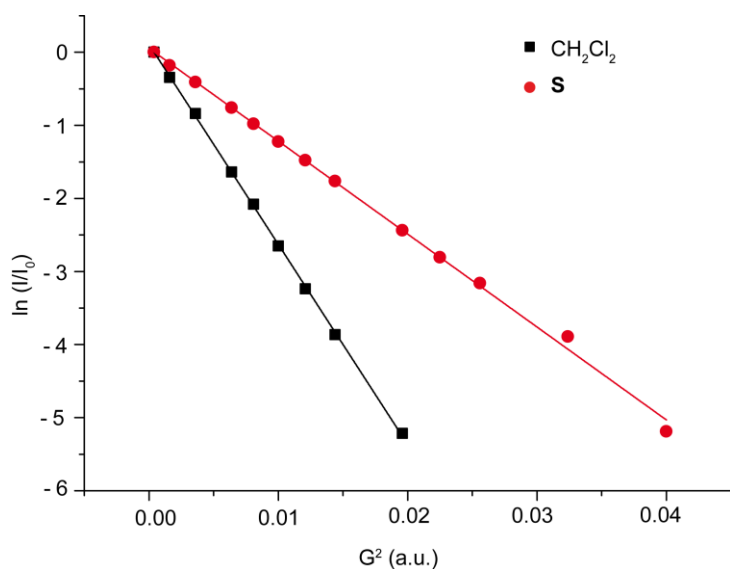
Figure S12. Plot of $\ln(I/I_0)$ *vs.* G^2 for a solution containing **1** (red circles, 3.2 mM) in C_6D_6 at 25°C. CH_2Cl_2 is used as internal reference (black squares).
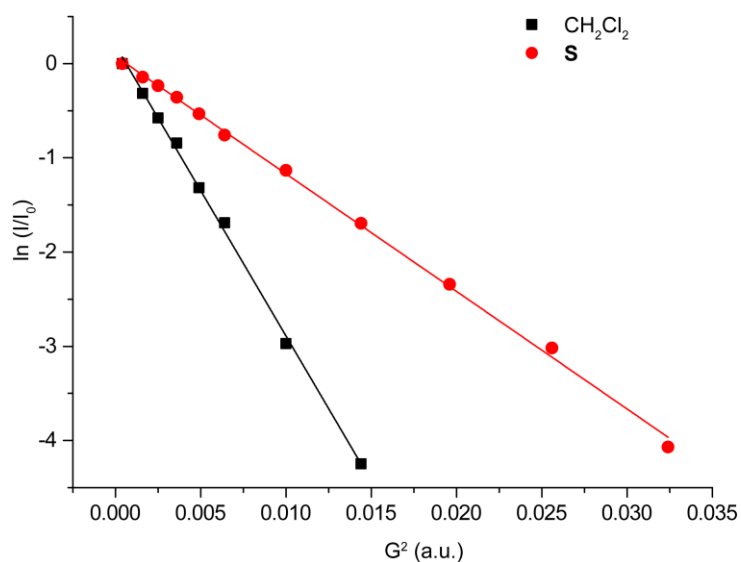
Figure S13. Plot of $\ln(I/I_0)$ *vs.* G^2 for a solution containing **1** (red circles, 3.2 mM) and **I** (247 mM) in C_6D_6 at 25°C. CH_2Cl_2 is used as internal reference (black squares).

Table S2. Diffusion coefficients (D_t, 10^{-10} m^2s^{-1}) and hydrodynamic volumes (V_H, $Å^3$) at different concentrations of **1** and **I** (mM).

[**1**]	[**I**]	D_t (**S**)	D_t (CH_2Cl_2)	V_H (**S**)
0.0	0.0	-	27.0	-
42	0.0	13.0	28.1	233
3.2	0.0	12.6	27.3	230
3.2	247	11.2	27.7	310

As it can be seen in Table S2, as an excess of **I** is added to a solution of **1**, the hydrodynamic volume of the latter increases from 230 to 310 $Å^3$. Considering that the V_H of **I** (in absence of any aggregation process) is 220 $Å^3$,[7] this means that the 37% of the molecules of **S** are involved in a XB adduct with a molecule of **I**. Consequently, the formation constant can be estimated to be 2.4 M^{-1} (The experimental error on volumes is about 10%).

Computational Studies.

TS(1)
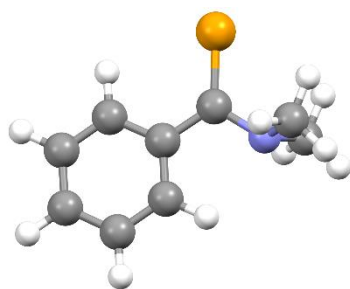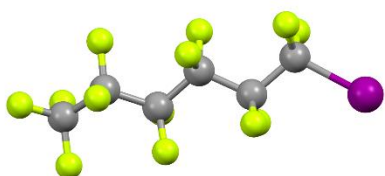
TS(1-I¹)
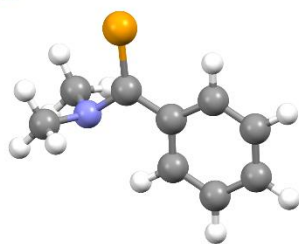
TS (1-CF₃)
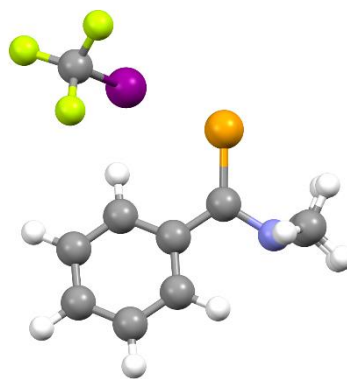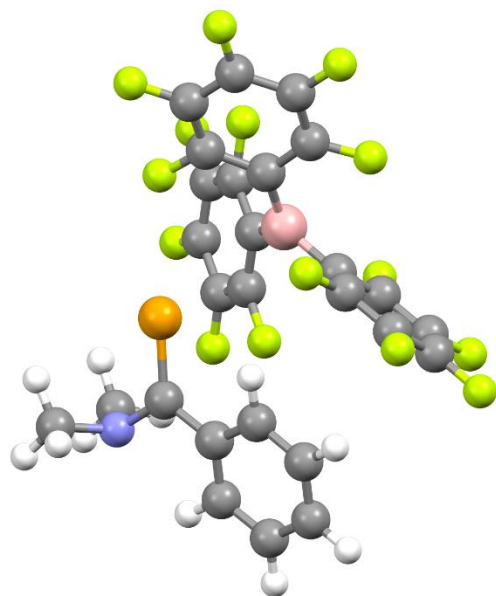
TS(1-B)

TS(1-BCl₃)
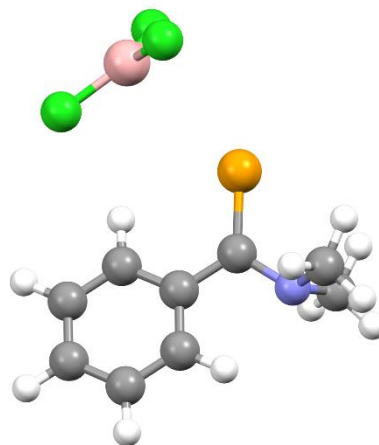
Figure S14. Optimized geometries for transition states.

Natural Energy Decomposition Analysis (NEDA).

Given the density matrix, the NBO procedure calculates a set of mutually orthogonal bond orbitals (the NBOs) that, aside from small orthogonalization tails, are strictly localized either on single atoms (core orbitals, lone pairs) or on atom pairs (bonds, antibonds). The molecular fragments of a cluster are naturally defined by the connectivity of the bonds. NEDA employs the Fock matrix expressed in the NBO basis.

The binding energy of a complex formed by the association of two fragments is defined as

$$\Delta E = E(\psi_{AB}) - E(\psi_A) - E(\psi_B) \qquad\qquad (1)$$

where ψ_{AB}, ψ_A, and ψ_B are respectively the variationally optimized wave functions for the AB complex and the isolated fragments A and B. Furthermore, we constrain the geometries of A and B to remain unchanged during the association reaction so that geometries of fragments within the complex are identical to those at infinite separation. The binding energy therefore contains no contribution from the geometrical distortion of A and B during formation of the complex.

NEDA partitions the corrected binding energy into electrical (*EL*), charge transfer (*CT*) and repulsive (*CORE*) contributions

$$\Delta E = EL + CT + CORE \qquad\qquad (2)$$

The key step of NEDA analysis is evaluation of perturbed ("deformed") wavefunctions ($\psi_A^{(def)}$, $\psi_B^{(def)}$) for each monomer as local eigenvectors of the NBO Fock matrix in the respective monomer blocks. (Each monomer wavefunction $\psi_A^{(def)}$, $\psi_B^{(def)}$ thereby inherits the overlap-free character of the underlying Natural Atomic Orbitals.) The antisymmetrized (determinantal) product of perturbed fragment wavefunctions

$$\psi^{(loc)} = \det|\psi A^{(def)} \psi B^{(def)}| \qquad\qquad (3)$$

defines the starting "localized" ($\psi(loc)$) wavefunction that underlies evaluation of each NEDA component. *CT* is directly defined as

$$CT = E(\psi) - E(\psi^{(loc)}) \qquad\qquad (4)$$

On the other hand, the difference between $E(\psi^{(def)})$ and $[E(\psi_A^{(def)}) + E(\psi_B^{(def)})]$ is defined as the sum of electrostatic (*ES*), polarization (*POL*) and exchange (*EX*) contributions.

