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SUPPLEMENTARY MATERIAL

Structure, Stability, and Cycloaddition Reactions of Nitrile Selenides

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Table S1: Calculated equilibrium structures[a] of small nitrile selenides

	HCNSe	**FCNSe**[b]	**ClCNSe**	**BrCNSe**	**NCCNSe**[c]	**CH_3CNSe**[d]
X–C	1.062	1.287	1.623	1.779	1.350	1.448
C≡N	1.156	1.175	1.160	1.161	1.169	1.156
N–Se	1.775	1.763	1.782	1.779	1.741	1.792
XCN	180.0	145.7	180.0	180.0	180.0	180.0
CNSe	180.0	170.9	180.0	180.0	180.0	180.0
E[e]	–2495.064975	–2594.301966	–2954.684082	–5068.681923	–2587.335694	–2534.411034
μ[f]	3.86	1.90	4.26	4.58	1.31	5.70
A[g]	----	271.6075	----	---	---	159.7443
B	4.0457	1.6137	0.9463	0.5659	0.9906	1.5945
C	4.0457	1.6137	0.9463	0.5659	0.9906	1.5945
BDE[h]	229 (199)	199 (173)	221 (191)	225 (196)	253 (224)	230 (200)

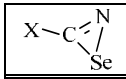
[a] Calculated at the B3LYP/cc-pVTZ level. Bond lengths are in angstrom and bond angles are in degrees.
[b] Barrier at linearity on the equilibrium FCN deformation potential curve is 267 cm^{-1}.
[c] r_e(N≡C)=1.161 Å, α(NCC)=180.0º. [d] r_e(CH)=1.091 Å, α(HCC)=110.4º. [e] Total energy in a.u.
[f] Dipole moment in Debye. [g] Rotational constants in GHz.
[h] The N–Se bond dissociation energy in kJ mol^{-1} (ΔG_{0K}); calculated by taking the difference between the ZPE corrected total energy of nitrile selenide and the sum of ZPE corrected total energies of nitrile and singlet selenium atom. In the unimolecular decomposition process the extrusion of singlet selenium atom is the 'spin-allowed' process. $\Delta G°_{298K}$ values are in parenthesis.

Table S2: Calculated equilibrium structures[a] of lowest energy excited triplet state nitrile selenides

	^{3}HCNSe	^{3}FCNSe	^{3}ClCNSe	^{3}BrCNSe	^{3}NCCNSe[b]	^{3}CH$_3$CNSe[c]
X–C	1.093	1.318	1.734	1.928	1.365	1.482
C≡N	1.225	1.255	1.239	1.231	1.224	1.227
N–Se	1.909	1.805	1.829	1.830	1.899	1.877
XCN	124.8	121.1	124.6	124.3	143.6	132.1
CNSe	125.2	129.0	128.4	130.1	126.1	122.5
E[d]	–2494.994346	–2594.272026	–2954.633685	–5068.631380	–2587.266862	–2534.340829
BDE[e]	–97 (–121)	–21 (–46)	–51 (–77)	–47 (–72)	–65 (–87)	–94 (–120)
AE[f]	1 (0) [0]	64 (63) [63]	27 (25) [25]	26 (25) [25]	0.02 (0) [3]	3 (1) [1]
Δ(S–T)[g]	181 (172)	76 (71)	128 (121)	128 (121)	174 (163)	180 (173)

