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Electronic Supplementary Information

Reactivity of dicationic N-heterocyclic chalcogen carbene analogues with methane and ethene: A theoretical investigation

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Table S1: The bond lengths, bond angles, Wiberg bond orders, and partial charges of the reactants, precursor complexes (if available), transition states, and products of the methane and ethene reactions are tabulated.[a]

(a) Reactants **Rea-M**

M	θ[b]	M−N_1[c]	M−N_2[d]	q(M)[e]
O	95.8	2.234 (0.214)	1.276 (1.316)	−0.279
S	90.6[p]	1.734 (0.963)	1.734 (0.963)	0.895
Se	85.5[q]	1.910 (0.856)	1.910 (0.856)	0.950
Te	78.9	2.145 (0.732)	2.145 (0.732)	1.080

(b) Transition States **TS-M-CH_4** (Reaction with CH_4)

M	θ	M−N_1	M−N_2	q(M)	ϕ[f]	M−C[g]	M−H[h]	C−H[i]	q(CH_4)[j]
[CH_4]								1.107 (0.949)	0.000
O	86.4	2.676 (0.078)	1.306 (1.191)	−0.393	157.2	2.212 (0.308)	1.838 (0.064)	3.972 (0.000)	0.926
S	79.8	2.298 (0.288)	1.883 (0.722)	0.463	46.6	2.135 (0.664)	1.458 (0.630)	1.552 (0.227)	0.443
Se	76.6	2.349 (0.309)	2.061 (0.620)	0.628	47.2	2.234 (0.707)	1.568 (0.677)	1.639 (0.212)	0.325
Te	72.3	2.460 (0.327)	2.224 (0.572)	0.989	46.7	2.423 (0.731)	1.749 (0.717)	1.766 (0.193)	0.123

(c) Products **Pro-M-CH_4** (Reaction with CH_4)

M	θ	M−N_1	M−N_2	q(M)	ϕ	M−C	M−H	C−H	q(CH_4)
O	89.3	2.702 (0.041)	1.394 (0.977)	−0.362	132.9	1.459 (0.842)	1.922 (0.037)	3.106 (0.001)	0.894
S	71.0	2.575 (0.183)	2.532 (0.180)	0.240	96.7	1.822 (1.018)	1.370 (0.917)	2.405 (0.007)	0.258
Se	71.3	2.511 (0.258)	2.495 (0.253)	0.518	93.9	1.961 (0.991)	1.498 (0.919)	2.548 (0.010)	0.137
Te	70.3	2.557 (0.272)	2.334 (0.470)	1.130	87.7	2.165 (0.983)	1.718 (0.889)	2.708 (0.006)	−0.095

(d) Precursor Complexes **PC-M-C_2H_4** (Reaction with C_2H_4)

M	θ	M−N_1	M−N_2	q(M)	ϕ'[k]	M−C_1[l]	M−C_2[m]	C_1−C_2[n]	q(C_2H_4)[o]
[C_2H_4]								1.343 (2.048)	0.000
O	94.4	2.322 (0.186)	1.272 (1.338)	−0.268	24.4	2.659 (0.078)	3.220 (0.015)	1.358 (1.833)	0.188
S	88.0	1.788 (0.864)	1.751 (0.937)	0.817	27.5	2.729 (0.151)	2.935 (0.109)	1.359 (1.837)	0.172
Se	75.8	2.440 (0.263)	2.027 (0.687)	0.788	39.3	2.146 (0.703)	2.116 (0.727)	1.433 (1.237)	0.233
Te	75.9	2.248 (0.557)	2.170 (0.684)	0.992	29.6	2.703 (0.310)	2.692 (0.308)	1.378 (1.655)	0.228

(e) Transition States **TS-M-C_2H_4** (Reaction with C_2H_4)

M	θ	M−N_1	M−N_2	q(M)	ϕ'	M−C_1	M−C_2	C_1−C_2	q(C_2H_4)
O	86.3	2.838 (0.050)	1.272 (1.339)	−0.271	31.2	2.652 (0.053)	2.174 (0.222)	1.379 (1.619)	0.336
S	81.5	2.182 (0.400)	1.819 (0.825)	0.572	37.2	2.211 (0.515)	2.191 (0.515)	1.403 (1.372)	0.372
Se	76.3	2.429 (0.273)	2.029 (0.687)	0.780	39.0	2.155 (0.691)	2.127 (0.712)	1.430 (1.248)	0.239
Te	75.7	2.262 (0.537)	2.179 (0.676)	0.980	29.8	2.686 (0.319)	2.673 (0.324)	1.380 (1.640)	0.222

(f) Products **Pro-M-C_2H_4** (Reaction with C_2H_4)

M	θ	M−N_1	M−N_2	q(M)	ϕ'	M−C_1	M−C_2	C_1−C_2	q(C_2H_4)
O	77.0	3.225 (0.026)	1.373 (1.016)	−0.300	34.3	2.486 (0.021)	1.437 (0.877)	1.532 (1.004)	0.701
S	70.3	2.547 (0.167)	2.550 (0.225)	0.427	47.7	1.837 (0.968)	1.838 (0.947)	1.485 (1.066)	0.147
Se	82.1	2.008 (0.691)	1.944 (0.807)	0.813	29.6	2.673 (0.222)	2.677 (0.227)	1.368 (1.725)	0.248
Te	75.7	2.251 (0.550)	2.174 (0.680)	0.989	29.8	2.679 (0.317)	2.689 (0.319)	1.379 (1.646)	0.228

[a] The bond lengths, bond angles, and partial charges are in the units of Å, degrees, and $|e|$, respectively.
[b] The bond angle between M−N_1 and M−N_2 bonds
[c] The bond length and Wiberg bond order (in parenthesis) of bond M−N_1
[d] The bond length and Wiberg bond order of bond M−N_2
[e] The partial charge of atom M
[f] The bond angle between M−C and M−H bonds
[g] The bond length and Wiberg bond order of bond M−C
[h] The bond length and Wiberg bond order of bond M−H
[i] The bond length and Wiberg bond order of bond C−H
[j] The partial charge of CH_4 fragment
[k] The bond angle between M−C_1 and M−C_2 bonds
[l] The bond length and Wiberg bond order of bond M−C_1
[m] The bond length and Wiberg bond order of bond M−C_2
[n] The bond length and Wiberg bond order of bond C_1−C_2
[o] The partial charge of C_2H_4 fragment
[p] Experimental values[1,2] for reactant **Rea-S** are θ(N_1−M−N_2)=87.7∼88.0 and M−N_1=1.655∼1.699.
[q] Experimental values[2,3] for reactant **Rea-Se** are θ(N_1−M−N_2)=81.8 and M−N_1=1.890.

Table S2: The activation energies and reaction enthalpies[a] (relative to the reactant energies) and their EDA analysis results[b] of the precursor complexes (if available), transition states and products of the reactions with methane and ethene are shown in parts (a) and (b), respectively.

(a) Reaction with CH_4 : **Rea-M** + CH_4 $\longrightarrow$ **TS-M-CH$_4$** $\longrightarrow$ **Pro-M-CH$_4$**

	Transition States **TS-M-CH$_4$**				Products **Pro-M-CH$_4$**			
Energy	**TS-O-CH$_4$**	**TS-S-CH$_4$**	**TS-Se-CH$_4$**	**TS-Te-CH$_4$**	**Pro-O-CH$_4$**	**Pro-S-CH$_4$**	**Pro-Se-CH$_4$**	**Pro-Te-CH$_4$**
ΔE	−3.61	35.18	30.27	30.65	−42.61	4.19	6.38	7.01
ΔE_{str}	170.94	73.86	79.12	86.94	170.94	174.96	163.07	147.93
$\Delta E_{\text{str}}^{\text{carb}}$	27.12	27.02	23.06	17.09	34.95	62.47	43.88	21.79
$\Delta E_{\text{str}}^{\text{meth}}$	143.82	46.84	56.05	69.85	135.99	112.48	119.19	126.14
ΔE_{int}	−171.13	−40.65	−43.81	−52.92	−208.48	−171.10	−149.43	−136.50
ΔE_{disp}	−9.12	−8.54	−8.49	−8.82	−7.29	−7.25	−7.58	−9.10
ΔE_{Pauli}	414.01	293.18	265.59	241.13	671.41	623.99	560.48	476.64
ΔE_{elstat}	−183.96	−124.79	−126.51	−123.77	−294.05	−247.00	−243.08	−236.14
ΔE_{orb}	−392.06	−200.50	−174.40	−161.46	−578.56	−540.84	−459.25	−367.90
ΔE_1	−282.57	−134.25	−111.20	−96.94	−406.81	−444.53	−387.31	−300.04
	(72.1%)	(67.0%)	(63.8%)	(60.0%)	(70.3%)	(82.2%)	(84.3%)	(81.6%)
ΔE_2	−69.49	−38.28	−39.81	−46.11	−107.99	−38.63	−28.78	−38.80
	(17.7%)	(19.1%)	(22.8%)	(28.6%)	(18.7%)	(7.1%)	(6.3%)	(10.5%)
ΔE_{rest}	−37.76	−25.70	−21.37	−15.68	−60.48	−55.94	−41.63	−27.50
	(9.6%)	(12.8%)	(12.3%)	(9.7%)	(10.5%)	(10.3%)	(9.1%)	(7.5%)

(b) Reaction with C_2H_4 : **Rea-M** + C_2H_4 $\longrightarrow$ **PC-M-C$_2$H$_4$** $\longrightarrow$ **TS-M-C$_2$H$_4$** $\longrightarrow$ **Pro-M-C$_2$H$_4$**

	Precursor Complexes **PC-M-C$_2$H$_4$**			
Energy	**PC-O-C$_2$H$_4$**	**PC-S-C$_2$H$_4$**	**PC-Se-C$_2$H$_4$**	**PC-Te-C$_2$H$_4$**
ΔE	−7.50	−16.23	−17.80	−24.64
ΔE_{str}	3.97	4.18	31.96	9.62
$\Delta E_{\text{str}}^{\text{carb}}$	3.67	3.75	24.58	8.34
$\Delta E_{\text{str}}^{\text{eth}}$	0.30	0.43	7.38	1.28
ΔE_{int}	−9.57	−19.23	−45.60	−31.61
ΔE_{disp}	−9.74	−10.71	−10.19	−11.03
ΔE_{Pauli}	20.60	34.93	267.32	73.62
ΔE_{elstat}	−8.99	−18.10	−132.39	−41.23
ΔE_{orb}	−11.44	−25.35	−170.34	−52.97
ΔE_1	−7.48	−19.05	−110.08	−37.54
	(65.4%)	(75.1%)	(64.6%)	(70.9%)
ΔE_2	−1.04	−1.49	−34.12	−6.05
	(9.1%)	(5.9%)	(20.0%)	(11.4%)
ΔE_{rest}	−1.33	−2.19	−23.72	−7.33
	(11.6%)	(8.6%)	(13.9%)	(13.8%)

	Transition States **TS-M-C$_2$H$_4$**				Products **Pro-M-C$_2$H$_4$**			
Energy	**TS-O-C$_2$H$_4$**	**TS-S-C$_2$H$_4$**	**TS-Se-C$_2$H$_4$**	**TS-Te-C$_2$H$_4$**	**Pro-O-C$_2$H$_4$**	**Pro-S-C$_2$H$_4$**	**Pro-Se-C$_2$H$_4$**	**Pro-Te-C$_2$H$_4$**
ΔE	−1.18	−9.11	−17.76	−23.70	−56.51	−13.10	−20.92	−24.56
ΔE_{str}	15.13	25.53	30.09	10.49	137.89	80.90	6.87	10.06
$\Delta E_{\text{str}}^{\text{carb}}$	13.72	22.29	23.10	9.10	37.99	63.37	6.17	8.73
$\Delta E_{\text{str}}^{\text{eth}}$	1.40	3.24	7.00	1.39	99.90	17.52	0.70	1.33
ΔE_{int}	−13.89	−35.52	−43.87	−31.64	−186.11	−94.26	−24.98	−32.04
ΔE_{disp}	−10.64	−10.60	−10.23	−10.88	−10.38	−10.66	−11.10	−10.98
ΔE_{Pauli}	54.47	178.71	260.29	77.81	815.37	580.21	56.13	76.15
ΔE_{elstat}	−23.16	−82.81	−128.86	−43.29	−367.15	−253.57	−30.23	−42.55
ΔE_{orb}	−34.56	−120.82	−165.08	−55.28	−623.94	−410.25	−39.76	−54.66
ΔE_1	−26.59	−85.91	−106.73	−38.90	−417.74	−320.55	−29.56	−38.58
	(76.9%)	(71.1%)	(64.7%)	(70.4%)	(67.0%)	(78.1%)	(74.3%)	(70.6%)
ΔE_2	−4.48	−16.82	−32.77	−6.65	−128.41	−32.46	−3.37	−6.39
	(13.0%)	(13.9%)	(19.9%)	(12.0%)	(20.6%)	(7.9%)	(8.5%)	(11.7%)
ΔE_{rest}	−1.82	−15.83	−23.19	−7.68	−75.07	−55.04	−4.25	−7.60
	(5.3%)	(13.1%)	(14.0%)	(13.9%)	(12.0%)	(13.4%)	(10.7%)	(13.9%)

[a] Activation energies, reaction enthalpies, and strain energies are calculated at the BP86/Def2-SVP theory level. All energies are in Kcal/mol. (Free energies are included in Table S3 of ESI.)

[b] Interaction energies and EDA results are obtained at the BP86/TZ2P//BP86/Def2-SVP theory level with ZORA.

Table S3: The activation energies and reaction enthalpies of the transition states and products of the reactions with methane and ethene (relative to the reactants energies) are shown in (a) and (b), respectively. ΔE are the total energies, and ΔG are the free energies at 298.15 K.

(a) Reaction with CH_4 : **Rea-M** + CH_4 $\longrightarrow$ **TS-M-CH$_4$** $\longrightarrow$ **Pro-M-CH$_4$**								
	Transition States **TS-M-CH$_4$**				Products **Pro-M-CH$_4$**			
Energy	**TS-O-CH$_4$**	**TS-S-CH$_4$**	**TS-Se-CH$_4$**	**TS-Te-CH$_4$**	**Pro-O-CH$_4$**	**Pro-S-CH$_4$**	**Pro-Se-CH$_4$**	**Pro-Te-CH$_4$**
ΔE	−3.61	35.18	30.27	30.65	−42.61	4.19	6.38	7.01
ΔG	11.46	43.01	37.65	39.00	−25.74	13.12	14.29	16.93
(b) Reaction with C_2H_4 : **Rea-M** + C_2H_4 $\longrightarrow$ **PC-M-C$_2$H$_4$** $\longrightarrow$ **TS-M-C$_2$H$_4$** $\longrightarrow$ **Pro-M-C$_2$H$_4$**								
	Precursor Complexes **PC-M-C$_2$H$_4$**							
Energy	**PC-O-C$_2$H$_4$**	**PC-S-C$_2$H$_4$**	**PC-Se-C$_2$H$_4$**	**PC-Te-C$_2$H$_4$**				
ΔE	−7.50	−16.23	−17.80	−24.64				
ΔG	2.74	−4.76	−7.21	−12.99				
	Transition States **TS-M-C$_2$H$_4$**				Products **Pro-M-C$_2$H$_4$**			
Energy	**TS-O-C$_2$H$_4$**	**TS-S-C$_2$H$_4$**	**TS-Se-C$_2$H$_4$**	**TS-Te-C$_2$H$_4$**	**Pro-O-C$_2$H$_4$**	**Pro-S-C$_2$H$_4$**	**Pro-Se-C$_2$H$_4$**	**Pro-Te-C$_2$H$_4$**
ΔE	−1.18	−9.11	−17.76	−23.70	−56.51	−13.10	−20.92	−24.56
ΔG	11.39	1.80	−4.05	−11.00	−36.91	−3.82	−9.51	−13.09

References

(1) Martin, C. D.; Jennings, M. C.; Ferguson, M. J.; Ragogna, P. J. Dicationic sulfur analogues of N-heterocyclic silylenes and phosphenium cations. *Angew. Chem. Int. Ed.* **2009**, *48*, 2210–2213.

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(3) Dutton, J. L.; Tuononen, H. M.; Jennings, M. C.; Ragogna, P. J. Extending the series: Synthesis and characterization of a dicationic *N*-heterocyclic selenium carbene analogue. *J. Am. Chem. Soc.* **2006**, *128*, 12624–12625.

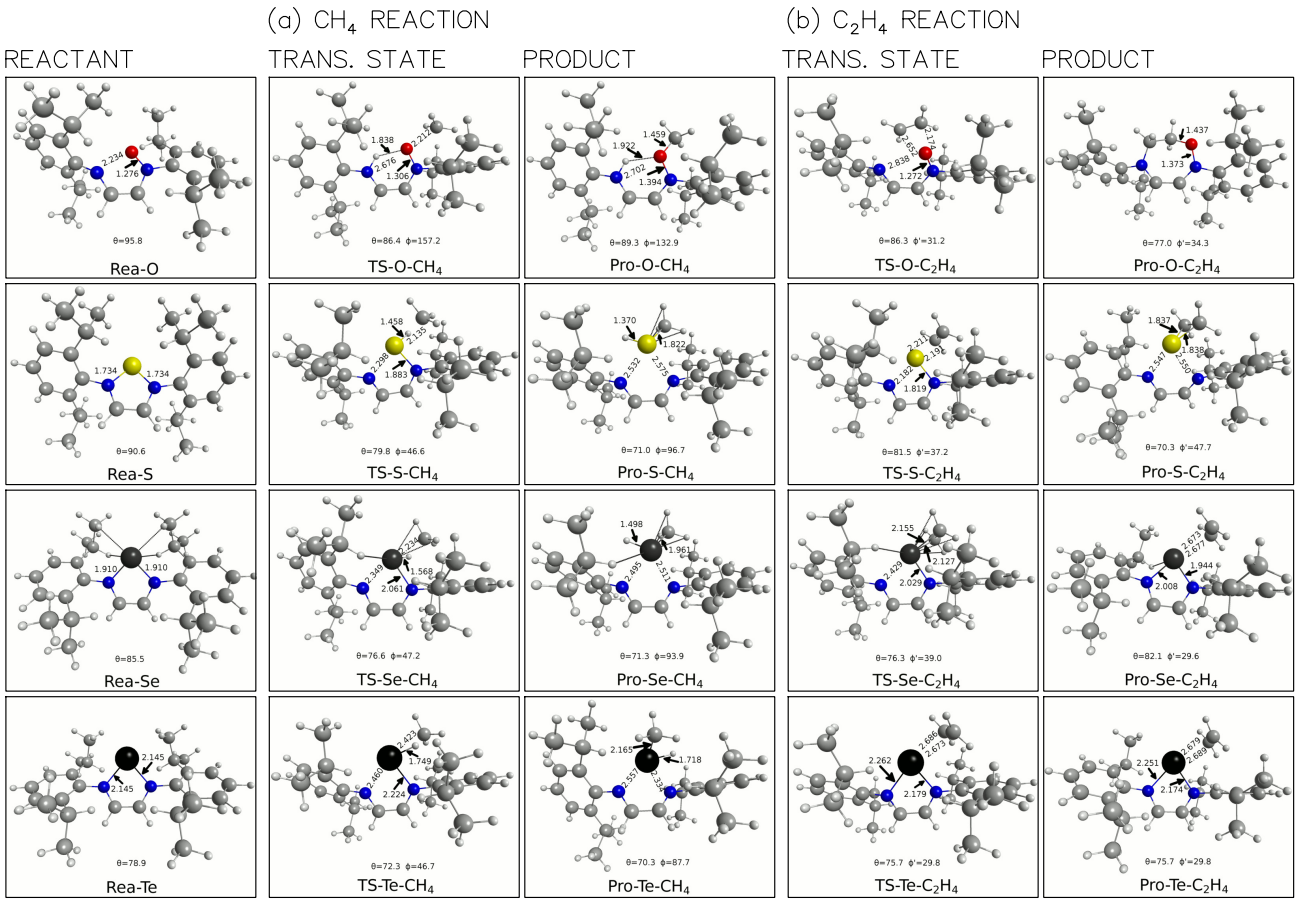

Figure S1: The optimized structures of the reactants, transition states, and products of the $(Dipp_2DAB)M^{+2}$ (M = O, S, Se, and Te) reactions with methane and ethene are plotted. The structures of the reactants **Rea-M** are shown in the first column. The structures of the transition states **TS-M-CH$_4$** and products **Pro-M-CH$_4$** of the reactions with methane are shown in the second and third columns, and the structures of the transition states **TS-M-C$_2$H$_4$** and products **Pro-M-C$_2$H$_4$** of the reactions with ethene are depicted in the fourth and fifth columns, respectively. Important geometric parameters labeled in each subplot include the lengths of the M−N$_1$ and M−N$_2$ bonds and the bond angles N$_1$−M−N$_2$ (θ), the lengths of the M−C and M−H bonds and the bond angles C−M−H (ϕ) for **TS-M-CH$_4$** and and **Pro-M-CH$_4$**, and the lengths of the M−C$_1$ and M−C$_2$ bonds and the bond angles C$_1$−M−C$_2$ (ϕ') for **TS-M-C$_2$H$_4$** and **Pro-M-C$_2$H$_4$**.