The deformation energy (*DEF*) is evaluated as

$$DEF = [E(\psi_A^{(def)}) - E(\psi_A) + E(\psi_B^{(def)}) - E(\psi_B)] \qquad\qquad (5)$$

In accordance with classical electrodynamics, one can employ linear response theory to evaluate the self-energy (*SE*) correction ("polarization penalty") for each center, thereby expressing the total electrical component as

$$EL = ES + POL + SE \tag{6}$$

However, the self-energy must then be removed (subtracted) from the deformation (*DEF*) penalty to obtain the net repulsive *CORE* component

$$CORE = EX + DEF - SE \tag{7}$$

Extended Transition State-Natural Orbitals for Chemical Valence (ETS-NOCV) analysis.[8] In the ETS-NOCV approach, the electron density rearrangement taking place upon formation of AB from fragments A and B is defined with respect to a reference system made up of the occupied ψ_i^A and ψ_i^B orbitals of A and B orthonormalized with respect to each other (ψ_i^0). In other words, rather than two separate A and B determinants, their antisymmetrized product is taken as the fragment–fragment non-interacting reference (the so-called "promolecule"). The resulting electron density rearrangement,

$$\Delta\rho_{tot} = \Sigma_i \left|\psi_i^{AB}\right|^2 - \left|\psi_i^0\right|^2 \tag{8}$$

where $\psi_i^{(AB)}$ is the set of occupied orbitals of the adduct, can be brought into diagonal form in terms of NOCVs. These are defined as the eigenfunctions, $\phi_{\pm k}$, of the so-called "valence operator" [9–11]

$$\hat{V} = \Sigma_i \left(|\psi_i^{(AB)}\rangle\langle\psi_i^{(AB)}| - |\psi_i^0\rangle\langle\psi_i^0| \right) \tag{9}$$

The fragmentation depends on the interaction under examination and is generally indicated in each case. The NOCVs can be grouped in pairs of complementary orbitals (ϕ_k, ϕ_{-k}) corresponding to eigenvalues with same absolute value but opposite sign (Eq. 10).

$$\hat{V}\phi_{\pm k} = \pm v_k \phi_{\pm k} (v_k > 0) \tag{10}$$

where k numbers the NOCV pairs ($k = 0$ for the largest value of $|v_k|$). In this framework, $\Delta\rho_{tot}$ can be defined as in Eq. 11.

$$\Delta\rho_{tot} = \Sigma_k v_k \tag{11}$$

Hence, on formation of AB from the promolecule, a fraction v_k of electrons is transferred from the ϕ_{-k} to the ϕ_k orbital. Only some NOCVs pairs have v_k significantly different from zero and this subgroup is generally enough to describe the A···B interaction. For each value of k, an energy contribution associated with the k-th NOCV pair is given.

The ETS-NOCV analysis has been performed with ORCA 4.1.0.

Table S3. Selected bond lengths (in Å) and components of NEDA (in kcal/mol) of partially optimized **1-Me$^+$** structures, fixing the Se-Me bond length.

Se-Me	C-Se	N-C	*CT*	*El*	*Core*	*E$_{int}$*
1.964	1.892	1.309	-394.01	-93.65	329.99	-157.67
2.298	1.881	1.31	-233.3	-77.55	177.52	-133.33
2.631	1.876	1.311	-147.92	-59.83	99.34	-108.41
2.946	1.87	1.311	-103.01	-45.55	59.1	-89.46
3.298	1.865	1.312	-79.423	-35.424	38.89	-75.96
3.631	1.86	1.313	-67.18	-27.45	27.7	-66.93
3.964	1.854	1.313	-61.55	-21.86	22.6	-60.81
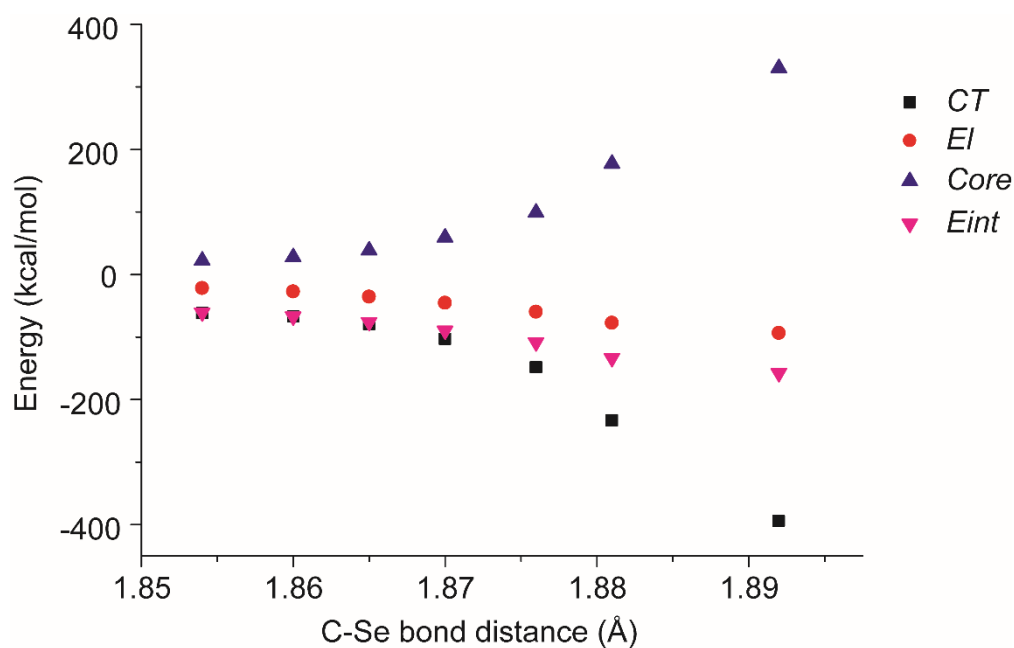
Figure S15. Trends of NEDA components *versus* the C-Se bond length.

Table S4. ETS-NOCV analysis of adducts, energies in kcal/mol

Adduct	E$_{oi}$	E$_1$	E$_2$	E$_{int}$
1-ICF$_3$	-9.6	-7.4	-0.6	-10.1
1-BCl$_3$	-82.8	-70.2	-3.5	-36.7

1-Me⁺	-211.6	-184.7	-10.0	-162.1
ICF₃···ICH₃	-3.8	-3.0	-0.4	-4.1

Table S5. Selected bond lengths (in Å) and components of NEDA (in kcal/mol) of TSs structures

TS	Se-X	C-Se	N-C	*CT*	*El*	*Core*	E_{int}
TS(1-ICF₃)	3.385	1.807	1.425	-15.3	-16.9	30.0	-2.2
TS(1-BCl₃)	3.346	1.803	1.429	-10.2	-11.0	22.4	1.1
TS(1-Me⁺)	1.967	1.870	1.397	-395.2	-79.8	328.2	-146.7

Optimized Cartesian Coordinates

1-I[1]

C	4.24729935724449	2.92963301795323	-1.84742293846709
C	3.89070158306746	2.41045804899205	-0.60765990518250
C	2.60564365017911	2.61206565099852	-0.11659871274731
C	1.68398223834881	3.33838910753834	-0.85746646343911
C	2.03443499043155	3.84971610552697	-2.10888280396432
C	3.32119191598463	3.63484363192468	-2.60232072251992
C	1.01395658163746	4.53296095959660	-2.93773744605525
N	0.47839780684913	5.66414809236428	-2.48203169932361
C	1.02545835505270	6.42466788465471	-1.35795005345403
Se	0.51174610664976	3.75599435402960	-4.52272562465555
C	-0.62149739754338	6.31757993679693	-3.18295023889833
H	-0.25192238259477	6.87084975748493	-4.04972124545358
H	-1.11006352169591	7.00520181833550	-2.49461066125193
H	-1.32912604601887	5.57056795759488	-3.53558565554340
H	1.19876081445246	7.45321957369513	-1.68015655229959
H	1.96195081349580	5.99321535916076	-1.02607574313060
H	0.31856680403041	6.43456724437462	-0.52555086243490
H	3.57831220988612	4.00477988752616	-3.58522007622252
H	0.67703542032261	3.47917432606675	-0.48533750516039
H	2.31691990714264	2.19482552441246	0.83894054014721
H	5.24335485516145	2.76649982139293	-2.23761716499602
H	4.60768355871684	1.84017483307676	-0.03156371394283
F	3.20443499424230	-1.63262721478395	-3.55321930603659
F	1.96307144114855	-1.40455745617201	-1.77123570677223
F	-0.21033774305357	-2.29796605924486	-3.05993463989209
F	0.84535559836114	-2.29973090167308	-4.98745758192668
F	2.46068509543879	-4.21027575112680	-4.29194860181170
F	1.97349986449290	-4.04317041978838	-2.16221906880121
C	0.87792637190299	-6.45569289278721	-3.78510697018946