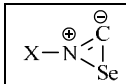
[a] Calculated at the UB3LYP/cc-pVTZ level. Bond lengths are in angstrom and bond angles are in degrees. XCNSe molecular frame is trans-bent planar.
[b] r_e(N≡C)=1.165 Å, α(NCC)=171.6º. [c] r_e(CH′)=1.094 Å, α(HCC′)=111.0º, r_e(CH″)=1.091 Å, α(HCC″)=109.9º, δ(HCCN″)=121.1°.
[d] Total energy in a.u.
[e] The N–Se bond dissociation energy in kJ mol^{-1} (ΔG_{0K}); calculated by taking the difference between the ZPE corrected total energy of nitrile selenide and the sum of ZPE corrected total energies of nitrile and triplet selenium atom. In the unimolecular decomposition process the extrusion of triplet selenium atom is 'spin-allowed' process. $\Delta G°_{298K}$ values are in parenthesis. Selenium atom loss is exothermic.
[f] Barrier on the potential energy surface for the rupture of the N–Se bond in kJ mol^{-1}; ΔG_{0K} and $\Delta G°_{298K}$ values are in parenthesis and brackets, respectively.
[g] Energy difference between the ground state singlet and the lowest energy triplet state (ΔG_{0K} values in kJ mol^{-1}); $\Delta G°_{298K}$ values are in parenthesis.

Table S3: Calculated equilibrium structures[a] of selenazirines

	**HC(NSe)**	**FC(NSe)**	**ClC(NSe)**	**BrC(NSe)**	**NCC(NSe)**[b]	**CH_3C(NSe)**[c]
X–C	1.082	1.302	1.696	1.865	1.405	1.474
C=N	1.222	1.231	1.229	1.226	1.233	1.223
C–Se	1.926	1.870	1.899	1.903	1.927	1.946
N–Se	2.114	2.144	2.118	2.119	2.088	2.098
XCN	139.6	136.5	137.3	136.8	140.2	142.5
XCSe	139.4	138.6	140.5	141.0	140.3	138.1
CNSe	64.2	60.3	62.7	62.8	65.1	65.7
E[d]	–2495.044936	–2594.313668	–2954.675565	–5068.671628	–2587.304352	–2534.391192

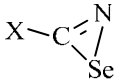
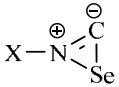
[a] Calculated at the B3LYP/cc-pVTZ level. Bond lengths are in angstrom and bond angles are in degrees.
[b] r_e(N≡C)=1.152 Å, α(NCN)=176.9º. [c] r_e(CH(ip))=1.090 Å, α(HCC(ip))=110.2º. r_e(CH(op))=1.090 Å, α(HCC(op))=109.3º.
[d] Total energy in a.u.

Table S4: Calculated equilibrium structures[a] of selenaziridinilidenes

	**HN(CSe)**	**FN(CSe)**	**ClN(CSe)**	**BrN(CSe)**	**NCN(CSe)**[b]	**CH_3N(CSe)**[c]
X–N	1.011	1.400	1.731	1.904	1.319	1.443
N=C	1.236	1.240	1.241	1.236	1.267	1.233
N–Se	1.968	1.853	1.914	1.917	2.000	1.976
C–Se	2.177	2.320	2.230	2.242	2.069	2.167
XNC	141.1	131.3	135.1	134.3	146.1	144.3
XNSe	136.8	133.5	137.7	137.9	139.1	134.3
NCSe	63.6	52.7	59.0	58.7	68.9	64.4
E[d]	–2495.007857	–2594.196522	–2954.595124	–5068.602039	–2587.250012	–2534.341886

[a] Calculated at the B3LYP/cc-pVTZ level. Bond lengths are in angstrom and bond angles are in degrees.
[b] r_e(N≡C)=1.156 Å, α(NCN)=177.9º. [c] r_e(CH(ip))=1.089 Å, α(HCC(ip))=108.4º. r_e(CH(op))=1.088 Å, α(HCC(op))=109.0º.
[d] Total energy in a.u.

Table S5: Total energies[a] of minima and transition states of unimolecular isomerisation and dissociation processes of nitrile selenides

X=	**H**	**F**	**Cl**	**Br**	**NC**	**CH_3**
TSu3 (XC(N)Se)	–2493.183909	–2592.316027	–2952.358201	–5065.285742	–2585.326114	–2532.463766
	–2493.277620	–2592.403757	–2952.409804	–5065.323465	–2585.357625	–2532.533017
TSu1 (XCNSe)	–2493.241875	–2592.349525	–2952.368353	–5065.283345	–2585.315514	–2532.504106
XCNSe	–2493.289488	–2592.383891	–2952.409359	–5065.325987	–2585.373881	–2532.544271
TSu2 (XN(C)Se)	–2493.203439	–2592.268500	–2952.313420	–5065.241493	–2585.244653	–2532.437221
	–2493.238203	–2592.281590	–2952.325136	–5065.249366	–2585.297908	–2532.481958
XCN	–93.274802	–192.380757	–552.397665	–2665.312128	–185.353554	–132.527459