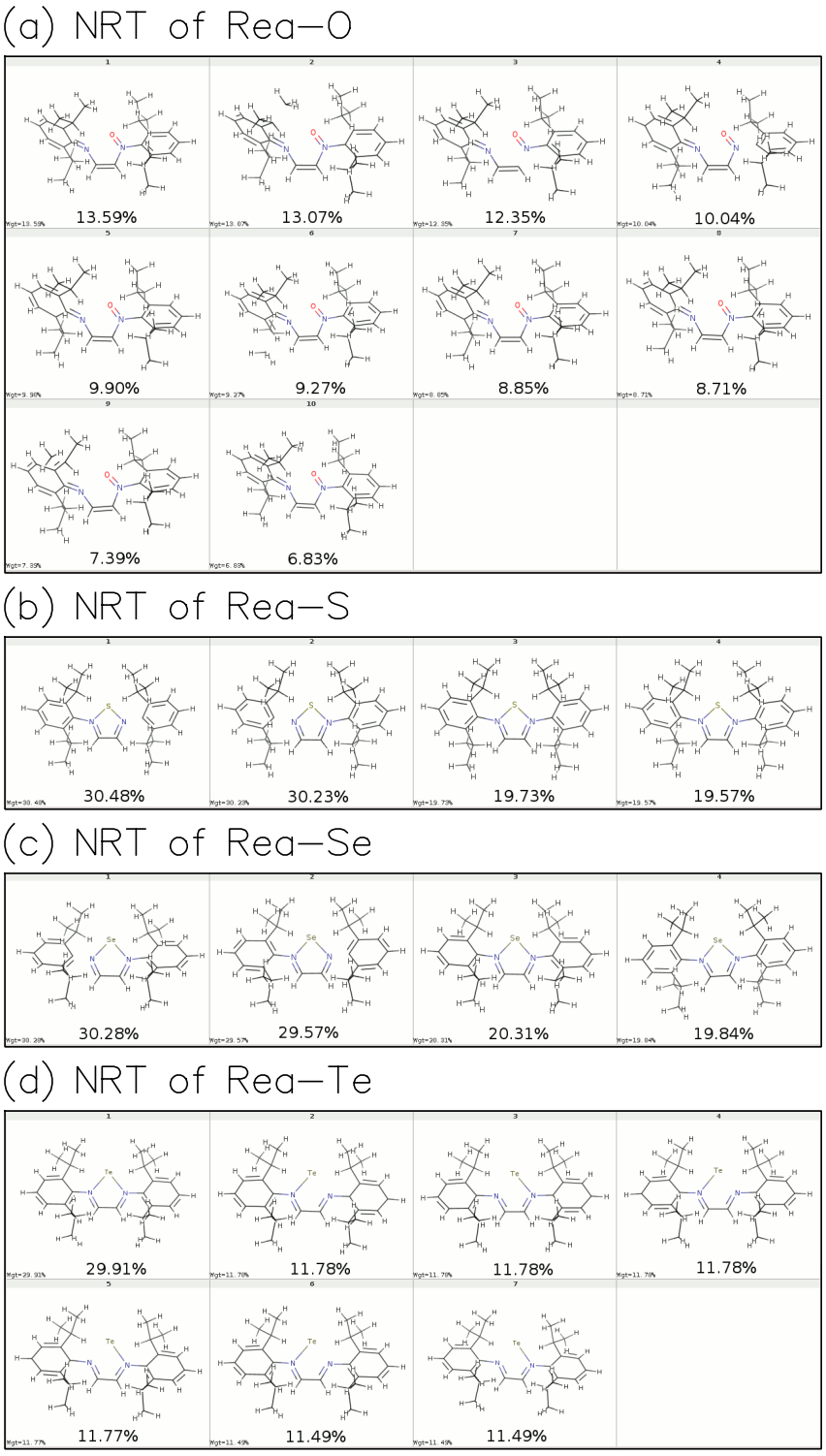

Figure S2: The NRT contributions of the resonance structures of reactants (a) **Rea-O**, (b) **Rea-S**, (c) **Rea-Se**, and (d) **Rea-Te** are illustrated. Only structures with resonance contributions exceeding 1% are shown. The most probable NRT structures of the reactants are employed for the subsequent theoretical computations.

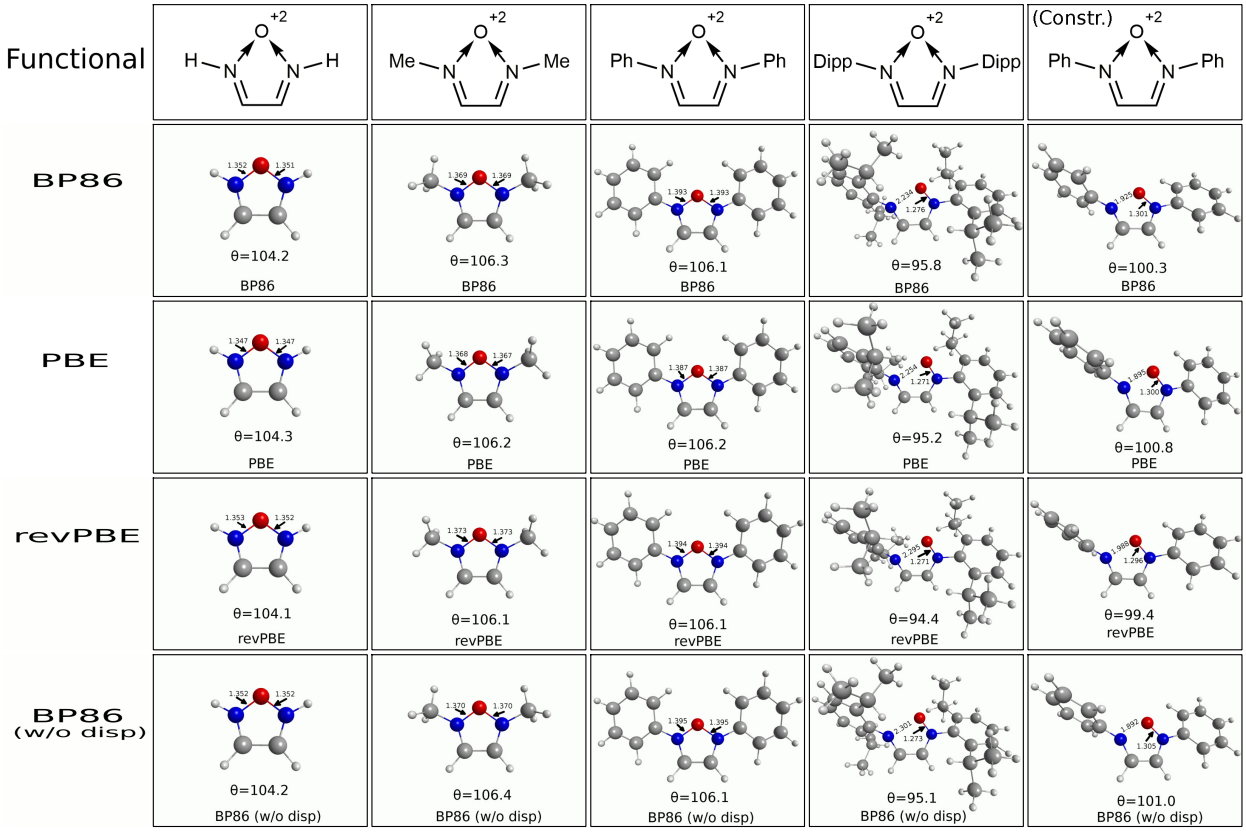

Figure S3: The N-H-, N-Me-, N-Ph-, and N-Dipp-substituted structures of $(R_2DAB)O^{+2}$ (R = H, Me, Ph, and Dipp) fully relaxed and optimized with the density functionals BP86, PBE, revPBE, and BP86 (without Grimme's dispersion correction) are shown in the first four subplots columns of this figure. In addition, the N-Ph-substituted structures $[(Ph_2DAB)O^{+2}]$ with the dihedral angle between the two phenyl planes constrained to the same value as the fully relaxed $(Dipp_2DAB)O^{+2}$ reactant (59.2°) are illustrated in the last subplot column of this figure for comparison. The lengths of bonds N_1-O and N_2-O and the bond angle N_1-O-N_2 (θ) are labeled in each subplot. Atoms N and O are colored in blue and red, respectively. The length differences of the N_1-O and N_2-O bonds for the N-H-, N-Me-, and N-Ph-substituted structures are less than 0.001 Å, but those for the relaxed N-Dipp-substituted and constrained N-Ph-substituted structures are, respectively, close to 0.958 and 0.624 Å, regardless of the density functionals employed in the computations. The comparison supports the reasoning presented in the main text that the enormous N-O bond length differences of $(Dipp_2DAB)O^{+2}$, or the rupture of the five-membered ring, are due to the smallness of the oxygen atom as well as the bulkiness of the substitution ligands.

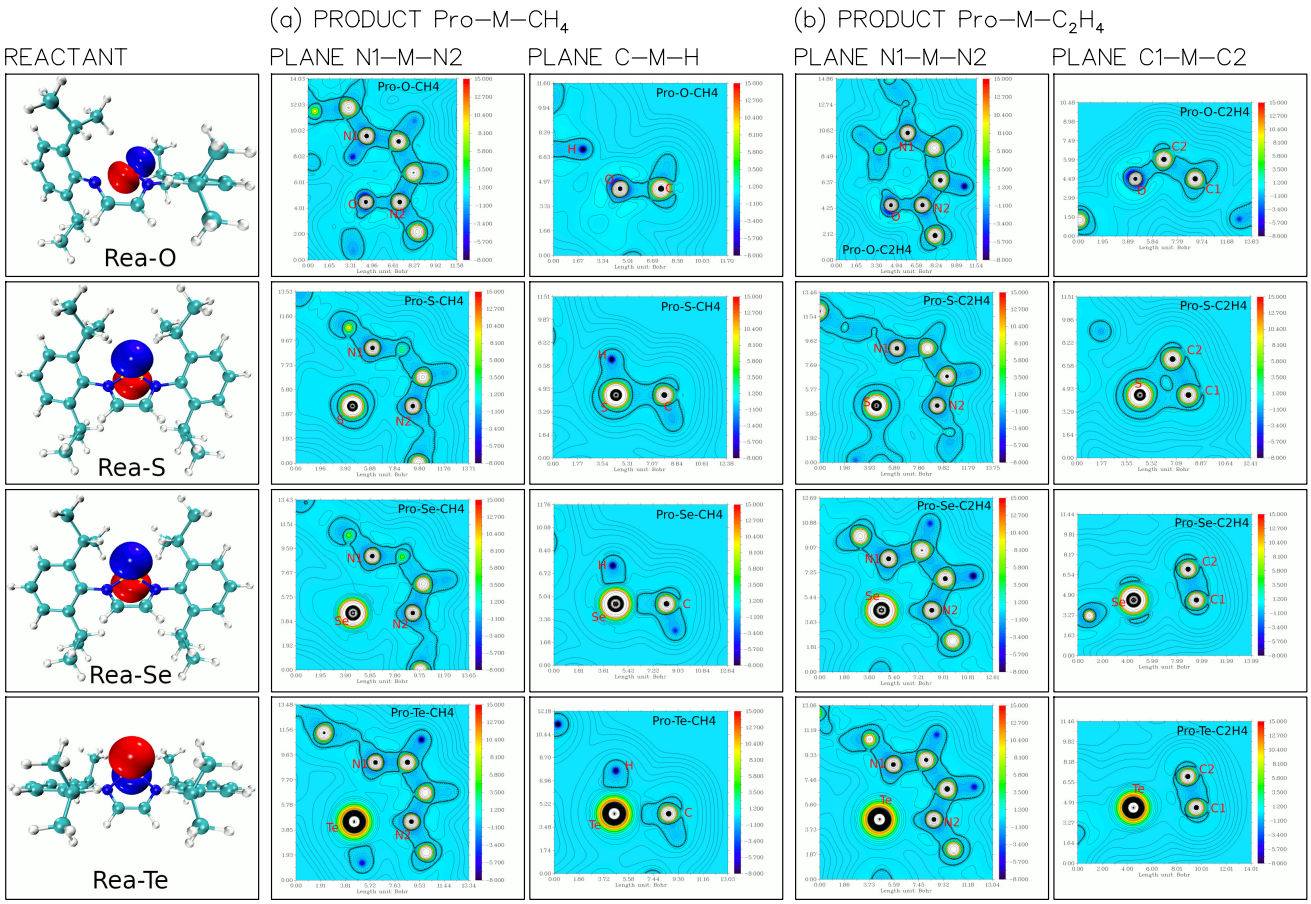

Figure S4: The asymmetric occupied lone-pair orbitals of the central chalcogen atoms of reactants **Rea-M** are plotted in the first column. (There are actually two occupied lone-pair orbitals on the central chalcogen atoms. Only the more asymmetric ones are shown in the subplots.) The Laplacians of the electron densities of (a) the products **Pro-M-CH$_4$** of methane reactions on N1-M-N2 and C-M-H planes are shown in the second and third columns, and (b) the products **Pro-M-C$_2$H$_4$** of the ethene reactions on N1-M-N2 and C1-M-C2 planes are depicted in the fourth and fifth columns, respectively. The solid and dashed contours in the Laplacians plots (a) and (b) are areas of positive and negative Laplacians, and represent regions with depleted and accumulated electron densities, respectively.

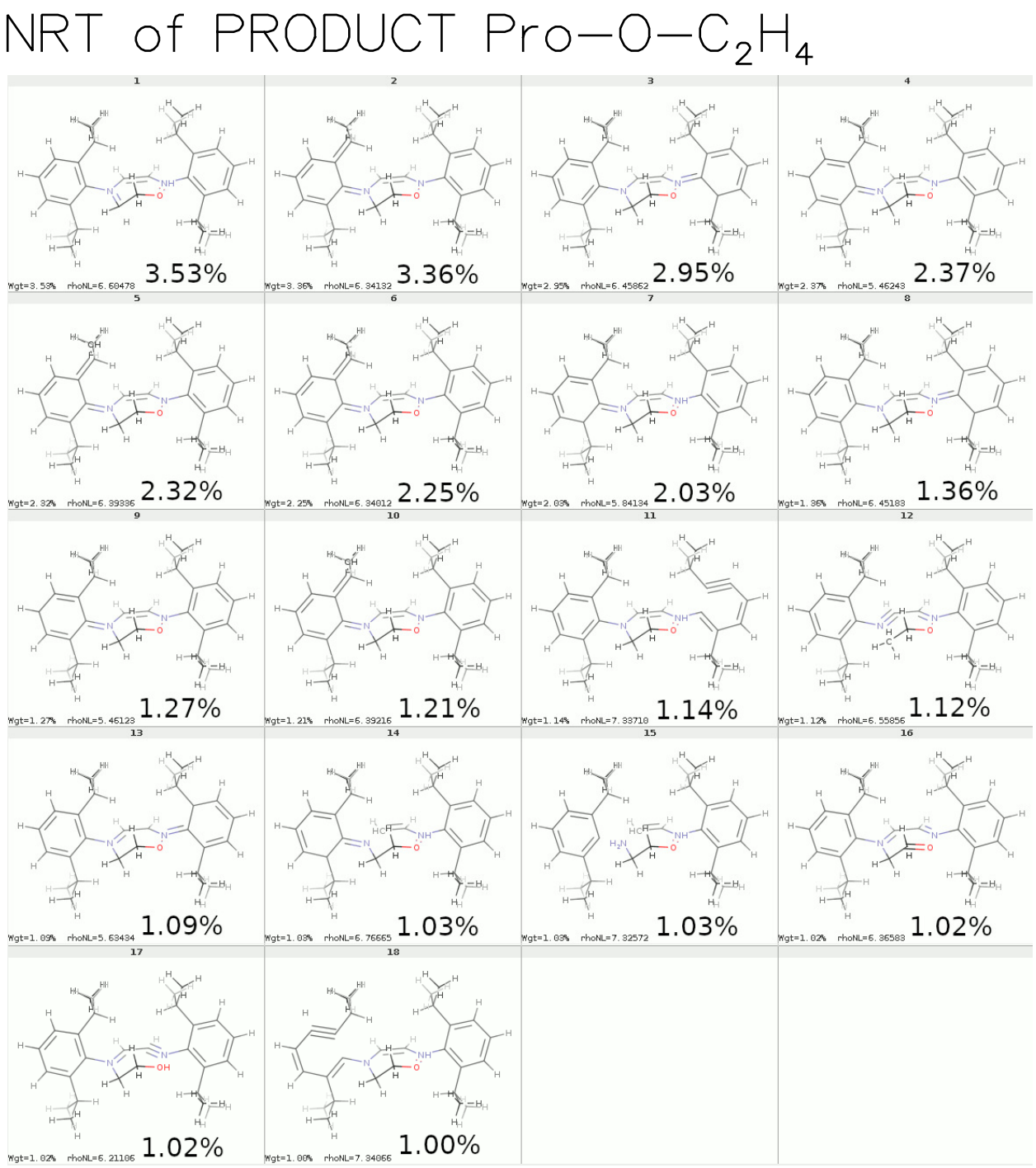

Figure S5: The NRT contributions of the resonance structures of the product **Pro-O-C_2H_4** of the $(Dipp_2DAB)O^{+2}$ reaction with ethene are plotted. Only structures with resonance contributions exceeding 1% are included.

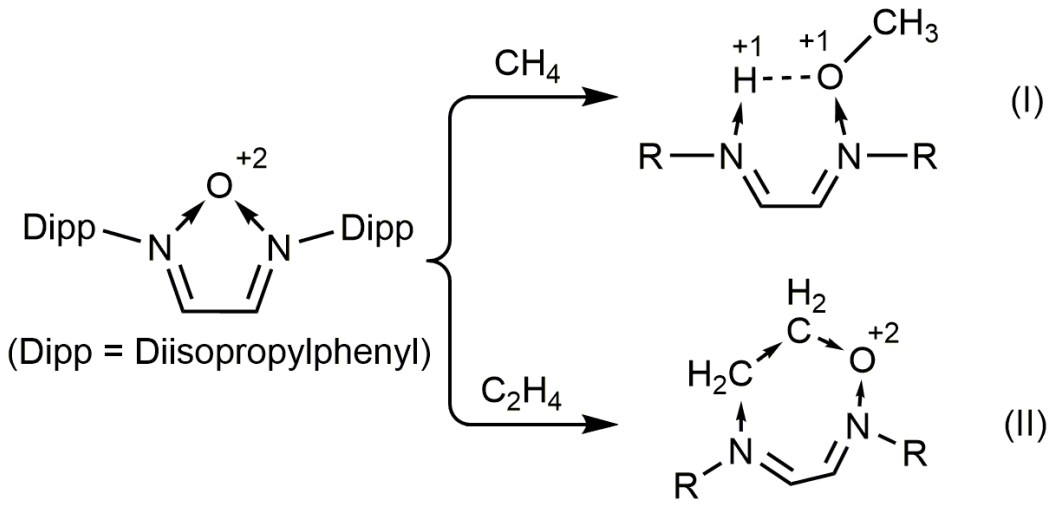

Figure S6: The reactions of the dicationic oxygen NHC analogues, $(Dipp_2DAB)O^{+2}$ with methane (I) and ethene (II) are computed for comparison.