F	-0.42884561809276	-4.98287744606335	-2.46547847815047
F	-0.42581619779739	-4.68415794378136	-4.63705032847611
C	-0.18887829282712	-7.57282972808383	-3.54506453093881
F	1.31637862226685	-6.58001135272624	-5.05149883047962
F	1.90274891500122	-6.69091395750412	-2.94014070492878
F	0.30855663007013	-8.73874036068237	-3.96721882758689
F	-0.48449037148424	-7.68436920185579	-2.25012181783734
F	-1.30750285832317	-7.31249900351157	-4.22718106689725
I	1.35205879819156	0.65671541702401	-3.77059048363958
C	1.95032904124059	-1.35842379961755	-3.12207977907360
C	0.99266214296020	-2.45906125391654	-3.65627227782069
C	1.47791542363818	-3.93165558844366	-3.41065600890408
C	0.34009052182239	-5.00034697875813	-3.57403974084126

TS(1-I¹)

C	4.53221543151614	2.98099484751477	-1.12510044748361
C	4.43368412741678	3.42066627710025	0.19437367833605
C	3.36184079275294	4.21869905579471	0.58214046522316
C	2.39125127176699	4.57590609336195	-0.33974842250269
C	2.46180425513405	4.11745859926228	-1.66791997334247
C	3.55902337253581	3.32203959311841	-2.04432333208572
C	1.40591933918587	4.46905398373164	-2.60827790150069
N	0.52316361660928	5.50093180773547	-2.17752310045199
C	0.52731969447833	6.67359007588671	-3.05265729620506
Se	1.16315607421584	3.65585601372192	-4.20575514883865
C	-0.83111322787960	5.01590179194068	-1.90466464712002
I	1.78394794871157	0.41660748643628	-3.58419795783766
C	2.06571674509903	-1.68750005836161	-3.02820262334941
C	1.06716082324778	-2.62037479904899	-3.77219109879748
C	1.35048194886651	-4.15460174942095	-3.59169809981318
C	0.13006453473702	-5.06290625538248	-3.97823516679632
F	3.32555298571622	-2.07291031692685	-3.32452764975492
F	1.89250438485790	-1.81970993395204	-1.69910379877914
F	-0.17616056686363	-2.35166251833762	-3.31797382148618
F	1.12000814439091	-2.35022591764639	-5.09148845430031
F	2.40207024283637	-4.48718715449084	-4.36810994406239
F	1.66582622201700	-4.40614321136084	-2.30625219261793
H	-1.35599253052675	4.70885585725515	-2.81866967318095
H	-1.39188249132844	5.81536360695980	-1.41848428436420
H	-0.78548694833355	4.16261757284396	-1.22810482004002
H	0.08258040082310	6.46715194434512	-4.03462266851754
H	1.55087222550072	7.01732811405971	-3.19746642207921
H	-0.03829727615492	7.46730526281978	-2.56317277821025
H	3.63866793215934	2.99358242892158	-3.06974724133787
H	1.56413946546621	5.20900534155565	-0.05605599311692

H	3.28664857414439	4.56664891542382	1.60418346719877
H	5.37259866826190	2.37299914974916	-1.43345876694301
H	5.19529610351681	3.14811770572232	0.91405302368568
C	0.52436353089039	-6.55566620867779	-4.23846821688383
F	-0.76938012895188	-5.02144781162548	-2.97416828873302
F	-0.44721273432211	-4.58374713104064	-5.09773508382711
C	-0.68186948799618	-7.54987335476854	-4.22312822266967
F	1.10963162755076	-6.64753972489228	-5.44680167034097
F	1.39631598790497	-6.96679356251383	-3.29510446458008
F	-0.26051896576607	-8.73929829680393	-4.66117277385962
F	-1.16453787808052	-7.70025866676486	-2.99001534323616
F	-1.65874723610728	-7.11849585324520	-5.02518384539737

1-I²

C	1.88689201299763	1.54954938862828	-3.19851186552770
C	3.13374742649144	1.78945389649603	-2.62950467821468
C	3.32085834201482	2.90367431476006	-1.81880689831912
C	2.27116306717668	3.78326187347580	-1.59359624735456
C	1.01442923791429	3.54324704951380	-2.15741509145533
C	0.82770816317410	2.41113027456868	-2.95249330968334
C	-0.11490364791370	4.45277986226309	-1.86034962996275
N	0.04062722305402	5.75259040831589	-2.10328378450139
C	1.05706902221519	6.29300037196463	-3.00809795119150
Se	-1.66184898492031	3.73937760615178	-1.16016664064996
C	-0.94801735675470	6.73486666565589	-1.67180383622920
I	-2.54752222442308	4.39011277112008	-4.35139685114822
C	-2.85926516301917	4.84493721783104	-6.48050015173280
C	-1.58990209968213	5.49250389178570	-7.10493509581993
C	-1.64318935300673	5.67876222480899	-8.66244085494270
C	-0.56366044614555	6.67949635737884	-9.20752143585173
F	-3.15161435407309	3.71723357391601	-7.16272211646403
F	-3.89851026465291	5.69225965667697	-6.61053214110588
F	-1.40903128683843	6.70465129868403	-6.52963227279120
F	-0.52218843493102	4.71724219943097	-6.82412500826266
F	-1.44844672830179	4.47555514112059	-9.23991995791297
F	-2.85650765293728	6.13994174882215	-9.01980535516226
H	-1.77640931567698	6.78302787828264	-2.38176825795902
H	-0.46091391802936	7.70781475759933	-1.61945840413992
H	-1.34550402453735	6.45440536261924	-0.70054967014966
H	0.55094407064697	6.85968953559368	-3.79245630952199
H	1.62893755553405	5.49415618961680	-3.46430895578388
H	1.73140797270349	6.96239961734684	-2.47042815877089
H	-0.14916488301393	2.21701266088002	-3.37124227319369
H	2.41577422543275	4.64759640379155	-0.95768156764430
H	4.28356575967963	3.08699593446987	-1.35940533979214

H	1.73590345708391	0.68229239576723	-3.82820966650407
H	3.95422241126895	1.10718335634881	-2.81152771624068
C	-0.30902348548936	6.54329799686167	-10.74671787337276
F	-0.97420324838458	7.93722274108273	-8.94639992737907
F	0.60662124835338	6.46662264401346	-8.57162810314553
C	0.43107628409148	7.76396527679580	-11.38360200747283
F	0.44523793156760	5.45114098640849	-10.96827399503204
F	-1.48529465432822	6.40382986704825	-11.39090471032093
F	0.78368795546175	7.44724890512162	-12.63172656375305
F	-0.35940835271503	8.83589722294382	-11.42541569673732
F	1.53315851291258	8.06145947403885	-10.68865362880224

TS(1-I^2)

C	1.75512031745737	1.05248534781180	0.64216420400711
C	2.77439401428591	1.80125783678114	1.23136531089783
C	3.12754215452391	3.03300921817203	0.69329409134366
C	2.46979298144440	3.51765692867433	-0.42647600179258
C	1.44199904661003	2.77439680669943	-1.03391215637119
C	1.09826318341594	1.52959367085823	-0.47481775158731
C	0.77128553974490	3.30825839450471	-2.21772835444847
N	1.21909530285047	4.58831686128338	-2.64124524176879
C	1.88121330942559	4.57733400588294	-3.94592170472532
Se	-0.53489435611261	2.41455352045142	-3.09432431832582
C	0.20405306634063	5.63375295147771	-2.51232592210633
I	-1.73789933944949	4.04144039020824	-5.79513402613635
C	-2.62030672734782	5.01047328190534	-7.55958068878490
C	-1.59015238993175	5.92972692339222	-8.27578583676969
C	-2.07286986131860	6.51128200481052	-9.65195055032139
C	-1.21777781630939	7.73237805590212	-10.14424097437763
F	-3.05483022306852	4.07870875562299	-8.43465846006242
F	-3.68105462969708	5.74753155423836	-7.17572603105166
F	-1.29956513062169	6.95899086576883	-7.44897782287031
F	-0.46424322480724	5.22391459172549	-8.50602377094844
F	-2.00085814643476	5.53193780587144	-10.57651900382748
F	-3.35332746079011	6.91525813746054	-9.54771044371176
H	-0.63621333357156	5.49865997477884	-3.20257803800190
H	0.67630074616211	6.59639287752895	-2.71332040579523
H	-0.18051994053612	5.64354566096286	-1.49251030738980
H	1.19584735003951	4.36220279307725	-4.77323211839883
H	2.67214121214028	3.82719766362448	-3.94418974954602
H	2.33385427253475	5.55659021361315	-4.10654613816519
H	0.30890891713861	0.95025357019625	-0.93255585011487
H	2.73198323617353	4.47246818693020	-0.85521948709381
H	3.91784856804955	3.61718135635355	1.14694080659881
H	1.47647537548380	0.09443776263018	1.06073015801746