[a] Calculated at the CCSD(T)//B3LYP/cc-pVTZ level. See Figure S1.
Total energy of singlet and triplet selenium atom, respectively: –2399.948783 and –2399.994409.

Table S6: SR-AQCC total energies[a] of nitrile selenides, nitriles, ethenes, and ethynes

HCNSe	–2493.25804	HCN	–93.25422	HC≡CH	–77.168359
FCNSe	–2592.34037	FCN	–192.35058	FC≡CF	–275.354238
ClCNSe	–2952.36682	ClCN	–552.36585	$H_3CC{\equiv}CCH_3$	–155.644750
NCCNSe	–2585.31743	NCCN	–185.30979	$H_2C{=}CH_2$	–78.421171
CH_3CNSe	–2532.50460	CH_3CN	–132.49828	*trans*-FHC=CHF	–276.655609
				trans-$H_3CHC{=}CHCH_3$	–156.889399

[a] Calculated at the SR-AQCC//B3LYP/cc-pVTZ level.

Table S7: MR-AQCC total energies of minima and transitional states of bimolecular processes of nitrile selenides

	HCNSe	**FCNSe**	**ClCNSe**	**NCCNSe**	**CH_3CNSe**
TS1	–4986.500352		–5904.719064	–5170.606554	–5064.983330
ctc	–4986.538671	–5184.789279	–5904.776043	–5170.657201	–5065.006668
TS2	–4986.532903	–5184.782187	–5904.773486	–5170.651601	–5065.004527
ttc	–4986.537573	–5184.792975	–5904.782931	–5170.660073	–5065.012079
TS5	–4986.525117	–5184.785061	–5904.780461	–5170.650667	–5065.006001
TS3	–4986.529242	–5184.786146	–5904.779667	–5170.653425	–5065.008381
ttt	–4986.538178	–5184.797725	–5904.790126	–5170.663648	–5065.018207
TS6	–4986.523817	–5184.789623	–5904.784443	–5170.651719	–5065.005377
tct	–4986.530836	–5184.794737	–5904.784405	–5170.657257	–5065.006778
TS7	–4986.524539	–5184.784674	–5904.776079	–5170.649221	–5064.999883
sfur	–4986.591205	–5184.825033	–5904.827028	–5170.705617	–5065.072355
TS4	–4986.526481	–5184.780419	–5904.776526	–5170.649820	–5065.006513
ss	–4986.596772	–5184.851395	–5904.839992	–5170.714049	–5065.072072
TSs1	–4986.497821	–5184.693122	–5904.720898	–5170.593897	–5064.992600
SP1	–4986.599744	–5184.827228	–5904.825654	–5170.705290	–5065.084508
TSs2	–4986.503741		–5904.722950	–5170.611872	–5064.993011
SP2	–4986.584193	–5184.833363	–5904.829658	–5170.701976	–5065.062266
TS-t	–4986.515768		–5904.735475	–5170.625766	–5065.010238

[a] Calculated at the MR-AQCC(2,2)//UB3LYP/cc-pVTZ level. Total energy of open-shell singlet Se_2: –4800.066348. See Figure S2 and S3.