Structure data

The Cartesian coordinates of the atomic positions of the structures of the reactants, precursor states (if available), transition states, and products. The first and second columns of the list are the atomic symbols and atomic numbers, respectively. The last three columns are the (x, y, z) coordinates of the atomic positions in Å.

Reactant **Rea-O**:

ATOM	CHARGE	X	Y	Z
H	1.0	-0.8852053711	-1.6769277288	-2.2665718675
C	6.0	-0.1301137119	-1.6742838601	-1.4726614271
C	6.0	1.2516626860	-1.5798454850	-1.6806577307
H	1.0	1.6490267624	-1.4860576182	-2.7111734215
N	7.0	2.1006047321	-1.5005614167	-0.6774966652
N	7.0	-0.5155250968	-1.8023634861	-0.1633149620
O	8.0	0.4061370957	-1.9531629640	0.7062102243
C	6.0	3.2970422900	-1.8652728344	-0.2867741847
C	6.0	5.8598926173	-2.5240655759	0.5838790012
C	6.0	4.0124966910	-0.9379306077	0.6234988352
C	6.0	3.8787565325	-3.1638238244	-0.7056235156
C	6.0	5.1569671857	-3.4417247995	-0.2411751480
C	6.0	5.3043258027	-1.2948980842	1.0013612638
H	1.0	5.6460675327	-4.3877694946	-0.5176589843
H	1.0	5.8943184659	-0.6265270087	1.6453351545
H	1.0	6.8767545836	-2.7903349467	0.9188650373
C	6.0	-1.8832981408	-1.7859899087	0.2466054440
C	6.0	-4.5903024832	-2.0108988133	0.8144388274
C	6.0	-2.7835258176	-0.8645690326	-0.3877899605
C	6.0	-2.2927069939	-2.7596748475	1.2324018488
C	6.0	-3.6774548553	-2.8599865551	1.4556522563
C	6.0	-4.1428467025	-1.0156159521	-0.0757373695
H	1.0	-4.0459428438	-3.6123431403	2.1680442757
H	1.0	-4.8742517956	-0.3249947688	-0.5221793016
H	1.0	-5.6661918428	-2.1015275448	1.0327818403
C	6.0	3.1428185526	-4.0846600809	-1.6457535555
H	1.0	2.0513013797	-3.9003904913	-1.5201416459
C	6.0	3.3990091231	-5.5770783331	-1.3619918219
H	1.0	4.4440627943	-5.8654128332	-1.5949023639
H	1.0	2.7447904958	-6.1954980731	-2.0081074611
H	1.0	3.1877999092	-5.8372494986	-0.3055703485
C	6.0	3.5249168875	-3.7232373820	-3.1105486378
H	1.0	3.3813942266	-2.6482124622	-3.3492435382
H	1.0	2.9118191741	-4.3218090375	-3.8143432465
H	1.0	4.5931761373	-3.9534597051	-3.2981101748
C	6.0	3.3241423696	0.2962319673	1.1327724109
H	1.0	2.5229989664	0.5522329788	0.4053148311
C	6.0	4.2653662796	1.5012894070	1.3029392437
H	1.0	4.9909941516	1.3471682196	2.1277891841
H	1.0	3.6701426066	2.3988294275	1.5648606200
H	1.0	4.8286362385	1.7215299452	0.3738912259
C	6.0	2.6122996857	-0.0595934115	2.4754486287
H	1.0	3.3557254713	-0.3477220092	3.2462257040
H	1.0	1.8876113532	-0.8878627041	2.3561098355
H	1.0	2.0673680798	0.8363841283	2.8360162214
C	6.0	-1.3499058130	-3.6538168119	2.0127045727
H	1.0	-0.3774567426	-3.6915331350	1.4671920998
C	6.0	-1.0376462293	-2.9955995248	3.3826391437
H	1.0	-0.2990279567	-3.6098378614	3.9363145143
H	1.0	-1.9594479279	-2.9299688028	3.9962869692
H	1.0	-0.6288971366	-1.9726523019	3.2639508325
C	6.0	-1.8600994771	-5.0944668968	2.1734222619
H	1.0	-1.0683212745	-5.7230309194	2.6287139465
H	1.0	-2.1486355709	-5.5469913607	1.2032992901
H	1.0	-2.7340580554	-5.1515660861	2.8556863746
C	6.0	-2.3592905608	0.3186093542	-1.2563498450
H	1.0	-1.2487278553	0.3512395650	-1.3007307887
C	6.0	-2.8003280378	1.6489351466	-0.6055030603
H	1.0	-2.4196268008	1.7409905043	0.4315403929
H	1.0	-3.9050787112	1.7429351818	-0.5749788442
H	1.0	-2.4139091052	2.5038543730	-1.1966956552
C	6.0	-2.8926933053	0.1898290648	-2.6987386467
H	1.0	-2.5852333260	-0.7582158237	-3.1921247175
H	1.0	-2.5325529544	1.0344497666	-3.3200053034
H	1.0	-4.0014322676	0.2125472435	-2.7172726219

Reactant **Rea-S**:

ATOM	CHARGE	X	Y	Z
H	1.0	1.3584646100	-1.5706976810	1.9705092152
C	6.0	0.6989312519	-1.0545232753	1.2577785570
C	6.0	-0.6997113761	-1.0540505976	1.2576653187
H	1.0	-1.3596319968	-1.5691957824	1.9707717791
N	7.0	-1.2325259454	-0.2078153665	0.3438737500
N	7.0	1.2324663206	-0.2088410746	0.3440048215
S	16.0	0.0003946905	0.5558479177	-0.6067450688
C	6.0	-2.6265817790	-0.0197609968	0.0964167752
C	6.0	-5.3473864288	0.2853508439	-0.3533335522
C	6.0	-3.1557926446	1.3115857039	0.0336220992
C	6.0	-3.4194669735	-1.2067280099	-0.0790292984
C	6.0	-4.7910392202	-1.0023280784	-0.3035660591
C	6.0	-4.5365168145	1.4220256496	-0.1877486724
H	1.0	-5.4392961266	-1.8772272339	-0.4621195094
H	1.0	-4.9952469046	2.4211370116	-0.2116931491
H	1.0	-6.4284371218	0.4062366508	-0.5247443728
C	6.0	2.6267958530	-0.0213586159	0.0971973917
C	6.0	5.3478630836	0.2824830915	-0.3510479193
C	6.0	3.1571170644	1.3096448895	0.0381815229
C	6.0	3.4185275936	-1.2085495478	-0.0811758761
C	6.0	4.7903632695	-1.0048323025	-0.3048090959
C	6.0	4.5380040478	1.4194593976	-0.1825548005
H	1.0	5.4378508077	-1.8798811992	-0.4656997726
H	1.0	4.9976393252	2.4182212387	-0.2033790904
H	1.0	6.4290629780	0.4028506337	-0.5218738058
C	6.0	-2.8725143167	-2.6313522856	-0.0913923941
H	1.0	-1.7586795940	-2.5947085903	-0.1097287698
C	6.0	-3.2931239129	-3.3925962900	-1.3657188437
H	1.0	-4.3884325860	-3.5617895040	-1.4027008135
H	1.0	-2.8110642405	-4.3910348078	-1.3854284387
H	1.0	-3.0006300972	-2.8470351517	-2.2853357786
C	6.0	-3.2971533874	-3.3901021081	1.1869335594
H	1.0	-2.9943324989	-2.8694250816	2.1219234691
H	1.0	-2.8579955154	-4.4081291034	1.1993639947
H	1.0	-4.4001480198	-3.4986097790	1.2324833427
C	6.0	-2.3100378980	2.5694964650	0.2062632221
H	1.0	-1.3636926757	2.2899324175	0.7239480580
C	6.0	-2.9893454692	3.6294291090	1.0947483161
H	1.0	-3.8816327552	4.0661955685	0.6020208758
H	1.0	-2.2881182665	4.4655192820	1.2896697516
H	1.0	-3.3038681097	3.2080378103	2.0703973654
C	6.0	-1.9511434054	3.1504144123	-1.1808682459
H	1.0	-2.8635162535	3.4886975931	-1.7136065038
H	1.0	-1.4609911956	2.4054704029	-1.8487931579
H	1.0	-1.2710277975	4.0204362228	-1.0801900158
C	6.0	2.8701084468	-2.6325515769	-0.0971130140
H	1.0	1.7563138033	-2.5948396607	-0.1143392015

C	6.0	3.2890409831	-3.3903493249	-1.3740504647
H	1.0	2.8058851781	-4.3881995258	-1.3966725419
H	1.0	4.3841501936	-3.5605822052	-1.4121714360
H	1.0	2.9966276819	-2.8415867753	-2.2917956921
C	6.0	3.2949833937	-3.3954673033	1.1786545405
H	1.0	2.8543463788	-4.4128855415	1.1886205854
H	1.0	2.9936258249	-2.8769532414	2.1153003104
H	1.0	4.3978561834	-3.5057554865	1.2229167007
C	6.0	2.3120664396	2.5676397734	0.2135375293
H	1.0	1.3655511613	2.2874396801	0.7305580016
C	6.0	1.9536076997	3.1517799967	-1.1723425505
H	1.0	1.4632553903	2.4084588753	-1.8419213098
H	1.0	2.8661775779	3.4908688545	-1.7042215020
H	1.0	1.2737818197	4.0218195194	-1.0698124445
C	6.0	2.9920667937	3.6252709632	1.1042530573
H	1.0	3.3070234383	3.2014099896	2.0786896948
H	1.0	2.2911754557	4.4610711127	1.3016110916
H	1.0	3.8841930737	4.0629728284	0.6120671536

Reactant **Rea-Se**:

ATOM	CHARGE	X	Y	Z
H	1.0	1.3200710698	1.6266533901	1.8837605057
C	6.0	0.7016387595	1.0363534844	1.1911746222
C	6.0	-0.7011938400	1.0364619995	1.1914531448
H	1.0	-1.3192004998	1.6269054817	1.8843093170
N	7.0	-1.2970857203	0.1621758691	0.3574750192
N	7.0	1.2969826769	0.1619519397	0.3568620944
SE	34.0	-0.0000848246	-0.8233391696	-0.6402365258
C	6.0	-2.7077279177	0.0824961419	0.1826695179
C	6.0	-5.4858561613	-0.0077829221	0.0480454965
C	6.0	-3.4233991406	1.3210238906	0.0249356315
C	6.0	-3.3541864980	-1.1999661839	0.2066554990
C	6.0	-4.7541774353	-1.2042668528	0.1590386527
C	6.0	-4.8244320245	1.2257001124	-0.0398457618
H	1.0	-5.2918859960	-2.1612476425	0.2175567106
H	1.0	-5.4136871755	2.1451614566	-0.1763623529
H	1.0	-6.5861200812	-0.0414674418	0.0150168452
C	6.0	2.7076878032	0.0822578728	0.1815478141
C	6.0	5.4857329378	-0.0079942949	0.0462877815
C	6.0	3.4232516515	1.3208066204	0.0236368985
C	6.0	3.3540895649	-1.2001964388	0.2053668622
C	6.0	4.7541000255	-1.2044686813	0.1574392433
C	6.0	4.8242806088	1.2254879607	-0.0414757182
H	1.0	5.2918859172	-2.1614142013	0.2158257078
H	1.0	5.4134683560	2.1449742781	-0.1781351667
H	1.0	6.5859901834	-0.0417124002	0.0130316480
C	6.0	-2.5754290947	-2.5080158550	0.2338941933
H	1.0	-1.6351180825	-2.3452160235	0.8096287121
C	6.0	-2.2015589317	-2.8838387436	-1.2205500489
H	1.0	-3.1054541189	-3.1794011559	-1.7941920897
H	1.0	-1.4735415383	-3.7202153689	-1.2572222867
H	1.0	-1.7827890717	-2.0246721542	-1.8099861407
C	6.0	-3.3053783760	-3.6697210287	0.9290720564
H	1.0	-3.6366635743	-3.3896791935	1.9487589441
H	1.0	-2.6260640581	-4.5410773397	1.0168427668
H	1.0	-4.1906716684	-4.0098361158	0.3538307279
C	6.0	-2.7731324852	2.6908808660	-0.1458151655
H	1.0	-1.6702580154	2.5604290980	-0.2306894914
C	6.0	-3.0465713908	3.5977734656	1.0753910277
H	1.0	-4.1293188665	3.8196279904	1.1677930456
H	1.0	-2.5133163700	4.5636115087	0.9674523508
H	1.0	-2.7365494784	3.1355708462	2.0380567446
C	6.0	-3.2243979319	3.3681374198	-1.4581796556
H	1.0	-4.3007492682	3.6340944832	-1.4348519790
H	1.0	-3.0519409404	2.7164754063	-2.3382774587
H	1.0	-2.6597790033	4.3106565518	-1.6070806883
C	6.0	2.5753251647	-2.5082477851	0.2326543320
H	1.0	1.6353147152	-2.3455946073	0.8089303183
C	6.0	2.2007104110	-2.8836717834	-1.2216899449
H	1.0	1.4725873138	-3.7199632632	-1.2582423461
H	1.0	3.1042905178	-3.1792553725	-1.7958288026
H	1.0	1.7818121713	-2.0243055415	-1.8107678679
C	6.0	3.3056884052	-3.6701408164	0.9270782446
H	1.0	2.6264878851	-4.5415806803	1.0149006542
H	1.0	3.6374676174	-3.3904310876	1.9466948470
H	1.0	4.1907007766	-4.0099635342	0.3512411179
C	6.0	2.7729444525	2.6906649397	-0.1469765682
H	1.0	1.6700378060	2.5602284559	-0.2314260881
C	6.0	3.2237909059	3.3677802125	-1.4595421677
H	1.0	3.0509965386	2.7160471884	-2.3395249888
H	1.0	4.3001682350	3.6336678628	-1.4366178550
H	1.0	2.6591751201	4.3103143546	-1.6083687832
C	6.0	3.0468065774	3.5976679354	1.0740470040
H	1.0	2.7370553268	3.1355972650	2.0368644352
H	1.0	2.5135392038	4.5635079893	0.9661775524
H	1.0	4.1295857984	3.8195065407	1.1661129919

Reactant **Rea-Te**:

ATOM	CHARGE	X	Y	Z
H	1.0	1.2878513893	1.5556623069	1.9581405067
C	6.0	0.7084599426	0.9405617370	1.2516478720
C	6.0	-0.7045849178	0.9431731181	1.2523910481
H	1.0	-1.2808566144	1.5602493305	1.9596941356
N	7.0	-1.3628959801	0.1138782503	0.4324805346
N	7.0	1.3626550845	0.1086624463	0.4311541687
TE	52.0	-0.0028070611	-1.0695216365	-0.7297308568
C	6.0	-2.7758598542	0.1789466302	0.2845672836
C	6.0	-5.5549052399	0.3717827141	0.1763216268
C	6.0	-3.3659688574	1.4786029200	0.1056719970
C	6.0	-3.5535459362	-1.0259454380	0.3355302616
C	6.0	-4.9471127216	-0.8914125240	0.3009499207
C	6.0	-4.7709259836	1.5272436206	0.0563627737
H	1.0	-5.5786818475	-1.7873437350	0.3813780712
H	1.0	-5.2640919080	2.5002340833	-0.0913881666
H	1.0	-6.6530973767	0.4499460984	0.1574782053
C	6.0	2.7758936711	0.1663551873	0.2823105836
C	6.0	5.5558759691	0.3446777337	0.1736058824
C	6.0	3.3727091055	1.4627666227	0.1028163699
C	6.0	3.5473455183	-1.0426251512	0.3331096067
C	6.0	4.9416131382	-0.9153465477	0.2985171754
C	6.0	4.7778982299	1.5041340922	0.0532204198
H	1.0	5.5687011534	-1.8144242262	0.3791980708
H	1.0	5.2761141853	2.4744470993	-0.0952660309
H	1.0	6.6544656181	0.4171430261	0.1546958832
C	6.0	-2.9019502079	-2.4026840760	0.3728675911
H	1.0	-1.9607943000	-2.3262823596	0.9632914136
C	6.0	-2.5467153533	-2.8038333959	-1.0771951817
H	1.0	-3.4637724147	-2.9744637724	-1.6811854816
H	1.0	-1.9149339633	-3.7146863244	-1.1271265423
H	1.0	-2.0372774791	-1.9765580591	-1.6569090739
C	6.0	-3.7518215083	-3.4985803219	1.0367040929
H	1.0	-4.0568774578	-3.2066281767	2.0612074824
H	1.0	-3.1702038192	-4.4392860194	1.1062715666
H	1.0	-4.6659782738	-3.7244267254	0.4509364787
C	6.0	-2.5855600925	2.7718766172	-0.1177871525
H	1.0	-1.4988097989	2.5357801665	-0.1795812992
C	6.0	-2.7817975665	3.7555688230	1.0567916675
H	1.0	-3.8417445331	4.0727891996	1.1361766908
H	1.0	-2.1707492004	4.6685643086	0.9070974625
H	1.0	-2.5079639069	3.3127656187	2.0387066695

C	6.0	-2.9626549635	3.4206116407	-1.4667515498
H	1.0	-4.0199146941	3.7552352884	-1.4795841095
H	1.0	-2.8171582390	2.7206324467	-2.3141193242
H	1.0	-2.3348385151	4.3174968628	-1.6440612207
C	6.0	2.8883239418	-2.4157037422	0.3702043787
H	1.0	1.9478310670	-2.3337839483	0.9609086073
C	6.0	2.5298874762	-2.8141308580	-1.0798243544
H	1.0	1.8919790217	-3.7207169375	-1.1300598361
H	1.0	3.4456658860	-2.9909725838	-1.6840651630
H	1.0	2.0266594034	-1.9829222711	-1.6593421912
C	6.0	3.7321348769	-3.5168206549	1.0330818554
H	1.0	3.1446267349	-4.4537969372	1.1035978071
H	1.0	4.0404180379	-3.2266587006	2.0571137565
H	1.0	4.6439852306	-3.7483491191	0.4459727800
C	6.0	2.5985797658	2.7595680772	-0.1210947835
H	1.0	1.5107175357	2.5285122009	-0.1814843454
C	6.0	2.9772138623	3.4049898068	-1.4712613328
H	1.0	2.8270779581	2.7047794286	-2.3176373962
H	1.0	4.0361596257	3.7342055760	-1.4859330133
H	1.0	2.3535804607	4.3047515150	-1.6485922922
C	6.0	2.8009512645	3.7434776763	1.0522301262
H	1.0	2.5269688285	3.3026543653	2.0350033579
H	1.0	2.1935355824	4.6589224968	0.9028015398
H	1.0	3.8623777249	4.0562450712	1.1295499872

Transition state **TS-O-CH$_4$**:

ATOM	CHARGE	X	Y	Z
O	8.0	-0.7461111727	-0.6296973672	-0.9013148930
N	7.0	-1.2879969054	0.0485251421	0.0747144814
C	6.0	-0.5668357499	0.6882796380	0.9974802277
C	6.0	0.8569479879	0.7413123999	1.0140047007
N	7.0	1.6143408644	0.1502250534	0.0897695699
H	1.0	-1.1348327113	1.1944413534	1.7890053511
H	1.0	1.3373579415	1.2519868064	1.8570978389
C	6.0	2.9930170345	0.0833784684	-0.0976035048
C	6.0	3.4229137190	-1.0061360785	-0.9508379641
C	6.0	4.7967934474	-1.1711540802	-1.1418403337
C	6.0	5.7193110607	-0.2899898768	-0.5452877942
C	6.0	5.2799460698	0.8025651412	0.2227122606
C	6.0	3.9197809674	1.0341982530	0.4697908885
H	1.0	6.0233684388	1.5039095963	0.6275722967
H	1.0	6.7988131975	-0.4461343549	-0.6993281161
H	1.0	5.1674728352	-1.9992580756	-1.7613329008
C	6.0	2.4203923280	-1.9913961770	-1.5440386195
H	1.0	1.5311159722	-1.4110710462	-1.8949962106
C	6.0	1.9454987820	-3.0030581619	-0.4702038615
C	6.0	2.9449740945	-2.7267881578	-2.7889813715
H	1.0	1.1842228842	-3.6874631902	-0.8956963815
H	1.0	2.7997419896	-3.6192980190	-0.1234406060
H	1.0	1.5086268768	-2.5123110910	0.4245763504
H	1.0	3.7546679258	-3.4413083567	-2.5347867817
H	1.0	2.1273834318	-3.3214816704	-3.2431523795
H	1.0	3.3262250087	-2.0248392920	-3.5572661929
C	6.0	3.5026867313	2.2705542665	1.2554332242
H	1.0	2.4754407722	2.5481758497	0.9241490186
C	6.0	4.3859491090	3.4993650061	0.9676387942
C	6.0	3.4728083963	1.9646589722	2.7746581895
H	1.0	3.9462203868	4.3939467503	1.4527121480
H	1.0	5.4089023157	3.3846849352	1.3798792689
H	1.0	4.4672785350	3.7023377613	-0.1190788590
H	1.0	4.5008792929	1.7618803290	3.1377807257
H	1.0	2.8732556699	1.0662488719	3.0383489386
H	1.0	3.0755272825	2.8319692278	3.3402061204
C	6.0	-2.7389688460	0.0122836054	0.0805248762
C	6.0	-3.3583334638	-1.0970207475	0.7538228197
C	6.0	-4.7587007029	-1.1438510209	0.6747447104
C	6.0	-5.4823009484	-0.1200407304	0.0324290835
C	6.0	-4.8357628092	0.9904718785	-0.5481765410
C	6.0	-3.4386579969	1.1160720173	-0.5120198982
H	1.0	-5.4374551708	1.7751858875	-1.0306068619
H	1.0	-6.5818770889	-0.1807752857	-0.0046152982
H	1.0	-5.2990454435	-1.9843965594	1.1349454224
C	6.0	-2.7144495539	2.3244076157	-1.0831508494
H	1.0	-1.6560248957	2.0313162998	-1.2584216939
C	6.0	-3.2987418131	2.7850699274	-2.4317053792
C	6.0	-2.7270660513	3.4731042266	-0.0454951536
H	1.0	-2.6720330485	3.5945940024	-2.8565608608
H	1.0	-4.3221625516	3.1976219944	-2.3198470389
H	1.0	-3.3405327961	1.9610075995	-3.1731160048
H	1.0	-2.1598248843	4.3436800927	-0.4324503162
H	1.0	-2.2783676284	3.1726820551	0.9237377421
H	1.0	-3.7654304474	3.8062371745	0.1578115496
C	6.0	-2.5481244338	-2.1331170738	1.5136971601
H	1.0	-1.5070506100	-2.0990022697	1.1259089245
C	6.0	-3.0743980663	-3.5665834398	1.3161909361
C	6.0	-2.5117366783	-1.7513784450	3.0151602544
H	1.0	-3.1569226073	-3.8369703085	0.2434711679
H	1.0	-4.0696703389	-3.7083806899	1.7839757582
H	1.0	-2.3868518002	-4.2892792113	1.7990678807
H	1.0	-2.0952845135	-0.7368563572	3.1834428229
H	1.0	-1.8878706098	-2.4757777639	3.5767565241
H	1.0	-3.5324762486	-1.7705035684	3.4482714164
C	6.0	-2.5733186551	-1.2285897495	-1.9954658525
H	1.0	1.0533159674	-0.3956936606	-0.6065746679
H	1.0	-2.1306816645	-0.5829430873	-2.7669442314
H	1.0	-2.1280491942	-2.2224191721	-1.8481676703
H	1.0	-3.6548380859	-1.1315789061	-1.8163665569

Transition state **TS-S-CH$_4$**:

ATOM	CHARGE	X	Y	Z
S	16.0	0.1405445893	-0.2345239330	1.1876254607
N	7.0	1.2423229538	0.3702332108	-0.2142026790
C	6.0	0.6048844479	0.8107563519	-1.2880202050
C	6.0	-0.8197365538	0.8034060619	-1.3865012704
N	7.0	-1.4379735660	0.1227003132	-0.4436628490
H	1.0	1.2388839060	1.1729379850	-2.1140274100
H	1.0	-1.3149629696	1.2411357557	-2.2689504516
C	6.0	-2.7622565081	-0.0040269742	-0.1291604793
C	6.0	-3.1413305907	-1.2351874068	0.5458999599
C	6.0	-4.4413831375	-1.3347698772	1.0461168526
C	6.0	-5.3553408212	-0.2741456494	0.8957249850
C	6.0	-4.9897701660	0.9095622025	0.2256326171
C	6.0	-3.7164223974	1.0822558111	-0.3283793158
H	1.0	-5.7272416863	1.7198835007	0.1337673063
H	1.0	-6.3782411725	-0.3769302143	1.2921627810
H	1.0	-4.7692691425	-2.2619951249	1.5401159587
C	6.0	-2.2159472445	-2.4420985751	0.5879871147
H	1.0	-1.2462486007	-2.1433434218	0.1335963206
C	6.0	-2.7802203582	-3.5779549132	-0.3000653336
C	6.0	-1.9540101002	-2.9231045932	2.0276847954
H	1.0	-2.0726670199	-4.4317317105	-0.3183769359
H	1.0	-3.7479082831	-3.9492491050	0.0942628727
H	1.0	-2.9442907786	-3.2376829338	-1.3422170654
H	1.0	-2.8802029343	-3.2849592344	2.5192390149
H	1.0	-1.2340858999	-3.7669531992	2.0277160540
H	1.0	-1.5447946216	-2.1087739114	2.6646300601
C	6.0	-3.3706256662	2.3699847707	-1.0522512810
H	1.0	-2.2776543496	2.5515151824	-0.9201032900
C	6.0	-4.0862441821	3.6120968756	-0.4916198492
C	6.0	-3.6512295384	2.2095080922	-2.5690072371

H	1.0	-3.6807853072	4.5244906560	-0.9730985429
H	1.0	-5.1747101977	3.5992648411	-0.7044816042
H	1.0	-3.9458685917	3.7093558973	0.6037416139
H	1.0	-4.7409337258	2.0986964755	-2.7434290030
H	1.0	-3.1719923021	1.3105738198	-3.0129938058
H	1.0	-3.3061904641	3.1055031677	-3.1241951326
C	6.0	2.6514481529	0.1501969354	-0.1629341303
C	6.0	3.1555189815	-1.0720347025	-0.6952969324
C	6.0	4.5490444865	-1.2526573656	-0.6265436292
C	6.0	5.3777157274	-0.2819705929	-0.0374491913
C	6.0	4.8382995358	0.8959205268	0.5094473252
C	6.0	3.4546430899	1.1396994621	0.4739173337
H	1.0	5.5092979809	1.6369604208	0.9685025799
H	1.0	6.4655151636	-0.4493865352	0.0023253831
H	1.0	4.9969963192	-2.1703879594	-1.0361968445
C	6.0	2.8455525442	2.4249426357	1.0214935193
H	1.0	1.7715928850	2.2201756737	1.2602762879
C	6.0	3.5233166969	2.9193757027	2.3112617231
C	6.0	2.8508421117	3.5217149975	-0.0690425110
H	1.0	2.9670293979	3.7814666223	2.7303006297
H	1.0	4.5588998368	3.2671628413	2.1210380116
H	1.0	3.5761414972	2.1325120519	3.0936617971
H	1.0	2.3637039178	4.4456884101	0.3024566857
H	1.0	2.3231385138	3.1996926172	-0.9909617884
H	1.0	3.8921750924	3.7733997281	-0.3570076598
C	6.0	2.2395612896	-2.1172387591	-1.3220720618
H	1.0	1.2029194719	-1.9231376249	-0.9617630274
C	6.0	2.6034043848	-3.5530874675	-0.8995666002
C	6.0	2.2297594960	-1.9684632140	-2.8601041854
H	1.0	2.6378332030	-3.6662789514	0.2039868032
H	1.0	3.5882085239	-3.8655523613	-1.3022365178
H	1.0	1.8525823401	-4.2675637021	-1.2930095338
H	1.0	1.9225492984	-0.9517576552	-3.1836976442
H	1.0	1.5337132970	-2.7007994511	-3.3171534750
H	1.0	3.2411686354	-2.1511369417	-3.2786393758
C	6.0	1.7880841310	-0.7516255503	2.4431425418
H	1.0	1.0127965719	0.5381449953	2.0645799795
H	1.0	2.3305835679	-1.4615412193	1.7954374861
H	1.0	2.4645977540	0.0403445558	2.8291975944
H	1.0	1.1717967940	-1.2227144096	3.2321939159

Transition state **TS-Se-CH$_4$**:

ATOM	CHARGE	X	Y	Z
SE	34.0	-0.0733357450	-0.3020500443	-1.2137304824
N	7.0	-1.2677626655	0.3759033804	0.3233060502
C	6.0	-0.6103953119	0.7779814132	1.3901812171
C	6.0	0.8235221476	0.7734775965	1.4679088044
N	7.0	1.4545961805	0.1188507136	0.5196436504
H	1.0	-1.2146495887	1.1225091629	2.2466238492
H	1.0	1.3204913494	1.2029427943	2.3537857432
C	6.0	2.7924914550	0.0324029949	0.2184653035
C	6.0	3.2225106054	-1.2006627818	-0.4149938728
C	6.0	4.5299965772	-1.2655850477	-0.9032079298
C	6.0	5.3992230543	-0.1647260678	-0.7823157110
C	6.0	4.9803033971	1.0230709033	-0.1529832428
C	6.0	3.6960644197	1.1608372839	0.3886795797
H	1.0	5.6822530002	1.8664077909	-0.0820998033
H	1.0	6.4282937369	-0.2385556133	-1.1687418569
H	1.0	4.8979813621	-2.1953085814	-1.3631801793
C	6.0	2.3479791904	-2.4465451734	-0.4121945110
H	1.0	1.3497294181	-2.1625969386	-0.0093311602
C	6.0	2.9214413392	-3.4904290614	0.5779260636
C	6.0	2.1620132076	-3.0417879748	-1.8194722091
H	1.0	2.2561675063	-4.3763466160	0.6240194342
H	1.0	3.9244952078	-3.8352793607	0.2535165195
H	1.0	3.0202611946	-3.0728187391	1.6001669895
H	1.0	3.1210755129	-3.3979604181	-2.2478747549
H	1.0	1.4783242334	-3.9143965384	-1.7829492675
H	1.0	1.7445488486	-2.2984611192	-2.5339768181
C	6.0	3.2929615152	2.4543789435	1.0723978046
H	1.0	2.1901231105	2.5745367931	0.9489306705
C	6.0	3.9391032918	3.7095894205	0.4594010897
C	6.0	3.5948153191	2.3618396799	2.5900668921
H	1.0	3.4975026411	4.6177643993	0.9164327433
H	1.0	5.0296933506	3.7552467255	0.6557729765
H	1.0	3.7802409993	3.7625768008	-0.6365441263
H	1.0	4.6898532784	2.3092561545	2.7587201589
H	1.0	3.1625175329	1.4564076146	3.0679200129
H	1.0	3.2101529054	3.2581181600	3.1179515875
C	6.0	-2.6694323948	0.1675174097	0.2698178370
C	6.0	-3.1914677343	-1.0454225777	0.8132753819
C	6.0	-4.5852466594	-1.2151291757	0.7356774383
C	6.0	-5.4021290933	-0.2461937141	0.1274860984
C	6.0	-4.8485274911	0.9189229232	-0.4335638267
C	6.0	-3.4641310039	1.1512612095	-0.3923597313
H	1.0	-5.5103473300	1.6586136545	-0.9075246548
H	1.0	-6.4910069583	-0.4052541415	0.0826484050
H	1.0	-5.0436401353	-2.1241933122	1.1528927253
C	6.0	-2.8386797500	2.4221388075	-0.9529396939
H	1.0	-1.7782107314	2.1853821719	-1.2194977475
C	6.0	-3.5348240410	2.9370333342	-2.2244102343
C	6.0	-2.7860671631	3.5168590064	0.1385320304
H	1.0	-2.9659862742	3.7849763646	-2.6554036103
H	1.0	-4.5555632886	3.3128263904	-2.0084371993
H	1.0	-3.6257906437	2.1527659548	-3.0054286097
H	1.0	-2.2858419065	4.4283495901	-0.2463409193
H	1.0	-2.2413103116	3.1816375080	1.0458237954
H	1.0	-3.8123161102	3.7948670195	0.4547818819
C	6.0	-2.2930775076	-2.0963217474	1.4556450259
H	1.0	-1.2521243245	-1.9260834659	1.0946710135
C	6.0	-2.6783966799	-3.5317026900	1.0506419706
C	6.0	-2.2833593985	-1.9301658572	2.9921286639
H	1.0	-2.7140956163	-3.6574213046	-0.0516078216
H	1.0	-3.6674353184	-3.8266911080	1.4562523867
H	1.0	-1.9378604706	-4.2521572028	1.4525409973
H	1.0	-1.9538807939	-0.9174394947	3.3061121759
H	1.0	-1.6054731680	-2.6731744942	3.4590295840
H	1.0	-3.2997365483	-2.0848169942	3.4096633225
C	6.0	-1.8927941935	-0.8339859944	-2.3952738444
H	1.0	-1.0624253626	0.5453064576	-2.0876341920
H	1.0	-2.3987713226	-1.5338537472	-1.7074970039
H	1.0	-2.5834922931	-0.0410519474	-2.7456110355
H	1.0	-1.3462640311	-1.3230626127	-3.2247705228

Transition state **TS-Te-CH$_4$**:

ATOM	CHARGE	X	Y	Z
TE	52.0	-0.0773184981	-0.7866927671	-1.0843899657
N	7.0	-1.2676306328	0.2324678996	0.4939216784
C	6.0	-0.5890806752	0.7144361754	1.5067298545
C	6.0	0.8543161420	0.7233733922	1.5415409262
N	7.0	1.4969736999	0.0795531794	0.5954123226
H	1.0	-1.1606612123	1.1378047069	2.3510085672
H	1.0	1.3660277953	1.2007968148	2.3943719465
C	6.0	2.8504087091	0.1306174571	0.3012884468
C	6.0	3.4647111878	-1.0732132265	-0.2142866314
C	6.0	4.7888153009	-0.9982207386	-0.6578624015
C	6.0	5.4978307453	0.2163286841	-0.6134992977
C	6.0	4.8914392001	1.3824892639	-0.1160637528
C	6.0	3.5777257575	1.3871253438	0.3747633381
H	1.0	5.4661367766	2.3205085675	-0.1117104246

H	1.0	6.5429866222	0.2531623604	-0.9596194055
H	1.0	5.2945401458	-1.9056220527	-1.0214354821
C	6.0	2.7732079504	-2.4268360531	-0.1404101726
H	1.0	1.7259804697	-2.2549101804	0.1992171338
C	6.0	3.4268517108	-3.3035280091	0.9537186022
C	6.0	2.7290498852	-3.1474424234	-1.5010433856
H	1.0	2.8734190053	-4.2578789684	1.0653032071
H	1.0	4.4755481137	-3.5487365027	0.6868128971
H	1.0	3.4381760874	-2.7885865060	1.9353957615
H	1.0	3.7424891590	-3.4425303072	-1.8425921373
H	1.0	2.1273275083	-4.0760144455	-1.4265039834
H	1.0	2.2966025102	-2.5087743776	-2.3032346342
C	6.0	2.9845093246	2.6894832220	0.8889479998
H	1.0	1.8723198573	2.6117147027	0.8396282056
C	6.0	3.3697903693	3.9132065117	0.0366777662
C	6.0	3.3703581985	2.9005294233	2.3740676216
H	1.0	2.8032904942	4.8025165804	0.3793665012
H	1.0	4.4450731334	4.1670925283	0.1326645463
H	1.0	3.1478949722	3.7533588516	-1.0378439218
H	1.0	4.4686904008	3.0213828636	2.4707323251
H	1.0	3.0904656848	2.0422985511	3.0226221708
H	1.0	2.8884091874	3.8154986642	2.7744672866
C	6.0	-2.6905633708	0.2486702353	0.3979333825
C	6.0	-3.4294965103	-0.8799522329	0.8488880208
C	6.0	-4.8273536528	-0.8181170539	0.6916584816
C	6.0	-5.4446846606	0.2991907045	0.1060826006
C	6.0	-4.6798782725	1.3897754692	-0.3431100049
C	6.0	-3.2798987067	1.3918461740	-0.2222529005
H	1.0	-5.1859930036	2.2549653092	-0.7962418911
H	1.0	-6.5402630470	0.3214066870	-0.0025464810
H	1.0	-5.4481616133	-1.6579368342	1.0403300245
C	6.0	-2.4327359994	2.5783119231	-0.6716114277
H	1.0	-1.4119740930	2.1956294773	-0.9130805309
C	6.0	-2.9723124396	3.2695955114	-1.9371647835
C	6.0	-2.2777944054	3.5958308519	0.4819144886
H	1.0	-2.2581066725	4.0449068050	-2.2795925540
H	1.0	-3.9365485336	3.7828325138	-1.7466460033
H	1.0	-3.1306616965	2.5567245507	-2.7735070023
H	1.0	-1.6414522134	4.4483498248	0.1684584839
H	1.0	-1.8256072920	3.1464260829	1.3910513129
H	1.0	-3.2673062421	3.9982619914	0.7811531865
C	6.0	-2.7678304326	-2.1137936022	1.4534082442
H	1.0	-1.6785643619	-1.9122272503	1.5586164096
C	6.0	-2.9233400490	-3.3281903949	0.5152022531
C	6.0	-3.3080119672	-2.4188587490	2.8661966768
H	1.0	-2.4988767783	-3.1310091495	-0.5005438242
H	1.0	-3.9888759019	-3.5969033744	0.3642626453
H	1.0	-2.3986035845	-4.2167499183	0.9209479285
H	1.0	-3.1989979277	-1.5451577409	3.5399953233
H	1.0	-2.7595606747	-3.2729524499	3.3124481198
H	1.0	-4.3827111932	-2.6920245065	2.8410857889
C	6.0	-2.0545528991	-0.5984160282	-2.4727880043
H	1.0	-1.5547449015	-1.7162225597	-1.2007907386
H	1.0	-1.6364583780	-1.0786386488	-3.3791789641
H	1.0	-2.9934400442	-1.0714030984	-2.1285385738
H	1.0	-2.1566997552	0.4976325873	-2.5502353103

Product **Pro-O-CH$_4$**:

ATOM	CHARGE	X	Y	Z
O	8.0	-0.7654266548	-0.8970969332	-0.7940829807
N	7.0	-1.3933019837	-0.0871566907	0.1508305203
C	6.0	-0.5788792943	0.5723764501	0.9677002471
C	6.0	0.8405482660	0.6718024823	0.9201066900
N	7.0	1.6284519478	0.0198899942	0.0594202770
H	1.0	-1.1007074942	1.1078562447	1.7742695675
H	1.0	1.3134906513	1.2824236018	1.6986718582
C	6.0	2.9996605096	0.0469476011	-0.1494946735
C	6.0	3.5165613944	-1.1153897078	-0.8517665281
C	6.0	4.8929658945	-1.1711821782	-1.0741386842
C	6.0	5.7354784687	-0.1230928350	-0.6505266084
C	6.0	5.2094442644	1.0249477140	-0.0288774453
C	6.0	3.8421017795	1.1577669015	0.2422717664
H	1.0	5.8890201695	1.8470157528	0.2370990609
H	1.0	6.8210039347	-0.1956442605	-0.8244144995
H	1.0	5.3316343277	-2.0433333878	-1.5781607492
C	6.0	2.6070886899	-2.2767542419	-1.2367044997
H	1.0	1.6447768422	-1.8501743472	-1.6215262275
C	6.0	2.2838197105	-3.1466293291	0.0044936103
C	6.0	3.1633109668	-3.1366797650	-2.3836538169
H	1.0	1.6002669458	-3.9742309553	-0.2717812930
H	1.0	3.2144022434	-3.5954368620	0.4071254639
H	1.0	1.8137526296	-2.5670154869	0.8263820654
H	1.0	4.0568530631	-3.7113137555	-2.0651161226
H	1.0	2.4042253227	-3.8806652285	-2.6976446853
H	1.0	3.4350692887	-2.5265674735	-3.2682437429
C	6.0	3.3205370225	2.4464925841	0.8603888791
H	1.0	2.2625156004	2.5734813638	0.5318930121
C	6.0	4.0695086041	3.7016805096	0.3745392531
C	6.0	3.3499182801	2.3578482493	2.4083571245
H	1.0	3.5473458903	4.6084889059	0.7404118578
H	1.0	5.1042372555	3.7513540993	0.7701785219
H	1.0	4.1141951708	3.7530981092	-0.7317652107
H	1.0	4.3995664905	2.3249022448	2.7656474649
H	1.0	2.8618110849	1.4463334907	2.8174121377
H	1.0	2.8661550145	3.2490503616	2.8573824548
C	6.0	-2.8167467764	0.0243510842	0.1778225131
C	6.0	-3.5648051521	-1.1217566746	0.5862974356
C	6.0	-4.9597968808	-0.9731580775	0.6097797350
C	6.0	-5.5686024427	0.2419356927	0.2433646887
C	6.0	-4.7973939814	1.3448762025	-0.1550537387
C	6.0	-3.3931848108	1.2751876032	-0.2055455743
H	1.0	-5.3007019369	2.2784982453	-0.4491560509
H	1.0	-6.6660434070	0.3294902278	0.2733096275
H	1.0	-5.5868351203	-1.8127953491	0.9449371377
C	6.0	-2.5774690459	2.4723929657	-0.6808975492
H	1.0	-1.5232082128	2.1474891048	-0.8241245140
C	6.0	-3.0719036429	2.9940629027	-2.0463245148
C	6.0	-2.5852159795	3.5912351251	0.3847604520
H	1.0	-2.4041911540	3.8016921717	-2.4083552749
H	1.0	-4.0928672724	3.4208469188	-1.9760481152
H	1.0	-3.0929836157	2.1931986207	-2.8138597262
H	1.0	-1.9631241802	4.4471753633	0.0521617952
H	1.0	-2.1993954449	3.2425491327	1.3659000578
H	1.0	-3.6135338042	3.9707259794	0.5549145341
C	6.0	-2.8902575512	-2.3810562552	1.1193035716
H	1.0	-1.8489691822	-2.4115439521	0.7314787831
C	6.0	-3.5918169612	-3.6747212064	0.6664827785
C	6.0	-2.8047382125	-2.2954001054	2.6623572151
H	1.0	-3.7022118368	-3.7282697525	-0.4367074774
H	1.0	-4.6025405964	-3.7728404420	1.1118433049
H	1.0	-3.0080625164	-4.5577713291	0.9951116895
H	1.0	-2.2610798167	-1.3881678305	3.0002626289
H	1.0	-2.2811915220	-3.1836251082	3.0708520499
H	1.0	-3.8196203748	-2.2607968290	3.1083271750
C	6.0	-1.5779036822	-1.2747504971	-1.9461873179
H	1.0	1.1262615787	-0.6595597822	-0.5470115516
H	1.0	-2.0206796259	-0.3763226280	-2.4179806587
H	1.0	-0.8443456387	-1.7545943542	-2.6196337681
H	1.0	-2.3596569916	-1.9984171614	-1.6509896965

Product **Pro-S-CH$_4$**:

ATOM	CHARGE	X	Y	Z

S	16.0	0.0460408230	0.5514203330	1.5454803472
N	7.0	1.5053816508	0.2254239730	-0.4972299491
C	6.0	0.7503746645	0.0016702846	-1.5244662718
C	6.0	-0.7106113624	0.0399961540	-1.4891729025
N	7.0	-1.4322498054	-0.1698875219	-0.4360914750
H	1.0	1.2004752235	-0.1296356186	-2.5284480047
H	1.0	-1.2089207604	0.1370868095	-2.4743955392
C	6.0	-2.7446149293	0.0443942625	-0.1663335869
C	6.0	-3.4527307456	-1.0417968229	0.4941458522
C	6.0	-4.7773484350	-0.8144609826	0.8686291271
C	6.0	-5.3825043205	0.4400408725	0.6374045742
C	6.0	-4.6826515380	1.4897669369	0.0046766395
C	6.0	-3.3606906883	1.3357749027	-0.4266188535
H	1.0	-5.1905021118	2.4521080210	-0.1582817379
H	1.0	-6.4255945195	0.6029435150	0.9529947729
H	1.0	-5.3597130945	-1.6167082271	1.3444877993
C	6.0	-2.7790280512	-2.3929935238	0.6232297810
H	1.0	-1.6879249440	-2.1940497384	0.7317868789
C	6.0	-2.9592182138	-3.1848963880	-0.6988567201
C	6.0	-3.2628560541	-3.2110036966	1.8297505958
H	1.0	-2.4206891640	-4.1520585122	-0.6334476607
H	1.0	-4.0312223739	-3.4010436521	-0.8830555515
H	1.0	-2.5701420590	-2.6289138808	-1.5766589454
H	1.0	-4.3112253223	-3.5510982043	1.7023450229
H	1.0	-2.6455436540	-4.1244811439	1.9447759393
H	1.0	-3.2062451449	-2.6361569439	2.7769649270
C	6.0	-2.6347321447	2.4588405732	-1.1413774931
H	1.0	-1.5423960024	2.2450775220	-1.1122240229
C	6.0	-2.8402358782	3.8309066985	-0.4712946497
C	6.0	-3.0674745122	2.4844841973	-2.6302153290
H	1.0	-2.2125532194	4.5930739382	-0.9751272342
H	1.0	-3.8907793512	4.1782923140	-0.5490868862
H	1.0	-2.5628993106	3.8094244656	0.6022071534
H	1.0	-4.1466414111	2.7249974138	-2.7176175246
H	1.0	-2.9089255781	1.5091998109	-3.1372389366
H	1.0	-2.4974125308	3.2601643950	-3.1809693049
C	6.0	2.8004233472	-0.0657153096	-0.2193176061
C	6.0	3.3616225376	-1.3681353513	-0.5618251187
C	6.0	4.6539431304	-1.6293120631	-0.0976633206
C	6.0	5.3845785207	-0.6736948785	0.6403753492
C	6.0	4.8389586030	0.5889619773	0.9500279401
C	6.0	3.5441239190	0.9230660347	0.5477211007
H	1.0	5.4465958230	1.3186149125	1.5055476990
H	1.0	6.4054072782	-0.9201593237	0.9745579408
H	1.0	5.1188035921	-2.6022453998	-0.3176453907
C	6.0	2.9783371722	2.3155138885	0.7465833423
H	1.0	1.8769492528	2.2513506308	0.5968873824
C	6.0	3.2391375569	2.8908602837	2.1487988748
C	6.0	3.5295369307	3.2445249254	-0.3653624962
H	1.0	2.7216020918	3.8649451580	2.2583709800
H	1.0	4.3174215650	3.0785284671	2.3291792387
H	1.0	2.8715566823	2.2148301386	2.9486216524
H	1.0	3.0703902422	4.2503594792	-0.2801079986
H	1.0	3.3150684113	2.8479706346	-1.3788434366
H	1.0	4.6289033699	3.3610639946	-0.2720723548
C	6.0	2.6126073734	-2.3979327344	-1.3846198368
H	1.0	1.5269296472	-2.1469258207	-1.3580119373
C	6.0	2.7486219360	-3.8295754433	-0.8311002309
C	6.0	3.0744539917	-2.3168123764	-2.8622657922
H	1.0	2.4601149865	-3.8852169979	0.2381162494
H	1.0	3.7833746456	-4.2172028301	-0.9290825730
H	1.0	2.0948589123	-4.5178091683	-1.4036532578
H	1.0	4.1408667210	-2.6093562666	-2.9478958375
H	1.0	2.9857220791	-1.2935090306	-3.2849647841
H	1.0	2.4772045314	-3.0086468554	-3.4904392453
C	6.0	-1.0427861228	-0.2823537042	2.7449080065
H	1.0	1.2257550917	0.0346063585	2.0128525351
H	1.0	-0.9192717553	0.2490991601	3.7127200635
H	1.0	-0.7969363101	-1.3541316306	2.8575471329
H	1.0	-2.0891754244	-0.1523047646	2.4081720982

Product **Pro-Se-CH$_4$**:

ATOM	CHARGE	X	Y	Z
SE	34.0	-0.0303279796	0.4975790195	-1.4414667704
N	7.0	-1.4727404863	0.1788880587	0.5691796806
C	6.0	-0.7334587590	-0.0710205641	1.6082090816
C	6.0	0.7234518471	-0.0611389549	1.5620867594
N	7.0	1.4123317954	-0.2405515486	0.4769275338
H	1.0	-1.1973676842	-0.2090254102	2.6035714230
H	1.0	1.2497257833	0.0041361861	2.5342213374
C	6.0	2.7457752654	-0.0250674806	0.2404961888
C	6.0	3.4786943624	-1.1137202999	-0.3727656895
C	6.0	4.8185954695	-0.8875241290	-0.6944999002
C	6.0	5.4145088596	0.3677420081	-0.4474647739
C	6.0	4.6854249579	1.4196621861	0.1415409976
C	6.0	3.3420175442	1.2673354730	0.5103631712
H	1.0	5.1818349792	2.3866466051	0.3142274249
H	1.0	6.4715494417	0.5272411951	-0.7140881811
H	1.0	5.4219964153	-1.6964696165	-1.1315877899
C	6.0	2.8258929917	-2.4789482314	-0.4912599044
H	1.0	1.7325195685	-2.3014052665	-0.6137767477
C	6.0	3.0022424399	-3.2493294273	0.8424215872
C	6.0	3.3344309337	-3.3055326751	-1.6819371527
H	1.0	2.4811512744	-4.2266822580	0.7872120026
H	1.0	4.0755055063	-3.4435389693	1.0434357636
H	1.0	2.5946417892	-2.6864780381	1.7077007979
H	1.0	4.3854433073	-3.6299560374	-1.5369907827
H	1.0	2.7307280957	-4.2285019177	-1.7936245391
H	1.0	3.2842395146	-2.7441781521	-2.6375949404
C	6.0	2.5778782550	2.4207834746	1.1369288593
H	1.0	1.4959198396	2.1597078216	1.1582392742
C	6.0	2.7055085581	3.7192450976	0.3133956355
C	6.0	3.0330836228	2.6270232208	2.6012952946
H	1.0	2.0732569247	4.5135205170	0.7587721164
H	1.0	3.7473291651	4.0997189640	0.3059961362
H	1.0	2.3876951058	3.5702550972	-0.7387818823
H	1.0	4.1006405536	2.9254606722	2.6450326965
H	1.0	2.9262746711	1.7053883417	3.2110938122
H	1.0	2.4371540443	3.4314297549	3.0785176585
C	6.0	-2.7950374220	-0.0795398688	0.3361414624
C	6.0	-3.3691492325	-1.3672583765	0.6941341479
C	6.0	-4.6891607645	-1.5950716760	0.2875113930
C	6.0	-5.4285618368	-0.6201300553	-0.4112006201
C	6.0	-4.8631470020	0.6281997494	-0.7397860448
C	6.0	-3.5430415805	0.9275178133	-0.3921884643
H	1.0	-5.4751780930	1.3778562176	-1.2629054269
H	1.0	-6.4697791762	-0.8378416440	-0.6985488149
H	1.0	-5.1645887507	-2.5595716412	0.5217394807
C	6.0	-2.9645139546	2.3146738556	-0.6074466163
H	1.0	-1.8577061650	2.2395199718	-0.5025952252
C	6.0	-3.2711621667	2.9014474589	-1.9954884905
C	6.0	-3.4501713499	3.2471012765	0.5305043546
H	1.0	-2.7359608263	3.8634049582	-2.1255484869
H	1.0	-4.3514822418	3.1159251447	-2.1259929086
H	1.0	-2.9578103940	2.2188204927	-2.8128734749
H	1.0	-2.9783231176	4.2458916351	0.4333445527
H	1.0	-3.2028624580	2.8393271820	1.5320061345
H	1.0	-4.5503153710	3.3821214078	0.4822778917
C	6.0	-2.6123633285	-2.4328694791	1.4655802110
H	1.0	-1.5238738218	-2.1964120590	1.4185032482
C	6.0	-2.7814724310	-3.8431606378	0.8680493316
C	6.0	-3.0314085681	-2.3961136538	2.9568665368

H	1.0	-2.5212855132	-3.8670526973	-0.2096811110
H	1.0	-3.8186953951	-4.2205849846	0.9787518514
H	1.0	-2.1232661311	-4.5593298159	1.4000304784
H	1.0	-4.0996998327	-2.6748250461	3.0635115011
H	1.0	-2.9152762202	-1.3887253027	3.4098118007
H	1.0	-2.4289076941	-3.1176353730	3.5452612365
C	6.0	1.0235804614	-0.5852739996	-2.6920865517
H	1.0	-1.3452518921	0.0083133817	-1.9661923636
H	1.0	0.8397049469	-0.1307543746	-3.6884304984
H	1.0	0.7023257903	-1.6420974649	-2.6781448855
H	1.0	2.0910794894	-0.4769946384	-2.4278397224

Product **Pro-Te-CH$_4$**:

ATOM	CHARGE	X	Y	Z
TE	52.0	-0.0665341107	-0.2937844975	-1.4302872877
N	7.0	-1.3313382861	0.0927987098	0.4934162525
C	6.0	-0.6762324826	0.0078492273	1.6269967085
C	6.0	0.7665373373	0.0122085063	1.6933400560
N	7.0	1.4740073908	-0.1797034361	0.6079402842
H	1.0	-1.2538404148	0.0582807534	2.5668661886
H	1.0	1.2390614080	0.1600567848	2.6807093132
C	6.0	2.7874658862	0.2100817082	0.4031023682
C	6.0	3.6042618291	-0.6255218692	-0.4438066355
C	6.0	4.8753660193	-0.1680164151	-0.8017281924
C	6.0	5.3415165391	1.0820518553	-0.3524425086
C	6.0	4.5385265196	1.8942584703	0.4672601889
C	6.0	3.2603212231	1.4951017069	0.8868601548
H	1.0	4.9237534914	2.8715953292	0.7938154402
H	1.0	6.3503667086	1.4222921115	-0.6346224635
H	1.0	5.5308465970	-0.7996489109	-1.4205100494
C	6.0	3.1454191266	-2.0194788091	-0.8373776265
H	1.0	2.1337056507	-2.1477873882	-0.3967980153
C	6.0	4.0443434261	-3.0982900119	-0.1892621767
C	6.0	3.0604168974	-2.2000819411	-2.3651882401
H	1.0	3.6424013815	-4.1104424355	-0.3992058604
H	1.0	5.0754684034	-3.0562974075	-0.5959599513
H	1.0	4.1072068371	-2.9691967428	0.9098891938
H	1.0	4.0546927416	-2.0895262884	-2.8437305146
H	1.0	2.6860066920	-3.2124769463	-2.6224134734
H	1.0	2.3933342335	-1.4452142084	-2.8391400556
C	6.0	2.4404986735	2.4350222315	1.7552306315
H	1.0	1.3705264705	2.1232311170	1.6959020351
C	6.0	2.4919374482	3.8977953167	1.2738394325
C	6.0	2.8714003729	2.3138063331	3.2367547671
H	1.0	1.7812350512	4.5134846100	1.8614313931
H	1.0	3.4955363808	4.3473979122	1.4169541918
H	1.0	2.2266110101	3.9859398223	0.2007732537
H	1.0	3.9212566371	2.6510150465	3.3581517655
H	1.0	2.8260303859	1.2706652323	3.6172266943
H	1.0	2.2314992036	2.9502077154	3.8812466459
C	6.0	-2.7170449193	0.0497775296	0.3176506804
C	6.0	-3.4935446899	-1.0483230625	0.8193212023
C	6.0	-4.8655688154	-1.0304849747	0.5138422489
C	6.0	-5.4365324975	0.0016432171	-0.2501464094
C	6.0	-4.6518804477	1.0678726050	-0.7319908724
C	6.0	-3.2792723331	1.1214598136	-0.4614740561
H	1.0	-5.1306983397	1.8767577623	-1.3026929392
H	1.0	-6.5165272095	-0.0179070086	-0.4655835773
H	1.0	-5.5082090980	-1.8463360424	0.8778762176
C	6.0	-2.4331666436	2.3322192035	-0.8232668470
H	1.0	-1.3779440782	1.9810786666	-0.9703577095
C	6.0	-2.8723631227	3.0415306837	-2.1103901221
C	6.0	-2.3722186567	3.3042069966	0.3811851571
H	1.0	-2.1483139424	3.8368684786	-2.3775098220
H	1.0	-3.8574827382	3.5366472327	-1.9875237166
H	1.0	-2.9500931948	2.3400161970	-2.9664872730
H	1.0	-1.7074213850	4.1608765624	0.1511814766
H	1.0	-1.9982433271	2.8058297033	1.2997395205
H	1.0	-3.3833276133	3.7009311223	0.6052634724
C	6.0	-2.9047722650	-2.1728273652	1.6584602791
H	1.0	-1.7955705296	-2.1446442328	1.5535108358
C	6.0	-3.3667440458	-3.5667610648	1.1913029883
C	6.0	-3.2350444370	-1.9496102230	3.1540848778
H	1.0	-3.1813311913	-3.7300751959	0.1087697926
H	1.0	-4.4503113677	-3.7235259664	1.3679507966
H	1.0	-2.8313250532	-4.3561510320	1.7562452522
H	1.0	-4.3298802182	-1.9987175483	3.3253062912
H	1.0	-2.8967083843	-0.9575423350	3.5214385901
H	1.0	-2.7576397729	-2.7327306032	3.7774281492
C	6.0	-0.4139944779	-2.4266903339	-1.3059900237
H	1.0	-1.6425593628	-0.1473273252	-2.0983785187
H	1.0	-0.3217552759	-2.8162313474	-2.3393736961
H	1.0	-1.4398509981	-2.5763152525	-0.9213713252
H	1.0	0.3514608228	-2.8695182673	-0.6454605901

Precursor state **PC-O-C$_2$H$_4$**:

ATOM	CHARGE	X	Y	Z
O	8.0	0.2878387615	-0.5281475924	0.3371290062
N	7.0	1.0777740978	0.1404189726	-0.4032091177
C	6.0	0.5735285181	0.7445658661	-1.5236254116
C	6.0	-0.7996344570	0.5867683381	-1.7537024459
N	7.0	-1.5565603335	-0.2122814229	-1.0371904418
H	1.0	1.2570054036	1.2678153631	-2.2015880441
H	1.0	-1.2580554415	1.0889298703	-2.6297227055
C	6.0	-2.7182927294	-0.3208263022	-0.4426414151
C	6.0	-3.2889770367	-1.6838853560	-0.3338632064
C	6.0	-4.4894576445	-1.8148207410	0.3575100631
C	6.0	-5.1098933428	-0.6870789969	0.9409687074
C	6.0	-4.5529837280	0.6171542169	0.8640256393
C	6.0	-3.3653526549	0.8552154098	0.1849832188
H	1.0	-5.0789971234	1.4492897819	1.3549800941
H	1.0	-6.0603268821	-0.8242804914	1.4836502879
H	1.0	-4.9617208879	-2.8025396779	0.4603891180
C	6.0	-2.6008246691	-2.8267472763	-1.0250928137
H	1.0	-1.5102215922	-2.6087234279	-1.0002040595
C	6.0	-3.0317871832	-2.8273208457	-2.5253697965
C	6.0	-2.8574627122	-4.1950598718	-0.3750426607
H	1.0	-2.4850810983	-3.6324123252	-3.0566439803
H	1.0	-4.1185444941	-3.0244094842	-2.6198835696
H	1.0	-2.8066240646	-1.8642982350	-3.0264177163
H	1.0	-3.9113503213	-4.5230703943	-0.4893173494
H	1.0	-2.2305140583	-4.9623700279	-0.8710189052
H	1.0	-2.6058742133	-4.1925011994	0.7049430334
C	6.0	-2.7650213917	2.2312754296	0.0501424505
H	1.0	-1.6632166608	2.1079646517	-0.0614384721
C	6.0	-3.0065928000	3.1328258175	1.2738749118
C	6.0	-3.3005140747	2.8978616629	-1.2500212178
H	1.0	-2.4430666616	4.0796315907	1.1563933999
H	1.0	-4.0753411258	3.4099584314	1.3796250107
H	1.0	-2.6774353552	2.6480763937	2.2151716869
H	1.0	-4.3854646361	3.1048335487	-1.1543502393
H	1.0	-3.1677907990	2.2645325507	-2.1518625645
H	1.0	-2.7763591249	3.8602366022	-1.4180194156
C	6.0	2.4756185157	0.2044755249	-0.0924974369
C	6.0	3.1529830694	-1.0322934442	0.1734778238
C	6.0	4.5186644074	-0.9313257315	0.4874370756
C	6.0	5.1704349949	0.3113979335	0.5299998363
C	6.0	4.4706070670	1.5010007808	0.2599045959
C	6.0	3.1054226426	1.4941517012	-0.0654757128
H	1.0	4.9995104669	2.4633949854	0.3341021293

H	1.0	6.2432245246	0.3567788537	0.7754471262
H	1.0	5.0925068734	-1.8511848541	0.6736598752
C	6.0	2.3778427309	2.8267142332	-0.2436771941
H	1.0	1.2853724658	2.6334722762	-0.3009150873
C	6.0	2.5877394717	3.7563047271	0.9707306569
C	6.0	2.8091154385	3.5172663176	-1.5564362454
H	1.0	1.9889757796	4.6815343158	0.8480939920
H	1.0	3.6465744632	4.0674449906	1.0774939789
H	1.0	2.2782479913	3.2718272869	1.9191572770
H	1.0	2.2414948794	4.4581642128	-1.7043605538
H	1.0	2.6550732385	2.8752944768	-2.4504160323
H	1.0	3.8874726028	3.7761344649	-1.5332713345
C	6.0	2.5089417585	-2.4056163384	0.0174862495
H	1.0	1.5344482911	-2.2788311520	-0.4982530818
C	6.0	2.2145921534	-3.0400694518	1.3960845063
C	6.0	3.3730540372	-3.3400821334	-0.8555606300
H	1.0	1.4931741539	-2.4318836288	1.9754924408
H	1.0	3.1449300806	-3.1467329325	1.9915811975
H	1.0	1.7859983051	-4.0540307751	1.2624842541
H	1.0	3.6508438499	-2.8665673516	-1.8189248674
H	1.0	2.8083619002	-4.2682023499	-1.0773930252
H	1.0	4.3064542319	-3.6478258789	-0.3412939508
C	6.0	0.6773261577	0.5109715482	2.7534710428
C	6.0	2.0100014498	0.3115386937	2.9247415621
H	1.0	-0.0585541545	-0.2685413854	3.0069515728
H	1.0	0.2805372879	1.4866452859	2.4235891960
H	1.0	2.4044173666	-0.6503140310	3.2895059108
H	1.0	2.7451307827	1.1117073631	2.7419097909

Precursor state **PC-S-C$_2$H$_4$**:

ATOM	CHARGE	X	Y	Z
S	16.0	-0.1015959162	-0.1519101422	0.7609073248
N	7.0	1.1039833894	0.4295025663	-0.3679925886
C	6.0	0.5635355062	1.0025839131	-1.4552422132
C	6.0	-0.8404634840	0.9534606458	-1.4894910088
N	7.0	-1.3486385725	0.2669517926	-0.4497950231
H	1.0	1.2248114704	1.3751149750	-2.2511822416
H	1.0	-1.4870609250	1.3029233746	-2.3079207114
C	6.0	-2.7112021467	-0.0001980541	-0.1785988788
C	6.0	-3.0834996128	-1.3475412152	0.1613889454
C	6.0	-4.4362090097	-1.5633744913	0.4600144103
C	6.0	-5.3706951422	-0.5124607424	0.4352762589
C	6.0	-4.9747829258	0.7923726226	0.0977439561
C	6.0	-3.6424098981	1.0979664547	-0.2212263555
H	1.0	-5.7230145147	1.5990323484	0.0986939811
H	1.0	-6.4258378441	-0.7155599486	0.6772615820
H	1.0	-4.7782347441	-2.5823960642	0.6944051362
C	6.0	-2.1208844235	-2.5330378183	0.1317970139
H	1.0	-1.1806614712	-2.2124053638	-0.3691711215
C	6.0	-2.6771804965	-3.7068639839	-0.7016054190
C	6.0	-1.7619468427	-2.9858909212	1.5644238291
H	1.0	-1.9080638080	-4.5003932583	-0.7893676987
H	1.0	-3.5648086220	-4.1662667444	-0.2216869156
H	1.0	-2.9645585506	-3.3853670697	-1.7226101307
H	1.0	-2.6582588412	-3.3526381301	2.1055761091
H	1.0	-1.0235927933	-3.8131144657	1.5355956385
H	1.0	-1.3364446473	-2.1590565693	2.1746617776
C	6.0	-3.2607813973	2.5373652214	-0.5449608569
H	1.0	-2.1514820207	2.6340695039	-0.5098256029
C	6.0	-3.8111056292	3.5361084443	0.4933895993
C	6.0	-3.7207173353	2.9043929049	-1.9762085897
H	1.0	-3.4330677289	4.5544553345	0.2713899918
H	1.0	-4.9181983926	3.5921091735	0.4674141247
H	1.0	-3.5041228353	3.2689032649	1.5244845601
H	1.0	-4.8270043366	2.8761714812	-2.0505307920
H	1.0	-3.3350554574	2.2038400215	-2.7488602416
H	1.0	-3.3893828573	3.9294251465	-2.2387590416
C	6.0	2.5044975054	0.1295641680	-0.2098279668
C	6.0	2.9175535754	-1.2036233082	-0.4996000824
C	6.0	4.2869343894	-1.4746665641	-0.3284969933
C	6.0	5.1737495265	-0.4819514547	0.1208570874
C	6.0	4.7204227524	0.8193345911	0.3951985730
C	6.0	3.3662699420	1.1695691264	0.2349194953
H	1.0	5.4343914377	1.5781267402	0.7480610300
H	1.0	6.2387959510	-0.7262134431	0.2576569021
H	1.0	4.6689358472	-2.4812101225	-0.5545322478
C	6.0	2.8738582640	2.5896773596	0.4906195050
H	1.0	1.7779038788	2.5397153527	0.6855522221
C	6.0	3.5330444819	3.2462405899	1.7181435300
C	6.0	3.0946874299	3.4627591457	-0.7676732618
H	1.0	3.0464648593	4.2182034181	1.9346075682
H	1.0	4.6075331521	3.4572180829	1.5431065152
H	1.0	3.4613607443	2.6162821885	2.6289159685
H	1.0	2.7128349689	4.4900617648	-0.5992978105
H	1.0	2.5921058212	3.0534620512	-1.6687716940
H	1.0	4.1755535369	3.5361765900	-1.0065763094
C	6.0	1.9717979937	-2.2523103520	-1.0753409536
H	1.0	0.9314910709	-1.9880937900	-0.7824530100
C	6.0	2.2353519899	-3.6680211518	-0.5332155255
C	6.0	2.0353013046	-2.2135690435	-2.6205551703
H	1.0	2.2304835279	-3.6935891819	0.5756150140
H	1.0	3.2091775580	-4.0685866538	-0.8805662324
H	1.0	1.4550049884	-4.3651856347	-0.8992228338
H	1.0	1.7963678076	-1.2069250922	-3.0248615358
H	1.0	1.3190712357	-2.9383813969	-3.0584778511
H	1.0	3.0510435794	-2.4786306796	-2.9781102028
C	6.0	1.4290416605	0.1791441893	2.9953100919
C	6.0	1.9684007982	-1.0203927093	2.6512464037
H	1.0	0.4708202436	0.2485341357	3.5398180053
H	1.0	1.9804201967	1.1218077718	2.8416194839
H	1.0	1.4491815575	-1.9708421419	2.8657222706
H	1.0	2.9684646907	-1.0910398419	2.1951146281

Precursor state **PC-Se-C$_2$H$_4$**:

ATOM	CHARGE	X	Y	Z
SE	34.0	0.1177553117	0.3008982040	-1.3291375606
N	7.0	1.2300639583	-0.4338158765	0.1982485414
C	6.0	0.5422386470	-0.9828896877	1.1843233782
C	6.0	-0.8876193158	-1.0042668233	1.2429044035
N	7.0	-1.5153328238	-0.1966279215	0.4142418590
H	1.0	1.1385580978	-1.4019842880	2.0131040961
H	1.0	-1.3836628337	-1.5588423701	2.0579183363
C	6.0	-2.8623244226	-0.0211290861	0.2350028407
C	6.0	-3.2813520023	1.3223708782	-0.1375491118
C	6.0	-4.6381959893	1.5396750032	-0.3839106999
C	6.0	-5.5657833770	0.4821310462	-0.2979423828
C	6.0	-5.1527621855	-0.8190364669	0.0422208055
C	6.0	-3.8163439033	-1.1158185436	0.3379391649
H	1.0	-5.9009604175	-1.6246529924	0.0732689455
H	1.0	-6.6319305684	0.6765976143	-0.4967107823
H	1.0	-4.9953530762	2.5493507868	-0.6311064230
C	6.0	-2.3031564785	2.4847261759	-0.0759529545
H	1.0	-1.3109181608	2.1018068147	-0.4067429595
C	6.0	-2.1170171982	2.9402989690	1.3919228134
C	6.0	-2.6750333688	3.6590789842	-0.9920674046
H	1.0	-1.3735008083	3.7617208670	1.4463465003
H	1.0	-3.0732190068	3.3190531941	1.8075089687
H	1.0	-1.7701132391	2.1106627068	2.0416518388
H	1.0	-3.5713698791	4.2019604533	-0.6273283607
H	1.0	-1.8494182939	4.3989349362	-1.0174553849

H	1.0	-2.8736618171	3.3284399453	-2.0319429265
C	6.0	-3.4259161816	-2.5432727684	0.6839095867
H	1.0	-2.3376683556	-2.6675114398	0.4802141904
C	6.0	-4.1535818053	-3.5970662062	-0.1733150150
C	6.0	-3.6629743507	-2.8041305873	2.1935738857
H	1.0	-3.7241142720	-4.6000450140	0.0231672123
H	1.0	-5.2329994387	-3.6608842673	0.0726841521
H	1.0	-4.0568965180	-3.3862533783	-1.2574587265
H	1.0	-4.7457650370	-2.7422229690	2.4257309987
H	1.0	-3.1576564611	-2.0646833885	2.8516392464
H	1.0	-3.3111485114	-3.8188601713	2.4702455134
C	6.0	2.6248259535	-0.1477671911	0.2816103336
C	6.0	2.9945091379	1.1518841694	0.7505420344
C	6.0	4.3702953237	1.4319438365	0.8009037016
C	6.0	5.3200809585	0.4706050397	0.4095535092
C	6.0	4.9201060881	-0.8003328782	-0.0333209189
C	6.0	3.5584634485	-1.1478854892	-0.1181345746
H	1.0	5.6842934321	-1.5406635593	-0.3134111539
H	1.0	6.3924424126	0.7165432822	0.4584421304
H	1.0	4.7114781439	2.4152635320	1.1566246970
C	6.0	3.1262265404	-2.5586827618	-0.5039874551
H	1.0	2.0452067535	-2.5254401702	-0.7716231667
C	6.0	3.8970037275	-3.1166314356	-1.7157078003
C	6.0	3.2646148928	-3.4990798066	0.7161698727
H	1.0	3.4713639495	-4.0923322059	-2.0243517900
H	1.0	4.9657427844	-3.2909920615	-1.4772670752
H	1.0	3.8657000422	-2.4355026723	-2.5928184225
H	1.0	2.8966648180	-4.5152371354	0.4674245199
H	1.0	2.6973562011	-3.1336620240	1.5976329646
H	1.0	4.3265055821	-3.5864744360	1.0248288726
C	6.0	1.9495066334	2.1557449870	1.2288693606
H	1.0	0.9973677169	1.9517413296	0.6870120335
C	6.0	2.3306285231	3.6172559606	0.9377239625
C	6.0	1.6649987129	1.9424334215	2.7340851339
H	1.0	2.5880123694	3.7763372367	-0.1295909279
H	1.0	3.1940553637	3.9473986955	1.5501363875
H	1.0	1.4858613499	4.2885855585	1.1918493779
H	1.0	1.3117492027	0.9134333822	2.9571128002
H	1.0	0.8888948650	2.6519801826	3.0856971976
H	1.0	2.5826914256	2.1093463646	3.3340671880
C	6.0	1.5494773101	-0.3266304220	-2.7999502863
C	6.0	1.8002142180	1.0233959242	-2.3901552215
H	1.0	0.9710631256	-0.5458423052	-3.7145890818
H	1.0	2.1601907604	-1.1493460278	-2.3939676291
H	1.0	1.4144262441	1.8731834994	-2.9812779998
H	1.0	2.6203445486	1.2474726614	-1.6841026651

Precursor state **PC-Te-C_2H_4**:

ATOM	CHARGE	X	Y	Z
TE	52.0	0.1143683245	-0.6317677687	-1.0395054757
N	7.0	-1.2693595275	0.2500070108	0.3800262456
C	6.0	-0.6831261546	0.7097174579	1.4728221037
C	6.0	0.7375924499	0.6644719153	1.6040284392
N	7.0	1.4266030862	0.0464219839	0.6547732162
H	1.0	-1.3212709210	1.1137256862	2.2756301890
H	1.0	1.2395780287	1.0672187863	2.4987540593
C	6.0	2.8284834012	0.0822649771	0.5574634634
C	6.0	3.5236497768	-1.1245362005	0.1969380593
C	6.0	4.9170884090	-1.0527820280	0.0739509257
C	6.0	5.6061438282	0.1579523082	0.2698530495
C	6.0	4.9064284354	1.3323999655	0.5874086370
C	6.0	3.5116767403	1.3429022647	0.7473570455
H	1.0	5.4643698684	2.2736951218	0.7050021050
H	1.0	6.7029120474	0.1848183810	0.1730842281
H	1.0	5.4861133446	-1.9648871399	-0.1594776042
C	6.0	2.8180412353	-2.4620205779	-0.0044245695
H	1.0	1.7836129742	-2.3788718479	0.3990590972
C	6.0	3.4837052370	-3.6084598665	0.7851806237
C	6.0	2.7354191384	-2.8017588115	-1.5097868664
H	1.0	2.8773933380	-4.5326109668	0.6976103511
H	1.0	4.4953079494	-3.8450117209	0.3966076740
H	1.0	3.5785336859	-3.3581605570	1.8606317834
H	1.0	3.7428796248	-2.9983185479	-1.9323534472
H	1.0	2.1121022647	-3.7034934087	-1.6811161676
H	1.0	2.3207453171	-1.9635383832	-2.1221767685
C	6.0	2.8160353322	2.6748759458	1.0050510652
H	1.0	1.7195243053	2.5404776223	0.8583087314
C	6.0	3.2527124379	3.7571778191	-0.0033948257
C	6.0	3.0323979723	3.1429417209	2.4628656676
H	1.0	2.6500044116	4.6763814212	0.1435153796
H	1.0	4.3151581051	4.0450682879	0.1312815500
H	1.0	3.1208944587	3.4179051135	-1.0507299818
H	1.0	4.1064536578	3.3432291035	2.6552514710
H	1.0	2.7128847094	2.3858115582	3.2109892049
H	1.0	2.4728065133	4.0806838053	2.6546860459
C	6.0	-2.6943421927	0.2023859424	0.2438329296
C	6.0	-3.3788939098	-0.9530676288	0.7215437922
C	6.0	-4.7776868627	-0.9582886352	0.5652704491
C	6.0	-5.4461149429	0.1206326042	-0.0366437373
C	6.0	-4.7349060305	1.2407618395	-0.4980763751
C	6.0	-3.3351205216	1.3141310808	-0.3755936812
H	1.0	-5.2820537139	2.0771782615	-0.9573855764
H	1.0	-6.5413799748	0.0887825421	-0.1459186954
H	1.0	-5.3571694294	-1.8224606116	0.9224294639
C	6.0	-2.5531175456	2.5532134164	-0.8032829515
H	1.0	-1.5155200861	2.2280472998	-1.0497421370
C	6.0	-3.1338431496	3.2430157022	-2.0512682932
C	6.0	-2.4544975194	3.5572758628	0.3691608195
H	1.0	-2.4530813711	4.0494431666	-2.3893628685
H	1.0	-4.1140910599	3.7167334928	-1.8403190504
H	1.0	-3.2799764340	2.5416334119	-2.8995339977
H	1.0	-1.8771912565	4.4533284292	0.0627498632
H	1.0	-1.9607039793	3.1227154035	1.2630567228
H	1.0	-3.4642367614	3.8913947454	0.6838668909
C	6.0	-2.6496058292	-2.1026995768	1.4111104489
H	1.0	-1.5910398791	-2.0967564607	1.0619523462
C	6.0	-3.2348853661	-3.4828513688	1.0611021288
C	6.0	-2.6341236877	-1.8823216275	2.9418477767
H	1.0	-3.2950813131	-3.6457850261	-0.0348570723
H	1.0	-4.2524166993	-3.6149569067	1.4809944330
H	1.0	-2.6029359268	-4.2851434915	1.4919543681
H	1.0	-2.1684180130	-0.9160361138	3.2277235452
H	1.0	-2.0731187943	-2.6952943994	3.4459833954
H	1.0	-3.6671111667	-1.8784776554	3.3462086580
C	6.0	-2.0435204382	-1.4651272958	-2.4154613516
C	6.0	-1.7251495003	-0.2502709186	-2.9829177714
H	1.0	-1.6128873027	-2.4092064974	-2.7957480009
H	1.0	-2.8340251853	-1.5460632883	-1.6487598114
H	1.0	-2.2505519468	0.6738916187	-2.6877684073
H	1.0	-1.0238994080	-0.1776207541	-3.8338632792

Transition state **TS-O-C_2H_4**:

ATOM	CHARGE	X	Y	Z
O	8.0	0.9778442718	-1.2958790854	0.2970079338
N	7.0	1.4523969549	-0.2865389734	-0.3141449576
C	6.0	0.6424322245	0.4170099575	-1.1818857732
C	6.0	-0.7613387461	0.3793165822	-1.2302765216
N	7.0	-1.5796408825	-0.3137129383	-0.4438328155
H	1.0	1.1785825559	1.0555531526	-1.8974309176
H	1.0	-1.2014109908	0.9511475128	-2.0726387114