H	3.28755193334033	1.42308652306319	2.10632899876034
C	-1.38146076152678	8.03233001316040	-11.67231094814301
F	-1.58961927906042	8.82551672836609	-9.44709592599264
F	0.08714957789525	7.49086315033354	-9.90622746170612
C	-0.87958456399948	9.44836631039865	-12.10434115603696
F	-0.67957143845624	7.12259897737454	-12.37287116227224
F	-2.68257051352567	7.94387939429322	-12.01594873170943
F	-0.86999604285463	9.51002978114873	-13.43841219036812
F	-1.68485919767448	10.40431691048824	-11.64238129779379
F	0.35985727203756	9.66671324217448	-11.65594454110937

1-I[3]

C	3.77462381905801	1.59690649049220	-0.58365271682531
C	2.56709591863025	1.10971768824469	-0.09415355025260
C	1.39602392544587	1.82343928222608	-0.32090804545964
C	1.43477655421352	3.02396344497387	-1.01814043409938
C	2.64437848120633	3.52106113326617	-1.51155478801790
C	3.81265071095100	2.78653615074581	-1.29466088118871
C	2.68016025044897	4.76515363811506	-2.31975115307203
N	2.08950012121249	5.86460100750661	-1.83173960691912
C	1.70290286342180	6.04555572981043	-0.43444683182199
Se	3.47302537131344	4.70962230627760	-3.96495840407406
C	1.97876000884627	7.06685087647059	-2.64799259859687
F	4.75260046191563	5.64669135398369	0.02114982954202
C	5.41917707280675	5.18767842034383	1.09481208255672
C	6.05229693120518	6.39798079172690	1.84800860713632
C	6.81321430445991	7.39508195744963	0.90101627469837
C	7.80160058104231	8.34320815386336	1.66540270623291
I	4.06027943489749	4.07821988241275	2.37884773401560
F	6.38746270097710	4.36556581216646	0.67079301122337
F	5.07571470131511	7.08702543818203	2.46889656445097
F	6.90850317005814	5.91739195738749	2.77118435820792
F	7.51740944251788	6.69759844234653	-0.00880846637107
F	5.89564873713448	8.14697261223734	0.25880086733120
H	2.95235871832248	7.55084312033280	-2.76014575493738
H	1.28403141637190	7.75089685514271	-2.16255717745952
H	1.62204573746624	6.80861792391443	-3.64286391278061
H	2.20424411595084	6.93194491369694	-0.03954387037644
H	1.99119886232292	5.18933029237725	0.16087362090407
H	0.62357703298240	6.19411087365432	-0.35066466362413
H	4.74372131214824	3.15829726254742	-1.69822399824362
H	0.51689685409331	3.56631601443859	-1.20542864678433
H	0.44831684489097	1.44219946423447	0.03737332501912
H	4.69117370074138	1.04723888400439	-0.41238416581401
H	2.53752249735619	0.17591337433498	0.45223160056933

C	8.20182865684944	9.61295813074517	0.84063520635893
F	7.22596660856137	8.75371747627388	2.81308249203079
F	8.91569902468404	7.64608110298977	1.96390527715338
C	9.47332567230875	10.34792501247713	1.37544803687079
F	8.44339995932663	9.26399419156327	-0.43897650127172
F	7.18014288625798	10.48845309157971	0.87215193964824
F	9.58532831288551	11.52071571213362	0.74784626586303
F	9.36935057900701	10.57061599263454	2.68853784835689
F	10.57248564439445	9.63315474069548	1.13946351982041

TS(1-I^3)

C	3.64119578998891	1.49268153928814	-0.51139601464201
C	2.42306650793987	1.48616232210558	0.16799658112554
C	1.56506649878344	2.57349584992288	0.05680246883362
C	1.91848364159964	3.66263744764863	-0.72633913880962
C	3.14655045392041	3.68925961869239	-1.40822809444242
C	4.00002414414102	2.57800672045960	-1.28727329773457
C	3.51461678649743	4.86590374286450	-2.19847835738456
Se	5.11169837040819	5.07831472915725	-2.99988061867775
N	2.50566384116800	5.87428461773728	-2.28251707223716
C	2.87733462727363	7.11991641527271	-1.61320709064930
C	2.02473791956794	6.09451003194322	-3.64531051620709
H	2.78774502926635	6.54642730910727	-4.29274331196053
H	1.15510996665080	6.75208843190288	-3.60219079572945
H	1.71691060656055	5.14380586431306	-4.08064670521665
H	3.70316656730519	7.63842250219151	-2.11822592957626
H	3.17635644571498	6.91039524054491	-0.58718855647328
H	2.00380611022308	7.77335397739470	-1.59284498022169
H	4.94679697775791	2.59170972302872	-1.80815439903862
H	1.26151384482161	4.51356863391423	-0.82330353168577
H	0.61839815531124	2.57447580988069	0.58159311481547
H	4.31167480271408	0.64695162250353	-0.42774596118207
H	2.14755544273915	0.63608385684239	0.77938473331973
I	4.93459041568953	3.14396740100011	3.05412695286769
C	5.32076135761318	4.74835223349603	1.64021762630783
C	6.12400717861455	5.90957986777184	2.30144441192495
C	6.25198116825824	7.18359570220127	1.38947203416643
C	7.38829958913732	8.16253563990253	1.84968069201836
C	7.24134072854499	9.60336937437318	1.25369413651582
C	8.53960073815890	10.46943056908547	1.34521359714939
F	4.15067081008104	5.23371810752343	1.19000974832376
F	6.01103571910023	4.25899473582433	0.60515052043824
F	5.50554212046544	6.27574024644240	3.43946309749208
F	7.35790207834131	5.45340552373573	2.59623194333803
F	6.50793708133250	6.80744829171947	0.12425221934757

F	5.07340886335530	7.84102588598257	1.41701689509580
F	7.37422611358190	8.26157927537883	3.19386790950469
F	8.57403688026549	7.65168819048624	1.46353350171465
F	6.89969721537546	9.52282006179256	-0.04788838764088
F	6.27083097775502	10.25326215575092	1.92286283007056
F	8.23822984800804	11.72665020185677	1.01118964610258
F	9.02398287167058	10.45953312039227	2.59004451866319
F	9.47486471429775	10.02099540856804	0.50921758037372

1-B

C	3.74889050154444	3.01846432932140	-4.72999174205580
C	3.02462380091306	1.86084018959401	-4.43772048631402
C	3.47773014300797	1.16580682377031	-3.31752197012029
C	4.53860653496317	1.59102217985322	-2.52980966798147
C	5.21491096291079	2.74992673332625	-2.86097245041778
C	4.82195151619979	3.46363267898416	-3.98163713107799
B	1.85402757481462	1.34829567511774	-5.39711948512719
C	0.89808695745658	0.17034604028339	-4.85930737173193
C	0.22168702812667	0.25302545863762	-3.64131788179716
C	-0.65603502056763	-0.70429812441185	-3.17080293884030
C	-0.87591226852508	-1.85182984071890	-3.91814357472114
C	-0.20051381834152	-2.00888324451656	-5.11537682079885
C	0.66452251473651	-1.014416117223015	-5.55774026411654
C	2.19935055736042	1.31066583762531	-6.97124611437236
C	3.49894014935267	1.21151427514977	-7.46703103213015
C	3.80175818182075	1.16200574833500	-8.82148107919547
C	2.78129915365671	1.19543275006596	-9.75603337856942
C	1.46844581308166	1.26036313795265	-9.31483270378432
C	1.21178145486398	1.30239086809855	-7.95590834147577
F	4.55509968537422	1.12401432871582	-6.63921131227253
F	5.07163540469286	1.07505821113939	-9.22918483148312
F	3.05482275612415	1.15234707199929	-11.05955485807370
F	0.46698454456602	1.26480140712575	-10.20025601523897
F	-0.08899534111218	1.30614518876398	-7.60200430719933
F	0.41542246527391	1.31274045343777	-2.82945793891780
F	-1.28189814037452	-0.54025197282977	-1.99725333214719
F	-1.71133660308047	-2.79282259380375	-3.47986477714667
F	-0.38204243880761	-3.11851796876023	-5.83623160124226
F	1.29449172819745	-1.27822019433281	-6.71365649230165
F	2.92069131058053	-0.00020229482688	-2.94534482769470
F	4.90990411607032	0.88942958923262	-1.45218545990893
F	6.22665143900673	3.18325389664310	-2.10696452265192
F	5.48192568787495	4.57631077477382	-4.32245454938783
F	3.43009272890070	3.75465191541155	-5.80663851852640
Se	0.15897168367954	3.14555612427256	-5.41472574459368

C	0.07321599705482	3.93428372836267	-3.73420744816043
N	-1.08328918504173	4.05061347622430	-3.10259165956255
C	-1.28360904949878	4.91041617078468	-1.93137479386214
C	1.27750487854797	4.50361028805791	-3.09933649189578
C	1.95388788452015	5.55127244319922	-3.72681581161519
C	3.04608371643216	6.14137576797303	-3.10701110465291
C	3.49376098584692	5.66577517403552	-1.87968010886828
C	2.84275744949476	4.59953154948751	-1.26769206122054
C	1.72937160581329	4.02719259175129	-1.86520089315587
C	-2.30510278131532	3.39353368198436	-3.56565062980394
H	-2.83943719167382	4.03103903325433	-4.27308656700153
H	-2.93870046002121	3.20622841005020	-2.70012456495824
H	-2.05472592641604	2.46107768597555	-4.06184784566338
H	-2.18424234835659	5.50369013585380	-2.09345329348669
H	-0.43558445736480	5.56925327717702	-1.79027904187677
H	-1.42174871339323	4.30000147234123	-1.03729542924603
H	1.61857025970511	5.89331123647149	-4.69566866460113
H	1.22262354080927	3.19871498893212	-1.39043256641563
H	3.20514920953384	4.20993451730482	-0.32560063919750
H	3.56342044835603	6.95598864189154	-3.59508139910231
H	4.36140137262505	6.11060644768733	-1.41082546223854

TS(1-B)

C	4.14879288962178	2.62078257758114	-4.99114266284995
C	3.46203746055049	1.43508470885360	-4.71886504100992
C	3.94425320401688	0.70659057205599	-3.62804496410142
C	5.00779203874020	1.12463454321518	-2.84640834548538
C	5.64343945425029	2.31998718594245	-3.14683595484535
C	5.21437101671651	3.06816053588741	-4.23195167186396
B	2.27272623463573	0.93250300659952	-5.60695463142428
C	1.10355733374645	0.10598177495343	-4.96886011168562
C	0.63378344606700	0.33261699134030	-3.66983679409843
C	-0.40260508995118	-0.38760190866892	-3.10319488618412
C	-1.00688848660289	-1.40423925222859	-3.82898367284089
C	-0.56252940979165	-1.68599542939681	-5.11215880933646
C	0.46841257027072	-0.93624149535914	-5.65353352675362
C	2.34592814635257	1.13024615136769	-7.16309326056984
C	3.55245332719181	1.04504292176605	-7.86316890835733
C	3.64716680033153	1.20425020034299	-9.23599610317532
C	2.50145865299376	1.47484472052984	-9.96968194727621
C	1.27738913603977	1.56473383544004	-9.32139062633087
C	1.21958486248112	1.37909775521269	-7.95125081370274
F	4.69530841567483	0.76669102820934	-7.21740202024576
F	4.82381266041690	1.10088360131833	-9.85641443482537
F	2.57399228065866	1.64099008615098	-11.28576693520090

F	0.17281254306949	1.82034235670966	-10.02390025583592
F	0.00726723559599	1.45880958473119	-7.38858766192124
F	1.18100177025322	1.28292100499419	-2.90348574243074
F	-0.81887018963167	-0.12556909453278	-1.86126145756956
F	-1.99516368675936	-2.11051335423375	-3.29221256597865
F	-1.12509310583701	-2.67659629003214	-5.80539044548693
F	0.86556363592925	-1.28538268460387	-6.88452883199830
F	3.39886096616874	-0.47512737183536	-3.30564974256884
F	5.42916414444069	0.39002379087700	-1.81542374392998
F	6.65942575948466	2.74441184094921	-2.40239801907904
F	5.82613264918024	4.21969109083834	-4.52526102006453
F	3.77685954808927	3.40011413569971	-6.01493002069720
Se	0.13489878153301	3.56262433866577	-5.09710501217808
C	0.01217176110996	4.24735159021520	-3.43160155625305
N	-1.25071183590571	4.34887375845706	-2.77744851492464
C	-2.19896257790625	5.21966931679960	-3.47196963072946
C	1.15412196211738	4.70849824544898	-2.64978025674418
C	2.40219601712610	4.95891494273249	-3.24549453223215
C	3.46688059308524	5.40978995973777	-2.48734550146252
C	3.31935274972511	5.59906320353775	-1.11438599683392
C	2.09054932805454	5.35669549068911	-0.50885329833236
C	1.01251372534278	4.93221574611824	-1.26849226875100
C	-1.83200633370141	3.04899045962218	-2.44249803736617
H	-2.13724631528591	2.48745855104037	-3.33625311328709
H	-2.70627238354017	3.21412536901447	-1.81180616078950
H	-1.11001725342521	2.45408108866637	-1.88528157382633
H	-2.53429084114243	4.79997329050150	-4.42884239175071
H	-1.73699307055670	6.18870198363695	-3.65751574588323
H	-3.06357809225749	5.36588774807243	-2.82371643314328
H	2.50515680678886	4.82088596732101	-4.31264307373091
H	0.04669765067874	4.76537963487661	-0.81566574185182
H	1.97095338680485	5.51058776681120	0.55591389554730
H	4.41356071728172	5.62615322382173	-2.96403243622406
H	4.15670800967818	5.94795820353843	-0.52345598952800

Free 1

C	1.88836307667943	1.57888223786532	-3.23718542987630
C	3.12860623711273	1.78311434715152	-2.64036228871821
C	3.31448133081981	2.87029791790589	-1.79362283412186
C	2.27128243305013	3.75558458657606	-1.55726153522925
C	1.02086692150373	3.55055731589084	-2.14711348404748
C	0.83701175445815	2.44878635659638	-2.98355349979005
C	-0.10818878086011	4.46095562510388	-1.83242358672039
N	0.03993612909572	5.76300068903165	-2.10981789877609
C	1.06362318392726	6.29280027252541	-3.00780557170319

Se	-1.59321814293078	3.76274055797084	-1.03514518592211
C	-0.96996480543922	6.72990974067675	-1.70092853677596
H	-1.86052300766875	6.65057530665066	-2.32972510295833
H	-0.54719275533984	7.72971186978835	-1.79045236650962
H	-1.27284947271134	6.53747138876842	-0.67403809584934
H	0.57685746099546	6.83009865294037	-3.82555179748896
H	1.66256329419507	5.49062477669162	-3.42242567359310
H	1.71684802633370	6.98947133342511	-2.47725504585640
H	-0.13833378845775	2.27757155077071	-3.41785390755350
H	2.41568032499148	4.59805671915165	-0.89224250194440
H	4.27176443150479	3.02805906296854	-1.31338398539733
H	1.73596724265135	0.73218795919001	-3.89442372325113
H	3.94290672263057	1.09504753646999	-2.82849420070677

TS(1)

C	3.94510041914061	2.10740849005546	-2.19241060669499
C	3.40308777520733	1.56683332632373	-1.02582128129984
C	2.29987434375996	2.16994198355543	-0.43347842101268
C	1.73917242642368	3.30581009219266	-0.99913465472818
C	2.27333867205188	3.86245219209976	-2.17396968663895
C	3.38903423472179	3.23777338602194	-2.76002378100422
C	1.66465415577726	5.06206970109421	-2.75290586626369
N	0.54794084283607	5.57895135634716	-2.02519125363291
C	0.79105879838132	6.90784631478142	-1.46700657010526
Se	2.24133440977446	5.85762813609663	-4.26160697751888
C	-0.70581137576328	5.51295697541924	-2.77460966139442
H	-0.71323400945578	6.19068694342976	-3.63837218102173
H	-1.52359388870246	5.77987113470381	-2.10308946103307
H	-0.86685962265847	4.49506776547780	-3.13000847929467
H	0.87998073505250	7.67892144422295	-2.24389783356442
H	1.71034542456514	6.89681659630653	-0.88125731742278
H	-0.03902854430011	7.16050821536444	-0.80533311595426
H	3.80466480216509	3.65998225582080	-3.66387102405904
H	0.88323403318227	3.78524449188115	-0.54956047219824
H	1.87543871993465	1.75530939723338	0.47164550633791
H	4.80420841066882	1.64068196493440	-2.65660079877767
H	3.84151223723725	0.68096383663735	-0.58426406271799

1-Me⁺

Se	0.49826615051560	5.63037037236387	6.43486951041406
N	-1.76939776852074	4.24835744622874	5.68278955169784