C	6.0	-2.8714858441	-0.1148120874	-0.1964065644
C	6.0	-3.6373152369	-1.3373275869	0.1353126255
C	6.0	-4.9952841833	-1.1972959075	0.4174654270
C	6.0	-5.5965888392	0.0784027888	0.4159772402
C	6.0	-4.8555953107	1.2601245483	0.1519498888
C	6.0	-3.4999434550	1.2182195941	-0.1558421386
H	1.0	-5.3726858886	2.2300457193	0.2053886979
H	1.0	-6.6725669714	0.1659430285	0.6406700611
H	1.0	-5.6065903142	-2.0833999985	0.6411438669
C	6.0	-2.9621780022	-2.6781764517	0.0415932398
H	1.0	-1.8886847260	-2.5198312803	0.2862325194
C	6.0	-3.0045081812	-3.1541765445	-1.4439524792
C	6.0	-3.5590390857	-3.7418543333	0.9772129588
H	1.0	-2.4680740592	-4.1208950982	-1.5297072080
H	1.0	-4.0511645676	-3.3075294577	-1.7758970350
H	1.0	-2.5223941822	-2.4258631385	-2.1264119472
H	1.0	-4.5799131271	-4.0474085930	0.6680851619
H	1.0	-2.9315747425	-4.6547167962	0.9468036394
H	1.0	-3.6057809848	-3.3920698577	2.0289183817
C	6.0	-2.7256004346	2.4968672196	-0.4031457409
H	1.0	-1.6397574776	2.2720779814	-0.2981765726
C	6.0	-3.0523791303	3.6025534533	0.6216866675
C	6.0	-2.9708944692	2.9897383007	-1.8540519972
H	1.0	-2.3880671124	4.4741805145	0.4550706288
H	1.0	-4.0935367880	3.9701150098	0.5180846128
H	1.0	-2.9120415799	3.2525821224	1.6643827655
H	1.0	-4.0321878461	3.2830028070	-1.9869722128
H	1.0	-2.7534493125	2.2154575651	-2.6204254956
H	1.0	-2.3406336418	3.8774060965	-2.0652274471
C	6.0	2.8270054292	0.0691348836	-0.1615382330
C	6.0	3.8076774032	-0.9771699638	-0.2872822353
C	6.0	5.1526129052	-0.5696297673	-0.2310199627
C	6.0	5.5061501475	0.7729980006	-0.0325208109
C	6.0	4.5170813393	1.7652583906	0.1197177523
C	6.0	3.1528199164	1.4474105646	0.0557391480
H	1.0	4.8228967907	2.8037994158	0.3180347558
H	1.0	6.5697362775	1.0542657193	0.0206693000
H	1.0	5.9432880899	-1.3246188214	-0.3528697274
C	6.0	2.1165542467	2.5340530541	0.3417507155
H	1.0	1.1025966751	2.0714740356	0.3180086141
C	6.0	2.2989123985	3.1011177293	1.7657935811
C	6.0	2.1375745705	3.6487522996	-0.7233847135
H	1.0	1.4939098794	3.8274800461	1.9990584060
H	1.0	3.2649100426	3.6377988619	1.8661377834
H	1.0	2.2817696826	2.3018085823	2.5350417320
H	1.0	1.3520166385	4.4021726583	-0.5106036970
H	1.0	1.9751784919	3.2573217574	-1.7496184736
H	1.0	3.1109040017	4.1806038833	-0.7287573078
C	6.0	3.4721262026	-2.4394959786	-0.5259953283
H	1.0	2.4021278727	-2.5158918857	-0.8209549799
C	6.0	3.6167363849	-3.2319951502	0.7981837659
C	6.0	4.3179458874	-3.0629136445	-1.6510917393
H	1.0	2.9753382369	-2.8130789288	1.5982971923
H	1.0	4.6673660141	-3.2098577175	1.1542391559
H	1.0	3.3311244944	-4.2909454274	0.6368336894
H	1.0	4.2725941045	-2.4656637179	-2.5842575591
H	1.0	3.9459722207	-4.0829098261	-1.8765035062
H	1.0	5.3842463165	-3.1699549793	-1.3626975990
C	6.0	-0.6545794784	-0.3609362439	2.1663529430
C	6.0	0.6058876916	-0.8695447819	2.3964908683
H	1.0	-1.5408666678	-1.0106781904	2.2130998418
H	1.0	-0.8190538012	0.7183334707	2.0123360762
H	1.0	0.7471884170	-1.9259836926	2.6728063862
H	1.0	1.4862482008	-0.2116021077	2.4881395572

Transition state **TS-S-C$_2$H$_4$**:

ATOM	CHARGE	X	Y	Z
S	16.0	0.0426168462	-0.2231620439	1.1149558192
N	7.0	1.1736696306	0.4243677255	-0.1546845608
C	6.0	0.5876498124	1.0218045399	-1.1877588459
C	6.0	-0.8314965478	1.0313180322	-1.2923425007
N	7.0	-1.4320111148	0.2357396754	-0.4269881972
H	1.0	1.2505631614	1.4327156988	-1.9655937809
H	1.0	-1.3483042151	1.5409739310	-2.1222134498
C	6.0	-2.7656671478	0.0063505858	-0.1978170599
C	6.0	-3.1281502374	-1.3339125528	0.2251418595
C	6.0	-4.4680877588	-1.5744672387	0.5399572879
C	6.0	-5.4268527445	-0.5457857617	0.4666722574
C	6.0	-5.0639125806	0.7542904506	0.0672426096
C	6.0	-3.7501291937	1.0754592982	-0.2937062261
H	1.0	-5.8336405820	1.5394678054	0.0421915873
H	1.0	-6.4775824558	-0.7612856531	0.7185144152
H	1.0	-4.7865813240	-2.5875225438	0.8290062446
C	6.0	-2.1341475402	-2.4874278091	0.2319643775
H	1.0	-1.1576704107	-2.1073357998	-0.1342420784
C	6.0	-2.5580895037	-3.6005009588	-0.7521853388
C	6.0	-1.9297586596	-3.0353725035	1.6589594594
H	1.0	-1.7865134444	-4.3969597258	-0.7745669371
H	1.0	-3.5145963033	-4.0757656568	-0.4520645002
H	1.0	-2.6813891826	-3.2089671345	-1.7820526749
H	1.0	-2.8600190900	-3.4869580470	2.0615023969
H	1.0	-1.1512369276	-3.8259733347	1.6634684646
H	1.0	-1.6288066119	-2.2340444185	2.3684458047
C	6.0	-3.4069580588	2.4962891643	-0.7072008685
H	1.0	-2.3188240784	2.6577245821	-0.5248475207
C	6.0	-4.1450009552	3.5672266642	0.1183210787
C	6.0	-3.6728150564	2.6885414803	-2.2226736638
H	1.0	-3.7578377122	4.5720078997	-0.1453022070
H	1.0	-5.2334043109	3.5818321288	-0.0929938814
H	1.0	-4.0038807061	3.4178080633	1.2077554682
H	1.0	-4.7585634574	2.6054310666	-2.4336222844
H	1.0	-3.1724343905	1.9256264579	-2.8575818775
H	1.0	-3.3364559468	3.6935887351	-2.5486525386
C	6.0	2.5855872250	0.1291144889	-0.1544863587
C	6.0	2.9741545993	-1.1758022525	-0.5785647826
C	6.0	4.3524778409	-1.4518144744	-0.5648061534
C	6.0	5.2824638127	-0.4779957177	-0.1599378554
C	6.0	4.8594265526	0.8024248507	0.2284394966
C	6.0	3.4932963366	1.1482268930	0.2450181916
H	1.0	5.6078254720	1.5533887550	0.5228218854
H	1.0	6.3567195846	-0.7199725162	-0.1576515482
H	1.0	4.7085352968	-2.4414722872	-0.8878213946
C	6.0	3.0470360596	2.5654355709	0.5935544924
H	1.0	1.9514988788	2.5428113280	0.7951611901
C	6.0	3.7464310060	3.1192569542	1.8505441626
C	6.0	3.2746104104	3.5029807162	-0.6149986131
H	1.0	3.3093034963	4.0974916465	2.1348647022
H	1.0	4.8283458265	3.2869098925	1.6754292460
H	1.0	3.6604385183	2.4390521132	2.7245029468
H	1.0	2.9107173799	4.5256847571	-0.3882299832
H	1.0	2.7567507438	3.1489508785	-1.5308717222
H	1.0	4.3545638577	3.5720810182	-0.8591191753
C	6.0	1.9594392776	-2.1877255043	-1.1017144432
H	1.0	0.9639141166	-1.9283329930	-0.6777009987
C	6.0	2.2653837446	-3.6337523285	-0.6751594420
C	6.0	1.8451192482	-2.0612489016	-2.6381007666
H	1.0	2.3832797798	-3.7268331989	0.4241289367
H	1.0	3.1912038971	-4.0188029520	-1.1489142585
H	1.0	1.4423307473	-4.3055214127	-0.9918562768
H	1.0	1.5708667737	-1.0325563923	-2.9548836429
H	1.0	1.0761321383	-2.7578820333	-3.0296904259
H	1.0	2.8109090850	-2.3074043182	-3.1255585759
C	6.0	1.3632402480	0.3196039508	2.8026147203
C	6.0	1.5979678703	-1.0147044195	2.4397284806

H	1.0	0.6209294216	0.5849585724	3.5754788745
H	1.0	2.0376232697	1.1215554783	2.4610602649
H	1.0	1.0331880770	-1.8394276296	2.9080441854
H	1.0	2.4740363692	-1.2882008960	1.8274840110

Transition state **TS-Se-C_2H_4**:

ATOM	CHARGE	X	Y	Z
SE	34.0	0.1199740762	0.4214428962	-1.2774791639
N	7.0	1.2292301498	-0.3396471156	0.2414277717
C	6.0	0.5368827652	-0.8628819162	1.2378566470
C	6.0	-0.8924215872	-0.8853034346	1.2892886643
N	7.0	-1.5285119628	-0.1284302794	0.4200100109
H	1.0	1.1283355559	-1.2777013090	2.0717116348
H	1.0	-1.3900949668	-1.4186757135	2.1172524967
C	6.0	-2.8826671033	-0.0358829161	0.2137088114
C	6.0	-3.3784468041	1.2669267970	-0.2007636435
C	6.0	-4.7427204070	1.3936166440	-0.4682400988
C	6.0	-5.6042536123	0.2828315235	-0.3659616258
C	6.0	-5.1146330444	-0.9815727885	0.0081175836
C	6.0	-3.7663720825	-1.1866276023	0.3284723842
H	1.0	-5.8092687062	-1.8334751432	0.0472974000
H	1.0	-6.6778661674	0.4063575348	-0.5804122939
H	1.0	-5.1579971380	2.3722399253	-0.7475874522
C	6.0	-2.4703602633	2.4855260656	-0.1674742858
H	1.0	-1.4592948713	2.1502465367	-0.4944719386
C	6.0	-2.3071133184	2.9887051546	1.2877773831
C	6.0	-2.9069179127	3.6155044031	-1.1106046752
H	1.0	-1.6068907156	3.8482738337	1.3186774620
H	1.0	-3.2815397359	3.3289036584	1.6943737763
H	1.0	-1.9173111059	2.1965203646	1.9596046560
H	1.0	-3.8400056455	4.1070887655	-0.7654481007
H	1.0	-2.1288240973	4.4046578611	-1.1404472836
H	1.0	-3.0721773525	3.2534852610	-2.1458845264
C	6.0	-3.2942622934	-2.5823399917	0.7052323704
H	1.0	-2.1947670195	-2.6360191160	0.5334529080
C	6.0	-3.9255103559	-3.6905326044	-0.1600527673
C	6.0	-3.5570855260	-2.8427419026	2.2099286726
H	1.0	-3.4467423266	-4.6631641118	0.0721644721
H	1.0	-5.0086463287	-3.8132162516	0.0440184837
H	1.0	-3.7980468684	-3.4918618293	-1.2433266631
H	1.0	-4.6478059369	-2.8476084742	2.4118967545
H	1.0	-3.1203921030	-2.0653524041	2.8734574728
H	1.0	-3.1500910764	-3.8299647714	2.5095169751
C	6.0	2.6409242212	-0.1458615957	0.2936332691
C	6.0	3.1173922557	1.1214640207	0.7531644932
C	6.0	4.5120097524	1.2908356560	0.7895603849
C	6.0	5.3777572858	0.2551364777	0.3942467529
C	6.0	4.8736777595	-0.9804617052	-0.0426318341
C	6.0	3.4882828278	-1.2175407640	-0.1159617645
H	1.0	5.5740355316	-1.7790334038	-0.3295568573
H	1.0	6.4669006425	0.4132807509	0.4344422008
H	1.0	4.9336077263	2.2442578984	1.1402718726
C	6.0	2.9415094280	-2.5857334709	-0.5141504994
H	1.0	1.8709781801	-2.4595214168	-0.7955161228
C	6.0	3.6780162458	-3.1936709849	-1.7229631802
C	6.0	2.9848346994	-3.5455937438	0.6976288584
H	1.0	3.1740494765	-4.1236192841	-2.0545077471
H	1.0	4.7235103922	-3.4648279741	-1.4727004267
H	1.0	3.7182817052	-2.4992324506	-2.5893698641
H	1.0	2.5564589446	-4.5318033436	0.4263765786
H	1.0	2.4191572159	-3.1531049235	1.5684624138
H	1.0	4.0296207326	-3.7078441148	1.0332625649
C	6.0	2.1596392049	2.2040320271	1.2415669089
H	1.0	1.1907510613	2.0734250748	0.7063671141
C	6.0	2.6531648453	3.6312570392	0.9482172515
C	6.0	1.8728354952	2.0124330127	2.7493065696
H	1.0	2.9225184764	3.7687253538	-0.1192813399
H	1.0	3.5401198589	3.8926790931	1.5601735515
H	1.0	1.8628547825	4.3663129660	1.2003911591
H	1.0	1.4420931034	1.0143415844	2.9757568980
H	1.0	1.1575505459	2.7798531437	3.1087479554
H	1.0	2.8062980660	2.1076012569	3.3410370902
C	6.0	1.5687210576	-0.1679428710	-2.7606436840
C	6.0	1.8160617449	1.1702878403	-2.3203000230
H	1.0	0.9903362241	-0.3690627068	-3.6794859687
H	1.0	2.1751771126	-0.9998565631	-2.3667492090
H	1.0	1.4279050777	2.0334087296	-2.8899505291
H	1.0	2.6325351223	1.3776462925	-1.6049581286

Transition state **TS-Te-C_2H_4**:

ATOM	CHARGE	X	Y	Z
TE	52.0	0.0828533383	-0.6564348994	-1.0802908992
N	7.0	-1.2594582916	0.2264214946	0.3916337740
C	6.0	-0.6463030203	0.6221119103	1.4930802129
C	6.0	0.7768680810	0.5599372342	1.5942079782
N	7.0	1.4473445003	-0.0146285812	0.6058287319
H	1.0	-1.2631049475	1.0033916313	2.3232750802
H	1.0	1.2967462788	0.9330519986	2.4914849798
C	6.0	2.8420441054	0.0781160815	0.4691510143
C	6.0	3.5713880469	-1.0824253865	0.0282671742
C	6.0	4.9602354666	-0.9596273083	-0.1015051942
C	6.0	5.6119895364	0.2623330063	0.1492821746
C	6.0	4.8776842860	1.3978990410	0.5238771080
C	6.0	3.4857168765	1.3533496082	0.7007469789
H	1.0	5.4031337737	2.3532863575	0.6726944495
H	1.0	6.7061012450	0.3298151501	0.0428261483
H	1.0	5.5558656607	-1.8376861446	-0.3908544007
C	6.0	2.9191897401	-2.4485888380	-0.1354143723
H	1.0	1.8285161642	-2.2977885105	-0.3281287117
C	6.0	3.0050571640	-3.2407690434	1.1891795167
C	6.0	3.4701333931	-3.2500330178	-1.3268558254
H	1.0	2.4881684315	-4.2168466919	1.0914909096
H	1.0	4.0651194574	-3.4389653787	1.4511791516
H	1.0	2.5495389190	-2.6848076312	2.0342716290
H	1.0	4.5182733007	-3.5703395909	-1.1565325870
H	1.0	2.8755149337	-4.1747337139	-1.4700445203
H	1.0	3.4440941252	-2.6659564530	-2.2696369934
C	6.0	2.7514156794	2.6522113731	1.0151851056
H	1.0	1.6560637925	2.4839771784	0.8955174488
C	6.0	3.1220985558	3.7764572847	0.0258644093
C	6.0	2.9923600881	3.0880496526	2.4791930680
H	1.0	2.4931597588	4.6696251285	0.2166200655
H	1.0	4.1778341980	4.0965950497	0.1387867407
H	1.0	2.9717160014	3.4615225133	-1.0265334691
H	1.0	4.0644635287	3.3174992395	2.6483257171
H	1.0	2.7167401791	2.3019359008	3.2147032656
H	1.0	2.4097663494	4.0024253530	2.7108607764
C	6.0	-2.6846419359	0.2127871374	0.2723690942
C	6.0	-3.3921009216	-0.9367629325	0.7317992749
C	6.0	-4.7918187656	-0.9059562767	0.5867772274
C	6.0	-5.4396348725	0.1999428839	0.0117127270
C	6.0	-4.7065242804	1.3135908438	-0.4318976734
C	6.0	-3.3050840279	1.3522083823	-0.3188335597
H	1.0	-5.2380146026	2.1723707826	-0.8676816338
H	1.0	-6.5361088385	0.1951508686	-0.0897598487
H	1.0	-5.3890060812	-1.7637792760	0.9300791709
C	6.0	-2.4967566936	2.5838401826	-0.7173591169
H	1.0	-1.4694783250	2.2425864506	-0.9845807685
C	6.0	-3.0715899523	3.3269192031	-1.9369822027
C	6.0	-2.3603326838	3.5463074740	0.4861016332

H	1.0	-2.3756500887	4.1287317393	-2.2543961198
H	1.0	-4.0388470951	3.8155009433	-1.7015422359
H	1.0	-3.2395984134	2.6564346848	-2.8060203199
H	1.0	-1.7491969858	4.4286944137	0.2076345851
H	1.0	-1.8847804116	3.0637783543	1.3653284273
H	1.0	-3.3569126959	3.9081759344	0.8119640358
C	6.0	-2.6854444190	-2.1205717514	1.3850843776
H	1.0	-1.6247137943	-2.1210371748	1.0429805185
C	6.0	-3.2908066778	-3.4780800144	0.9828317189
C	6.0	-2.6765754626	-1.9529738235	2.9225055248
H	1.0	-3.3486489234	-3.5994032444	-0.1185948558
H	1.0	-4.3122744965	-3.6104259302	1.3930917338
H	1.0	-2.6725875312	-4.3048835981	1.3862300642
H	1.0	-2.1961981671	-1.0050929793	3.2437539782
H	1.0	-2.1331530175	-2.7922340954	3.4022654648
H	1.0	-3.7119868376	-1.9448370971	3.3206871783
C	6.0	-2.0995845656	-1.4311748329	-2.4156081024
C	6.0	-1.7741958622	-0.2093819528	-2.9682229317
H	1.0	-1.7045076196	-2.3763988735	-2.8306255343
H	1.0	-2.8716473467	-1.5110860196	-1.6301545843
H	1.0	-2.2709542734	0.7162899849	-2.6317187098
H	1.0	-1.1004627860	-0.1295824310	-3.8404756342

Product **Pro-O-C_2H_4**:

ATOM	CHARGE	X	Y	Z
O	8.0	1.3401526408	-0.8330559845	1.2567812939
N	7.0	1.5960288399	-0.1225885981	0.1095213385
C	6.0	0.6801419787	0.2726541008	-0.7792746628
C	6.0	-0.7377943398	0.1563655517	-0.8480601165
N	7.0	-1.5732249545	-0.5691166486	-0.1009384444
H	1.0	1.1440924070	0.7789620511	-1.6392843256
H	1.0	-1.2008419103	0.6968790694	-1.6873508377
C	6.0	-2.9721667707	-0.2839444132	-0.1184839876
C	6.0	-3.8906107890	-1.3822814828	-0.2067567179
C	6.0	-5.2540689362	-1.0866553996	-0.0726423670
C	6.0	-5.6952761885	0.2342217867	0.1265214788
C	6.0	-4.7760823816	1.2953733366	0.1826876238
C	6.0	-3.3941362142	1.0870534991	0.0426286001
H	1.0	-5.1467161504	2.3181873515	0.3490683079
H	1.0	-6.7730084600	0.4425476130	0.2178297571
H	1.0	-5.9949645328	-1.8957687552	-0.1594731256
C	6.0	-3.4588989828	-2.7991586262	-0.5693578668
H	1.0	-2.3559820951	-2.8135255929	-0.6948888196
C	6.0	-4.0463130449	-3.2031537911	-1.9428613031
C	6.0	-3.8386936259	-3.8149511639	0.5279212226
H	1.0	-3.6644620764	-4.2015048864	-2.2373985484
H	1.0	-5.1530475431	-3.2660706642	-1.9073927042
H	1.0	-3.7718927382	-2.4781819279	-2.7357510073
H	1.0	-4.9392391252	-3.8915828140	0.6427423542
H	1.0	-3.4641495895	-4.8240205045	0.2622475490
H	1.0	-3.4237124043	-3.5430113153	1.5215745943
C	6.0	-2.4642579573	2.2917603409	0.1343442822
H	1.0	-1.4096499334	1.9324382184	0.2064825554
C	6.0	-2.7132659552	3.1412384454	1.3958262999
C	6.0	-2.5540809694	3.1409129842	-1.1543960645
H	1.0	-1.9622801016	3.9546618140	1.4575609719
H	1.0	-3.7107624224	3.6259792364	1.3763084211
H	1.0	-2.6505794795	2.5345753117	2.3221274592
H	1.0	-3.5700393583	3.5717530291	-1.2676554975
H	1.0	-2.3562997830	2.5467417506	-2.0723019546
H	1.0	-1.8325650170	3.9821158774	-1.1194058419
C	6.0	2.9779245022	0.2137341515	-0.0283548496
C	6.0	3.9386940539	-0.8474955613	0.0018305980
C	6.0	5.2860057779	-0.4653477115	-0.0804983228
C	6.0	5.6581228452	0.8865651085	-0.1818129962
C	6.0	4.6840434965	1.8987413113	-0.2150507815
C	6.0	3.3123237161	1.6060773091	-0.1454204680
H	1.0	5.0027255754	2.9503437239	-0.2748917035
H	1.0	6.7242536855	1.1553741762	-0.2444732273
H	1.0	6.0647193360	-1.2425834759	-0.0918496179
C	6.0	2.3078041083	2.7564296394	-0.1271322919
H	1.0	1.3014185916	2.3583833087	0.1358644710
C	6.0	2.6545438133	3.8017448357	0.9532531060
C	6.0	2.1995122090	3.4052041859	-1.5258496177
H	1.0	1.8640014847	4.5781761199	0.9979840489
H	1.0	3.6069630179	4.3223426656	0.7274335366
H	1.0	2.7476776945	3.3399716394	1.9568475300
H	1.0	1.4405390143	4.2137913119	-1.5238057657
H	1.0	1.9270301163	2.6758983742	-2.3195856787
H	1.0	3.1670070616	3.8554805870	-1.8281440334
C	6.0	3.5600217203	-2.3238588011	0.0312720156
H	1.0	2.4650564483	-2.4063191859	-0.1382621676
C	6.0	3.8688167248	-2.9348591164	1.4168125034
C	6.0	4.2517364273	-3.1102787634	-1.1017245078
H	1.0	3.3543642627	-2.3873534251	2.2315543946
H	1.0	4.9575850119	-2.9103030801	1.6286648699
H	1.0	3.5470674375	-3.9959903884	1.4453835777
H	1.0	4.0571328293	-2.6601335061	-2.0962729439
H	1.0	3.8783307122	-4.1542684939	-1.1152809261
H	1.0	5.3500922627	-3.1628894801	-0.9583188302
C	6.0	-1.0367250245	-1.4827412736	0.9267358752
C	6.0	0.0096356051	-0.7779620774	1.7958778757
H	1.0	-0.5825640376	-2.3744673395	0.4478414362
H	1.0	-1.8819870629	-1.8151803130	1.5556974879
H	1.0	0.1321219339	-1.3237925603	2.7510117995
H	1.0	-0.2680905825	0.2760284928	2.0144166651

Product **Pro-S-C_2H_4**:

ATOM	CHARGE	X	Y	Z
S	16.0	0.1570435602	0.1191046574	-1.5088568216
N	7.0	-1.3635209803	-0.3280428969	0.4891654158
C	6.0	-0.6614537325	-0.2312449640	1.5750553654
C	6.0	0.7973022184	-0.2254760848	1.6358367719
N	7.0	1.5263419381	0.1613283131	0.6379790615
H	1.0	-1.1859355939	-0.2722678112	2.5501819909
H	1.0	1.2430007173	-0.4687465293	2.6207521945
C	6.0	2.8159122927	-0.0390387123	0.2788945970
C	6.0	3.4807919860	-1.3164726743	0.5107409771
C	6.0	4.7532182858	-1.4685971896	-0.0469198090
C	6.0	5.3763078649	-0.4280371714	-0.7710431158
C	6.0	4.7293104942	0.8050231112	-0.9856001455
C	6.0	3.4435687040	1.0272188306	-0.4897133338
H	1.0	5.2477180549	1.5981621794	-1.5446139398
H	1.0	6.3898258462	-0.5851733702	-1.1736984903
H	1.0	5.2885989774	-2.4199016067	0.0891746879
C	6.0	2.8437154894	-2.4370579994	1.3079122080
H	1.0	1.7392575852	-2.2807323157	1.2983819722
C	6.0	3.3143815049	-2.3651064578	2.7830397744
C	6.0	3.0979076968	-3.8321971038	0.7066799825
H	1.0	2.7891896077	-3.1281416668	3.3928355166
H	1.0	4.4035612390	-2.5645896294	2.8471072914
H	1.0	3.1437456992	-1.3683415598	3.2431909354
H	1.0	4.1627777741	-4.1320798014	0.7873045588
H	1.0	2.5105812586	-4.5929955592	1.2590521253
H	1.0	2.8060512357	-3.8772891277	-0.3620627777
C	6.0	2.7579099757	2.3714716153	-0.6221256451
H	1.0	1.6839958260	2.2079292066	-0.3816052996
C	6.0	2.8647857278	2.9596807901	-2.0393341576
C	6.0	3.3152417917	3.3452043709	0.4469370884
H	1.0	2.2717027274	3.8943062641	-2.1129061083

H	1.0	3.9085149962	3.2296031013	-2.3011884173
H	1.0	2.5021793917	2.2455942521	-2.8083409221
H	1.0	4.3966639870	3.5333081205	0.2860539068
H	1.0	3.1888696918	2.9455364124	1.4735966640
H	1.0	2.7874887132	4.3189853586	0.3851449246
C	6.0	-2.6832180714	-0.1194578322	0.2398007276
C	6.0	-3.3596390928	-1.1449349913	-0.5418045161
C	6.0	-4.7006739084	-0.9278952073	-0.8701439966
C	6.0	-5.3497239587	0.2601869203	-0.4772945838
C	6.0	-4.6766975943	1.2579279333	0.2596814949
C	6.0	-3.3400367760	1.1097460922	0.6477118388
H	1.0	-5.2221456476	2.1710834343	0.5425790231
H	1.0	-6.4067264018	0.4139605507	-0.7479785247
H	1.0	-5.2570825559	-1.6892098784	-1.4359226788
C	6.0	-2.6479229560	2.1776266674	1.4757444833
H	1.0	-1.5519097561	1.9816557918	1.4588445867
C	6.0	-2.8616151465	3.5970433997	0.9112816043
C	6.0	-3.1155919813	2.0843839702	2.9493548720
H	1.0	-2.2590366584	4.3289830992	1.4855175161
H	1.0	-3.9200500698	3.9194290132	0.9862680713
H	1.0	-2.5653072458	3.6682242820	-0.1563418611
H	1.0	-2.5607721049	2.8130801840	3.5745842722
H	1.0	-2.9671641928	1.0715819298	3.3789889506
H	1.0	-4.1966537775	2.3188400421	3.0297345838
C	6.0	-2.6325566251	-2.4365317848	-0.8501495052
H	1.0	-1.5529235574	-2.1794598695	-0.9538320697
C	6.0	-3.1017852749	-3.1234336114	-2.1414459906
C	6.0	-2.7539734561	-3.3876561022	0.3704246638
H	1.0	-3.0712217396	-2.4390978938	-3.0142868089
H	1.0	-4.1344530838	-3.5180616835	-2.0489095323
H	1.0	-2.4490429942	-3.9907311054	-2.3647660967
H	1.0	-2.3905680032	-2.9160134944	1.3066173318
H	1.0	-2.1624626999	-4.3088692153	0.1945757111
H	1.0	-3.8111651655	-3.6830954026	0.5290326856
C	6.0	-1.3154528499	0.4738613669	-2.5501443234
C	6.0	-0.6857368916	1.6854015366	-1.9662465309
H	1.0	-2.2904157461	0.1361493688	-2.1494791750
H	1.0	-1.1365906094	0.2145990257	-3.6093078141
H	1.0	-1.1969225075	2.1729240423	-1.1161760880
H	1.0	-0.0675480371	2.3556519747	-2.5882914301

Product **Pro-Se-C_2H_4**:

ATOM	CHARGE	X	Y	Z
SE	34.0	0.0750849326	-0.4340837464	0.9184759541
N	7.0	-1.1854585826	0.2659790521	-0.3847368929
C	6.0	-0.5921734201	0.7750563468	-1.4597094342
C	6.0	0.8247136045	0.7393083818	-1.5067756252
N	7.0	1.4032878805	0.1176825099	-0.4825127740
H	1.0	-1.2217594713	1.1590695991	-2.2768499941
H	1.0	1.4151686411	1.1030203448	-2.3620462784
C	6.0	2.7862190603	0.0379859411	-0.2343111859
C	6.0	3.5824037630	1.2373825852	-0.3582042383
C	6.0	4.9395580548	1.1211118480	-0.0178176140
C	6.0	5.4964639269	-0.0971730740	0.4024910952
C	6.0	4.6992636188	-1.2519677065	0.5018335060
C	6.0	3.3326237811	-1.2215994041	0.1967179702
H	1.0	5.1646609552	-2.2028982174	0.8013626334
H	1.0	6.5688480847	-0.1509884458	0.6477478205
H	1.0	5.5795027431	2.0145529411	-0.0714250492
C	6.0	3.0401826722	2.5994160310	-0.7712857750
H	1.0	1.9265492152	2.5738469588	-0.7226572050
C	6.0	3.4375476980	2.9142056584	-2.2334389130
C	6.0	3.4837810348	3.7256772986	0.1833687148
H	1.0	3.0007410161	3.8810712793	-2.5558001030
H	1.0	4.5400831703	2.9911636042	-2.3275088632
H	1.0	3.1147665598	2.1276151886	-2.9498176552
H	1.0	4.5744599700	3.9164474800	0.1225086786
H	1.0	2.9778558979	4.6725461482	-0.0940097145
H	1.0	3.2332947902	3.4940506838	1.2382170933
C	6.0	2.5217394933	-2.5135220602	0.2480642179
H	1.0	1.5445079768	-2.3357125625	-0.2520319825
C	6.0	2.2456603683	-2.9311041712	1.7089403891
C	6.0	3.2008444780	-3.6537894503	-0.5401051536
H	1.0	1.6016472882	-3.8334493486	1.7432801712
H	1.0	3.1880113739	-3.1649345780	2.2463003298
H	1.0	1.7478108801	-2.1231238971	2.2942801983
H	1.0	4.1576029219	-3.9690947128	-0.0763339198
H	1.0	3.4088496006	-3.3560244915	-1.5873066314
H	1.0	2.5396636430	-4.5437135030	-0.5581216063
C	6.0	-2.6114073656	0.1435608774	-0.2771695560
C	6.0	-3.3314986429	1.2529569099	0.2490314386
C	6.0	-4.7306136073	1.1109839821	0.3097495933
C	6.0	-5.3607290475	-0.0693978383	-0.1170012333
C	6.0	-4.6107688912	-1.1461203225	-0.6198010686
C	6.0	-3.2090273858	-1.0744300405	-0.7125559457
H	1.0	-5.1269837044	-2.0598811101	-0.9492756025
H	1.0	-6.4569741090	-0.1530557115	-0.0548252424
H	1.0	-5.3404720449	1.9384443566	0.7014638570
C	6.0	-2.3837773749	-2.2117062395	-1.3058849761
H	1.0	-1.3553278186	-2.1404349480	-0.8842229067
C	6.0	-2.9282852363	-3.6058776962	-0.9473596947
C	6.0	-2.2728512092	-2.0401660052	-2.8396693443
H	1.0	-2.2265285319	-4.3894118859	-1.2968298279
H	1.0	-3.9016302379	-3.8050077156	-1.4397382439
H	1.0	-3.0676654959	-3.7327910681	0.1459327454
H	1.0	-1.6444205538	-2.8420969155	-3.2775768607
H	1.0	-1.8288690139	-1.0635516528	-3.1263485990
H	1.0	-3.2753173620	-2.0944925952	-3.3106548618
C	6.0	-2.6355368242	2.5427721763	0.6747118211
H	1.0	-1.5879026099	2.2826804756	0.9529332734
C	6.0	-3.2920759363	3.2031869310	1.9013302739
C	6.0	-2.5746637196	3.5410638106	-0.5053104768
H	1.0	-3.4205081016	2.4968083715	2.7479852170
H	1.0	-4.2914344927	3.6177233621	1.6583320038
H	1.0	-2.6705082372	4.0492448184	2.2566238590
H	1.0	-2.0307813259	3.1356632511	-1.3840647251
H	1.0	-2.0669940213	4.4764270278	-0.1937808150
H	1.0	-3.5962973380	3.8042572366	-0.8479243355
C	6.0	-1.7275059730	-0.2318356560	2.8868065261
C	6.0	-1.9016505153	-1.4890356795	2.3755829728
H	1.0	-2.4052618147	0.5948272613	2.6166872864
H	1.0	-0.9647648472	-0.0208209111	3.6574545963
H	1.0	-2.7256037031	-1.7121611570	1.6772895299
H	1.0	-1.2846658835	-2.3399974239	2.7146792220

Product **Pro-Te-C_2H_4**:

ATOM	CHARGE	X	Y	Z
TE	52.0	0.0827266195	-0.5917028126	1.0648355410
N	7.0	-1.2238450907	0.2932079578	-0.4309170506
C	6.0	-0.5859036134	0.7209269745	-1.5068650890
C	6.0	0.8388226746	0.6502789452	-1.5764521433
N	7.0	1.4728387049	0.0261661493	-0.5946089373
H	1.0	-1.1837475369	1.1168742359	-2.3441135243
H	1.0	1.3863816433	1.0362728760	-2.4518673251
C	6.0	2.8684405301	0.0468954190	-0.4262092220
C	6.0	3.5704471707	1.3037060952	-0.5575142513
C	6.0	4.9499964209	1.2807936352	-0.2970750012
C	6.0	5.6164587710	0.0974019203	0.0577709421
C	6.0	4.9086269122	-1.1121431474	0.1835028276
C	6.0	3.5273797471	-1.1718034966	-0.0424743308

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H           1.0    5.4556038872  -2.0315657669   0.4405553532
H           1.0    6.7033413705   0.1153876037   0.2348523304
H           1.0    5.5217324327   2.2189186905  -0.3634888129
C           6.0    2.9025353309   2.6393762972  -0.8616106086
H           1.0    1.7977765275   2.5124513273  -0.7826735544
C           6.0    3.2114985278   3.0966509319  -2.3065689190
C           6.0    3.2839577722   3.7255085777   0.1648674565
H           1.0    2.6682871978   4.0348091556  -2.5392437285
H           1.0    4.2962129932   3.2932873286  -2.4299152878
H           1.0    2.9373201908   2.3351302277  -3.0681131812
H           1.0    4.3519652931   4.0135711863   0.0848469806
H           1.0    2.6897676282   4.6438642550  -0.0170720497
H           1.0    3.0976377339   3.3898119872   1.2050775679
C           6.0    2.8008517662  -2.5102140511   0.0539303950
H           1.0    1.7906690488  -2.3918719483  -0.3981159513
C           6.0    2.6295033051  -2.9342368414   1.5282881471
C           6.0    3.5048056826  -3.6162575362  -0.7612398173
H           1.0    2.0395341844  -3.8705078694   1.6062856588
H           1.0    3.6102283477  -3.1053884743   2.0187403836
H           1.0    2.1202392392  -2.1505710642   2.1409622596
H           1.0    4.4952970080  -3.8753169597  -0.3346026752
H           1.0    3.6548559752  -3.3090138987  -1.8154215201
H           1.0    2.8931698672  -4.5407633251  -0.7522315773
C           6.0   -2.6534024946   0.2476016838  -0.3588847997
C           6.0   -3.3241957380   1.3702832561   0.2062559900
C           6.0   -4.7273767573   1.2915580381   0.2754736193
C           6.0   -5.4142404550   0.1551504620  -0.1830005227
C           6.0   -4.7168679417  -0.9346771023  -0.7301732593
C           6.0   -3.3132318861  -0.9245883583  -0.8319342573
H           1.0   -5.2771800867  -1.8114467023  -1.0872671626
H           1.0   -6.5127348433   0.1189454861  -0.1156254389
H           1.0   -5.2963675375   2.1362406149   0.6910027367
C           6.0   -2.5529306698  -2.0868618962  -1.4640318909
H           1.0   -1.5070166362  -2.0628330610  -1.0802873825
C           6.0   -3.1388496181  -3.4619377326  -1.0957145638
C           6.0   -2.4889019105  -1.9055186392  -2.9989797911
H           1.0   -2.4875992155  -4.2702337664  -1.4845148682
H           1.0   -4.1414921803  -3.6139998259  -1.5436949281
H           1.0   -3.2327672667  -3.5951386290   0.0018611368
H           1.0   -1.9083670882  -2.7274723612  -3.4649517369
H           1.0   -2.0192842047  -0.9435708039  -3.2931352070
H           1.0   -3.5089224696  -1.9168308921  -3.4344561789
C           6.0   -2.5660898941   2.6247546612   0.6320457928
H           1.0   -1.5349507471   2.3137348053   0.9211946585
C           6.0   -3.1941896275   3.3378100274   1.8433457395
C           6.0   -2.4342424689   3.6016492324  -0.5599045916
H           1.0   -3.3624661368   2.6549333512   2.7026380255
H           1.0   -4.1705476217   3.7976000191   1.5882865321
H           1.0   -2.5321467851   4.1583113126   2.1847605706
H           1.0   -1.9155860620   3.1468049718  -1.4292623760
H           1.0   -1.8666503140   4.5053079304  -0.2577285795
H           1.0   -3.4349149971   3.9273406106  -0.9105715966
C           6.0   -1.8125821278  -0.1408699602   2.9186764282
C           6.0   -2.1251689166  -1.3663223627   2.3686762403
H           1.0   -2.2990287148   0.7815508703   2.5591180408
H           1.0   -1.1588902996  -0.0520484764   3.8054094066
H           1.0   -2.8789633315  -1.4513257830   1.5658184832
H           1.0   -1.7383193272  -2.3083070719   2.7985136904
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