C	-1.03780446967410	5.29457262491956	5.39827333943919
C	1.34957673998640	7.04928705616975	5.38089661045061
C	-1.37911452480079	6.19507528382979	4.28733063673180
C	-1.26637117093441	5.73796324420740	2.97104247992438
C	-1.54822981485973	6.59810945449459	1.91898132016893
C	-1.95777176794693	7.90264255064496	2.17454286405096
C	-2.07605540134546	8.35484512411589	3.48514595719088
C	-1.77410284816119	7.50988371623893	4.54326422325308
C	-3.06858131876917	3.97775197785374	5.04522424475873
C	-1.37972194999075	3.29665386874522	6.73018227062494
H	-0.94550861661417	4.72296717578839	2.77419220084814
H	-1.44997354370458	6.24819974600467	0.90003429435267
H	-2.18325816188685	8.56792529852978	1.35191100314098
H	-2.40080603585757	9.36720835654308	3.68378035842394
H	-1.85791304216613	7.86092070726632	5.56409036502914
H	2.35908432172405	7.10665708122173	5.78241808486574
H	1.37410168720419	6.75810686608636	4.33587306151055
H	0.82833997749320	7.98930909414293	5.52302513816767
H	-3.37696859418762	4.82278319319010	4.44184809253112
H	-3.80159880843851	3.79765527945511	5.83049346527869
H	-2.98685092352746	3.08642171226234	4.42276363731855
H	-1.55477001403753	3.72997409143780	7.71722197011598
H	-1.97690977329821	2.39623838145195	6.62398039827322
H	-0.32485832820152	3.04250629680684	6.62686392143810

TS(1-Me$^+$)

Se	0.54258679469981	4.38505403322163	5.18496589738791
N	-2.15222397069835	4.51280094992236	5.62782012327010
C	-1.13270901623599	5.15331216271046	4.92115482343526
C	1.94571441886095	5.57223910422583	4.49678180189021
C	-1.45817728065307	6.30125326232471	4.13945606488302
C	-0.62232852657334	6.81491836607127	3.11990724532987
C	-0.99828487818403	7.93048607664771	2.40449389850859
C	-2.20297426139112	8.57387230772673	2.69585834519983
C	-3.05213327893618	8.07394736661963	3.68207888591397
C	-2.70138651496226	6.93859769000105	4.38109230127394
C	-2.41029685462462	3.11234718247567	5.25663395906217
C	-2.15497386547392	4.75507551133865	7.08019663252530
H	0.28227160969753	6.29778703945853	2.84814753934313
H	-0.36792070193919	8.29905058550086	1.60674745934937
H	-2.48840346050339	9.45543182851388	2.13664484424390
H	-3.99215064361923	8.56661086900714	3.88918364164163
H	-3.36172451800429	6.52318417470577	5.12646956774052
H	2.82104985137982	5.30591979918448	5.08586237935029
H	2.13150223944784	5.37350313095651	3.44558146735412

H	1.66811247027876	6.60768317609258	4.67165368057754
H	-2.43429332635040	3.01913635715244	4.17255514649468
H	-3.38968825930858	2.84059662475812	5.64792433687979
H	-1.66586907495889	2.41825593229648	5.66340290363764
H	-2.01719813257400	5.81675163719766	7.27925349229926
H	-3.12627917719377	4.45114563338759	7.46891672094999
H	-1.36941964217985	4.19342519850111	7.59825584145715

Free CH$_3$$^+$

C	1.47781486326742	7.22583641158960	5.25555517118144
H	2.36966573265782	7.03975222894900	5.85773436737401
H	1.31895951122178	6.67035189149143	4.32885155042297
H	0.74466261926082	7.96741956559073	5.58007180601614

Free I

F	3.20032854995721	-1.62138000687389	-3.56224035847800
F	1.97509078738148	-1.40879737288536	-1.77559102571670
F	-0.21047109546420	-2.29145110870226	-3.06135571559803
F	0.84390835013794	-2.29147373964299	-4.98743853571626
F	2.46082027848849	-4.20267022452827	-4.29410650334064
F	1.97258680695585	-4.03667920808878	-2.16482506492088
C	0.87825829672670	-6.45643900837706	-3.78346379833558
F	-0.43196336231742	-4.97583184051519	-2.47138594859691
F	-0.42114673728806	-4.68105454492524	-4.64343186387277
C	-0.18933722031693	-7.57308129032336	-3.54318553732899
F	1.32076222711934	-6.58011802159743	-5.04797368452151
F	1.90104775038870	-6.68452803217016	-2.93471141067694
F	0.30930057676009	-8.73867928729179	-3.96105379569670
F	-0.48776244891787	-7.67864468802916	-2.24891891638174
F	-1.30502246509208	-7.31145622246295	-4.22943715554679
I	1.34263843635823	0.61514551580713	-3.75437118777475
C	1.95884740622430	-1.37040496308228	-3.11487811981415
C	0.98599334007297	-2.46142866008378	-3.66003144287904
C	1.47746998839075	-3.93324369085504	-3.41283326527425
C	0.33849291363404	-5.00097549886894	-3.57728142053382

Free B

F	-3.17521791433037	2.69278490792203	-6.55011851684313
F	-3.31589579597990	1.27445428040193	-8.81576004915000
F	-2.30859215562264	2.28658724568040	-11.12569908138642
F	-1.14238214900891	4.73894374153242	-11.15016774128968
F	-0.96900809107358	6.17004237314982	-8.89506026030158
F	-1.92684054840386	7.97601611607039	-5.11033999407984
F	0.28909449269086	9.37526048074784	-4.56707357435920
F	2.73453397230324	8.32881919827233	-5.11560257903619

F	2.94680552902455	5.86350993087194	-6.23483199843435
F	0.74579897176822	4.45252167708633	-6.81154625856582
F	-4.78667664320043	5.40534556280508	-7.04263866608960
F	-6.82837758858507	5.43609661892984	-5.31225962463019
F	-6.35601056042996	5.37000802878408	-2.63978309922245
F	-3.80752402433049	5.28149573022621	-1.70293499352117
F	-1.74623116101476	5.26889639564571	-3.41015507543311
B	-1.97636211904917	5.32806966064298	-6.30422486554162
C	-2.98507953888998	5.31929684472787	-3.91942858955865
C	-3.17427476082211	5.33770316704342	-5.30360785344439
C	-4.50297092056813	5.36652859072579	-5.73336901701753
C	-5.57594878416323	5.38859015301540	-4.85908011175308
C	-5.33803138936844	5.35963968309579	-3.49102613582445
C	-4.03362738109476	5.31906079487967	-3.01594187385738
C	-0.68928064189320	6.15110349478450	-5.98536284212885
C	-0.74313497750955	7.41642592453211	-5.39620640626619
C	0.38750750417308	8.16234417818811	-5.11063911164106
C	1.63964178855366	7.63265487950997	-5.39456687876837
C	1.74399689851743	6.37340855729311	-5.97113208454953
C	0.59069933200098	5.66606651171310	-6.26405938942185
C	-2.06541156786349	4.49541837419440	-7.62120312256290
C	-2.66866230730862	3.23615255840178	-7.66559163251338
C	-2.74914852933962	2.48069178875366	-8.82266693407791
C	-2.23129943249380	2.99318232069938	-10.00500875646406
C	-1.63131299925443	4.24572140266371	-10.01259292913073
C	-1.54916405431967	4.96363882689750	-8.83176886944836

1-ICF₃

C	-1.10210919899910	0.32034129425678	-4.88848610647857
C	-0.14076112238671	1.29051185461806	-4.62873938076560
C	-0.52601341920752	2.51689204723603	-4.10085199389461
C	-1.86446823044559	2.77760071402113	-3.84326401838773
C	-2.83370020985951	1.80331197620152	-4.10002265222687
C	-2.43894761351690	0.56968137002124	-4.61626643483727
C	-4.24715946229035	2.04042252094250	-3.72251300800635
N	-4.88741936375411	3.07506705936974	-4.26806118776113
C	-4.39430792595717	3.82075370001895	-5.42696726025608
Se	-5.01880464606146	0.94198651619174	-2.46772239193458
C	-6.23250425152109	3.43839155556946	-3.83204214585199
H	-6.96677935201805	2.72721535096131	-4.21753162991999
H	-6.45921777982903	4.43443606481577	-4.20637914130686
H	-6.28461581031724	3.41991551304451	-2.74563086431824
H	-5.16386775350259	3.81842556991375	-6.20178226130767
H	-3.49433542178484	3.36472048961967	-5.82030854050103
H	-4.18014003265024	4.85482975901801	-5.14859419531289

H	-3.18411933177251	-0.19773360342018	-4.77526199864205
H	-2.15628247962479	3.72482452725776	-3.40782834537429
H	0.22057036532394	3.26637191064748	-3.87281360598901
H	-0.80887508971939	-0.64166895202025	-5.28866895711866
H	0.90552680191931	1.08553206455044	-4.81656704938482
F	0.30300366599148	-1.08594161340442	0.10970492358285
F	0.87787406719196	0.64789672212909	-1.05321348082816
I	-2.04750540201763	0.34729883306311	-0.95237946374541
C	-0.02229210075191	0.18659024251780	-0.16453515891820
F	0.12343109756099	0.89756651285902	0.96525634948523

1-ICF₃ (TS)

C	-1.80918433704341	0.73849232177419	-5.44485842068530
C	-1.24486982353507	1.77178065738769	-6.19118653774448
C	-1.72151970383482	3.07165780946833	-6.05044288807197
C	-2.76331000212310	3.33713010250086	-5.17911221212465
C	-3.31922644371427	2.31245909798445	-4.39039495972937
C	-2.81992266169028	1.00670519817897	-4.53940275620497
C	-4.39669677738813	2.62591271481225	-3.46114679889989
N	-5.05701557108558	3.86460349775153	-3.70370388693920
C	-6.47673274422092	3.71280847455143	-4.01669230346331
Se	-4.88122304650436	1.56481713952741	-2.08147200526920
C	-4.81132355573087	4.87553891865134	-2.67699311707982
I	-1.95042035995732	0.39490899147218	-0.85746063819351
C	-0.00045790603713	0.07049523426955	0.07192801187442
F	-0.07411502666577	0.21152177699027	1.40153312313262
F	0.46800713676631	-1.15923038475538	-0.18080086138509
F	0.89522019921327	0.95732550132616	-0.38675254046559
H	-5.30211786809974	4.63441408006835	-1.72422628736037
H	-5.18754492195549	5.83295041647195	-3.03997937658525
H	-3.74031049677779	4.96869351361283	-2.50096709344851
H	-7.06395551536825	3.37677973470776	-3.15167610204112
H	-6.59918135031587	2.98997278993578	-4.82244140038515
H	-6.85872977457527	4.67634271404214	-4.35622985364495
H	-3.26189419602752	0.20760908383227	-3.96172943065968
H	-3.16323584234275	4.33556497378121	-5.08471456978573
H	-1.28945089854995	3.87474368851180	-6.63429031554811
H	-1.45503046690675	-0.27693050126516	-5.56618741877125
H	-0.44449804552918	1.56344245440986	-6.89089936052053

Free ICF₃

F	0.44026521636814	-1.19007403646809	-0.38008846116243
F	0.87315351889000	0.92667616882037	-0.38528968809798
I	-1.97066550349720	0.40181786673837	-0.77163750817477
C	0.00492990282372	0.00113550852453	0.02587703840879

F	-0.02688313458466	0.00625449238483	1.35884861902638

1-BCl₃

B	2.09322752642701	2.29448994193084	-5.68794959374722
Cl	1.71697957884438	0.97010937798029	-6.90577173194982
Cl	2.96388512315499	3.70863446960071	-6.47162295305252
Cl	2.90401784494219	1.68094812833686	-4.17183856977500
Se	0.01405330804362	2.87122715190359	-5.23535972966038
C	-0.04421433795162	3.83161328521961	-3.64634566593132
N	-1.21206412094374	4.02662518325109	-3.04410721649494
C	-1.41491369266494	5.02290414454658	-1.98999129372551
C	1.17696974687088	4.35494582618538	-3.01385693075632
C	2.04493902189190	5.18574290320492	-3.71957694082853
C	3.21934413902892	5.62543495571793	-3.12668328416660
C	3.53210725985553	5.24367145433738	-1.82879636813245
C	2.66574539771597	4.41984891391483	-1.11503262514761
C	1.49440998893606	3.97434705763938	-1.70463767035065
C	-2.43717285527399	3.37461039200674	-3.49771654525976
H	-2.87137593735832	3.90931083201099	-4.34619842591564
H	-3.14746546606766	3.37276221369773	-2.67274821144990
H	-2.22179671538095	2.35351860920144	-3.80459167444387
H	-2.27699048123380	5.63415705051591	-2.26233244567530
H	-0.54321445516416	5.66015640546089	-1.89423246837789
H	-1.61799213818061	4.53767564712579	-1.03381076609989
H	1.80663390134656	5.46844588886310	-4.73237575198429
H	0.83680242601028	3.30341231372882	-1.16626573729903
H	2.91523106235493	4.10978783060085	-0.10898458388936
H	3.89523872185758	6.25853444315448	-3.68679381805239
H	4.45761515293907	5.57508557986387	-1.37537899783376

1-BCl₃ (TS)

Cl	0.96410332337115	0.89986727687467	-1.52924516958234
B	-0.12086363872971	-0.05380910668063	-0.53834306264733
Cl	0.34854049082193	-0.51411804533008	1.08229240246667
Cl	-1.58512319480095	-0.70891822168478	-1.23309203188180
Se	-1.91057926685599	2.41295739338244	0.84234570549939
C	-1.48613973514838	4.15412963166349	1.03869870754056
N	-2.08148609106705	4.95018563646228	2.06516011005491
C	-3.52515877590022	5.11523628417319	1.89190719545079
C	-0.52258330144580	4.85494337300773	0.19309564294465
C	-0.00738097116651	4.27459859259362	-0.97863351817677
C	0.92759456140236	4.94651389756792	-1.74245247637350
C	1.36550000903945	6.21400856358892	-1.36202005197490
C	0.84830314939013	6.81281503251866	-0.21883115872262
C	-0.08444030015134	6.14025112780750	0.55442543561752

C	-1.74198517508974	4.51641697108668	3.42107448491032
H	-2.17609138515223	3.53817862739808	3.66795490894488
H	-2.11997471440825	5.26113478492773	4.12248700221142
H	-0.65964029125157	4.45557678756122	3.52987213317800
H	-4.07615430205595	4.18596064991138	2.09140329801264
H	-3.74224171424667	5.43639833341535	0.87351387681450
H	-3.87107261896311	5.88814803796754	2.57985147567356
H	-0.35987908573301	3.29899451945392	-1.27803245931457
H	-0.49262760674988	6.58892303261054	1.44729644281452
H	1.17899509291883	7.79950266376870	0.07762886368771
H	1.31160465366165	4.48716285581687	-2.64449214227905
H	2.10190088831085	6.73486130013706	-1.96156561486914

Free BCl₃

B	1.97123617797647	1.20319538327536	-5.41024950808264
Cl	2.14468049239537	1.42247149852098	-7.13460423180454
Cl	3.05385928494114	2.02598914914857	-4.31547548397333
Cl	0.71222404468704	0.16734396905510	-4.78367077613949

Partially optimized structures for 1-Me⁺

Se-Me distance 2.298

Se	0.70841945003713	0.22925989807614	-0.02478612269396
C	0.24794545782927	0.11537419187833	2.22334925850205
N	-0.38101783890338	2.17485213741767	-1.67174438362715
C	-0.14771316026839	1.85580303408134	-0.42329572654963
C	-0.55145986258690	2.75373697638701	0.66969504649258
C	0.40276098632150	3.39560040416564	1.46102575995522
C	-0.01002737488813	4.22376964723816	2.49494943459611
C	-1.36690390115445	4.38877809963587	2.76069384729447
C	-2.31723533263497	3.73606871311739	1.98334279063203
C	-1.91414952664222	2.92777123028289	0.93030111370997
C	-0.81046360358045	3.52153848182962	-2.08718926881423
C	-0.13250829053889	1.24545151745339	-2.77872221459633
H	1.45657464253229	3.25341940588862	1.25621805682566
H	0.72596411671125	4.73700239402784	3.09863219060578
H	-1.67941312109316	5.02787229988577	3.57639558816881
H	-3.37207855055240	3.85475092656963	2.19209653553961
H	-2.65055432388910	2.41738692548480	0.32278734250158
H	0.63782330213605	-0.86944889861719	2.45096895904624
H	0.79819118716655	0.94069965528852	2.65004958744559
H	-0.82915559085363	0.20201816199084	2.25800846884123
H	-0.72754090790313	4.21602275585021	-1.26005505961909
H	-1.84148655674293	3.48607053445522	-2.43962168136208
H	-0.16552091959432	3.84329865123667	-2.90434457379189
H	-0.37469649053068	0.22873457432932	-2.47362698839154

| H | -0.75938683034994 | 1.53107169816110 | -3.61908830819339 |
| H | 0.91527303997302 | 1.29528658388522 | -3.08232965251764 |

Se-Me distance 2.631

Se	0.72571168370800	0.23531478072174	-0.09882373150858
C	0.18824052957298	0.11740979604981	2.47395857199133
N	-0.38101130800467	2.19813550741583	-1.72078428525361
C	-0.13129361245637	1.86021998033185	-0.47921607828152
C	-0.53198540144201	2.74293658646642	0.63002610229741
C	0.42227967985848	3.38689103437420	1.41938600986712
C	0.01092828264113	4.19141496419591	2.47282423118915
C	-1.34474284162645	4.33427772312879	2.75738540094564
C	-2.29500611321002	3.68381851998416	1.97826919158423
C	-1.89326217236565	2.89898308367097	0.90666471115066
C	-0.81309142473384	3.55077348215685	-2.11129848926571
C	-0.14491338150211	1.28576523884680	-2.84355510162806
H	1.47526192480617	3.25978581508564	1.20141874265757
H	0.74727244465513	4.70539475673134	3.07556513775747
H	-1.65648565071762	4.95568313818189	3.58702220502717
H	-3.34903785273641	3.78686370925245	2.19960287423795
H	-2.63008456458974	2.38984970938578	0.29847883575335
H	0.63629074342602	-0.84956835075070	2.65495400599957
H	0.72397177184345	0.99628977607593	2.79688970561482
H	-0.88742418423762	0.17400559671066	2.40412067554977
H	-0.72522679319703	4.23208103706644	-1.27380169336117
H	-1.84622245134950	3.52193154641815	-2.45847628290702
H	-0.17305612956773	3.88657872314775	-2.92671872614233
H	-0.36943975732797	0.26293272798641	-2.54521065868921
H	-0.79203162333902	1.57477795739876	-3.66748668453271
H	0.89599820189241	1.34964315996619	-3.16748467005333

Se-Me distance 2.964

Se	0.71798267281070	0.23191662039828	-0.17703322053334
C	0.11927972208854	0.14360674992626	2.72483357078618
N	-0.37855499630806	2.22469007442637	-1.77734787847274
C	-0.12118495428557	1.86295733384541	-0.54343814082860
C	-0.51538500331327	2.72802460897168	0.58485616850966
C	0.44063764871093	3.38627517064159	1.35961053731307
C	0.03504161524565	4.16174306613064	2.43727377603370
C	-1.31643799973615	4.26464955253933	2.75762246246533
C	-2.26807426139363	3.60468721301127	1.98849593473670
C	-1.87290314381534	2.84758409167290	0.89425553907161
C	-0.81135003568205	3.58397318831975	-2.14026185677336
C	-0.15054853141469	1.33071210750495	-2.91564623487214
H	1.49098558341918	3.28865021200791	1.11605617177422

H	0.77283039848013	4.68738073373621	3.02834421185778
H	-1.62421019778675	4.86533864952504	3.60396362901798
H	-3.31904553829812	3.68029018957976	2.23483850997016
H	-2.61116279695691	2.33120766775029	0.29394009177551
H	0.58819699410910	-0.81576810404218	2.88838863397098
H	0.66234309394363	1.04690842258375	2.95586549742694
H	-0.94897664952780	0.19500081357246	2.58117967739209
H	-0.72397523886921	4.24850801820408	-1.28925912483913
H	-1.84444550535100	3.56191743845417	-2.48837926412758
H	-0.17155742944027	3.93782178733645	-2.94831039201183
H	-0.37480346455112	0.30379539143769	-2.63090261433919
H	-0.80185963553817	1.63388605855180	-3.73122090098135
H	0.88881765346024	1.39643294391412	-3.24401478432267

Se-Me distance 3.298

Se	0.67712617586480	0.21289993713052	-0.26258678117222
C	0.07451162646150	0.16785870935318	2.97920474200315
N	-0.37707305447445	2.25434347362840	-1.83592000292797
C	-0.12527889755320	1.85958041666868	-0.61069259995469
C	-0.51004413953798	2.70404803716540	0.53850955388207
C	0.44862599084455	3.37639289445749	1.29727041602415
C	0.05197311663881	4.12999460461645	2.39386049061418
C	-1.29349712524488	4.19995043382549	2.74685880355813
C	-2.24759688150580	3.52818566939199	1.99112719161914
C	-1.86199425026207	2.78960058217525	0.88052501603567
C	-0.80060075429879	3.62429089276801	-2.16609946405621
C	-0.15556579064478	1.38318095135553	-2.99259284322974
H	1.49500516416173	3.30450873220776	1.02938545416402
H	0.79225036151174	4.66761116745706	2.97120753001077
H	-1.59553580392780	4.78624845182912	3.60534109953098
H	-3.29447794060452	3.58119236546256	2.26046621431531
H	-2.60273908076716	2.26543405164233	0.29027835090841
H	0.56650206351659	-0.78085345966218	3.13987134310492
H	0.62040195564252	1.08864267760166	3.12251029144626
H	-0.99202517767646	0.20175961644205	2.81438122149043
H	-0.70889317586229	4.26820410251394	-1.29971679211347
H	-1.83368285625124	3.61777132124104	-2.51522650451250
H	-0.15811441869475	3.99382317691997	-2.96497131995613
H	-0.39952052583545	0.35415751291945	-2.73228163406966
H	-0.79547322432102	1.71602269403140	-3.80563816706507
H	0.88735664282038	1.43734098685746	-3.31136160964993

Se-Me distance 3.631

| Se | 0.70051291680090 | 0.27147065340055 | -0.30747924525064 |
| C | 0.13200647120187 | -0.02835050520070 | 3.26615012597197 |

N	-0.39682859844384	2.28932602318899	-1.88568795371902
C	-0.12695861637074	1.89902940912769	-0.66175849175105
C	-0.51349526523848	2.73569861699828	0.49214350903667
C	0.44786626560418	3.37321185278219	1.27800717476539
C	0.04902534066795	4.13174856258415	2.36996217275970
C	-1.30152673507803	4.23933967450227	2.69308635493411
C	-2.25912064297374	3.59976866845602	1.91335041652979
C	-1.87006859940905	2.85617847919972	0.80807850260179
C	-0.83032529154026	3.65517663588937	-2.21598364191543
C	-0.17069533653828	1.41932602931035	-3.04168025480295
H	1.49672567728917	3.27467546548796	1.02976404779228
H	0.79066643487504	4.64594857296323	2.96650162654387
H	-1.60462084054868	4.83068112925254	3.54772490015872
H	-3.30948923183560	3.68089458115270	2.16095086965642
H	-2.61203894751413	2.35569442166062	0.19930132959710
H	0.73342353755241	-0.92331476620070	3.34065049905569
H	0.58798876281235	0.94038875504890	3.41193825590412
H	-0.93610547344105	-0.10289976444139	3.12510363239943
H	-0.74586092213734	4.29979763741567	-1.34925006127853
H	-1.86257401841196	3.64199070270328	-2.56750871428847
H	-0.18905973082062	4.03049531308204	-3.01336949016598
H	-0.39748545540303	0.38748305398716	-2.77746999665254
H	-0.81990026895186	1.74159195440432	-3.85167510907453
H	0.86957856785280	1.48683884324478	-3.36714045880794

Se-Me distance 3.964

Se	0.67944712017072	0.32992715819590	-0.32011663966132
C	0.18771843143591	-0.29377373232051	3.56380846657765
N	-0.40380284302072	2.33217799925476	-1.93809839237761
C	-0.13609264317458	1.94825766140232	-0.71150802468699
C	-0.52423861923130	2.78768368101437	0.43981424486471
C	0.43575477886381	3.43766935941575	1.21828210798485
C	0.03462007362118	4.20269686483501	2.30427901733687
C	-1.31567625174923	4.30093975282601	2.63123373028742
C	-2.27187362132658	3.64543931757056	1.86150234903346
C	-1.88130022497398	2.89637191496366	0.76196435556517
C	-0.84033117207521	3.69474903649941	-2.27458536773116
C	-0.17451014669460	1.45597516135345	-3.08826485261484
H	1.48405270777905	3.34399326962165	0.96587678455181
H	0.77342578920297	4.72744789498121	2.89509248136986
H	-1.61991963300177	4.89712853895509	3.48199148372867
H	-3.32164801686025	3.71923593010540	2.11376739221519
H	-2.61989979429266	2.38168689630549	0.16098749755979
H	0.74570326681860	-1.21804616106563	3.50572105070729
H	0.70444438710586	0.63314159641430	3.76790487868446

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H   -0.88809045991838    -0.30302104496781    3.46595676591132
H   -0.76091723809664     4.34264899642900   -1.40958355564416
H   -1.87146788305783     3.67796440178751   -2.62931466995317
H   -0.19769444702123     4.07052652118983   -3.07074916651302
H   -0.39226742215390     0.42436710982991   -2.81645238738234
H   -0.82821671762091     1.76809836692564   -3.89876114046558
H    0.86442057927166     1.52890350847770   -3.41703840934835
```

ICF₃···ICH₃

```
I   -0.79790801727323    -0.32802747798119    1.78125092026511
C    0.07507921298842     0.19647939376679   -0.14131201719458
F    0.98695870568453     1.16328673607830    0.00829398926492
F    0.67671795642972    -0.85937998243432   -0.69643915012007
F   -0.86098719549002     0.63427161322336   -0.98757396471092
I   -1.73046486310623    -0.96071312778116    5.29981372368359
C    0.19810072031786    -0.06158351516796    5.65615955993165
H    0.94823504828480    -0.78887269213673    5.36896157634676
H    0.25157337443720     0.17487185537233    6.71298661270503
H    0.25169505772692     0.82966719706058    5.04185874982840
```

Free ICH₃

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I    0.00002696774473     0.00000001526192    3.75242754735217
C   -0.00004355316341    -0.00000000383521    5.90989082137353
H    1.03450983208507    -0.00000002995087    6.23384025034636
H   -0.51724660069432    -0.89596262955836    6.23392074294110
H   -0.51724664597207     0.89596264808252    6.23392063798683
```

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