Table S8: MR-AQCC total energies of cycloadducts and relevant transition states for reactions of FCNSe and CH_3CNSe with dipolarophiles

dipolarophile	FCNSe		CH_3CNSe	
	TS	adduct	TS	adduct
FC≡CF	–2867.683636	–2867.893656	–2807.832951	–2808.009712
HC≡CH			–2609.647186	–2609.786803
$H_3CC{\equiv}CCH_3$			–2688.114117	–2688.254705
FHC=CHF	–2868.992055	–2869.115310	–2809.129699	–2809.229460
$H_2C{=}CH_2$			–2610.903510	–2610.992948
$H_3CHC{=}CHCH_3$			–2689.368111	–2689.459846
FC≡N	–2784.691457	–2784.830921	–2724.844242	-2724.944943
HC≡N			–2625.740899	–2625.823814
$H_3CC{\equiv}N$			–2664.982852	–2665.062457

[a] Calculated at the MR-AQCC(2,2)//(U)B3LYP/cc-pVTZ level.

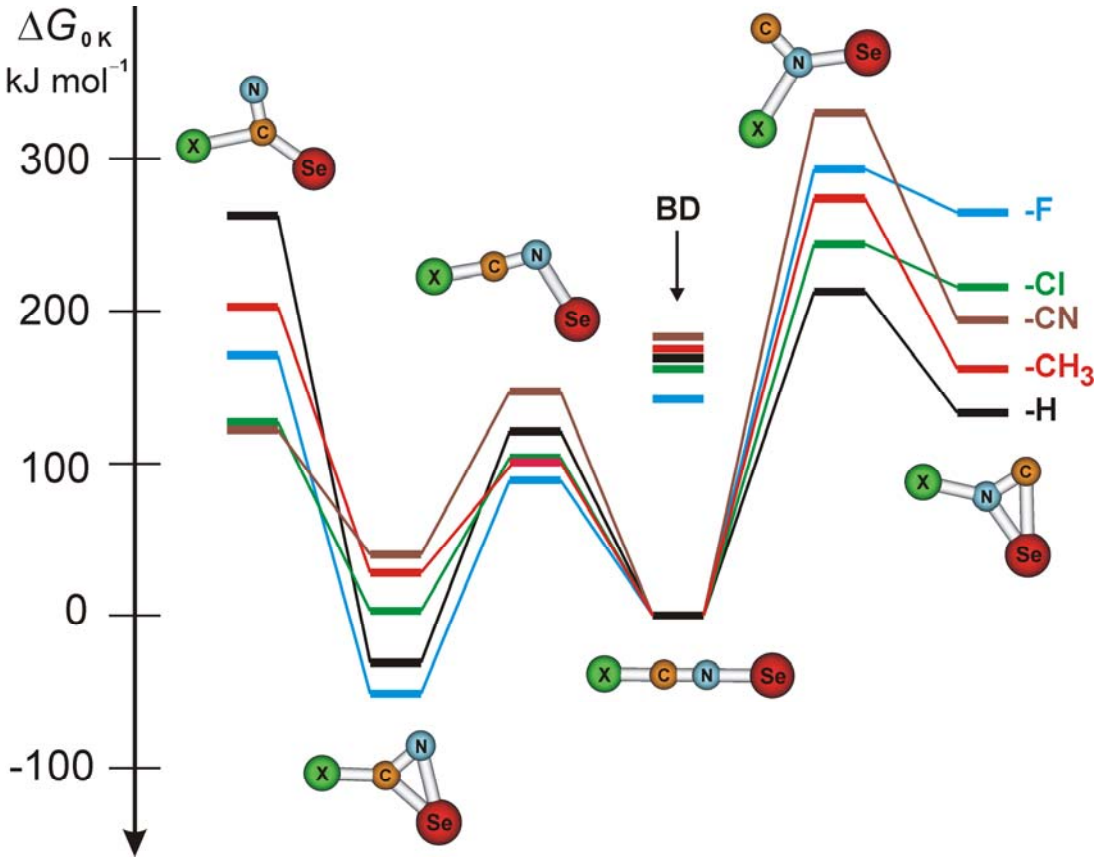


Figure S1.

Unimolecular isomerisation of nitrile selenides (XCNSe). N–Se bond dissociation energies are indicated (BD). Results for BrCNSe are omitted from the figure for clarity. Calculated at the CCSD(T)//B3LYP/cc-pVTZ level.

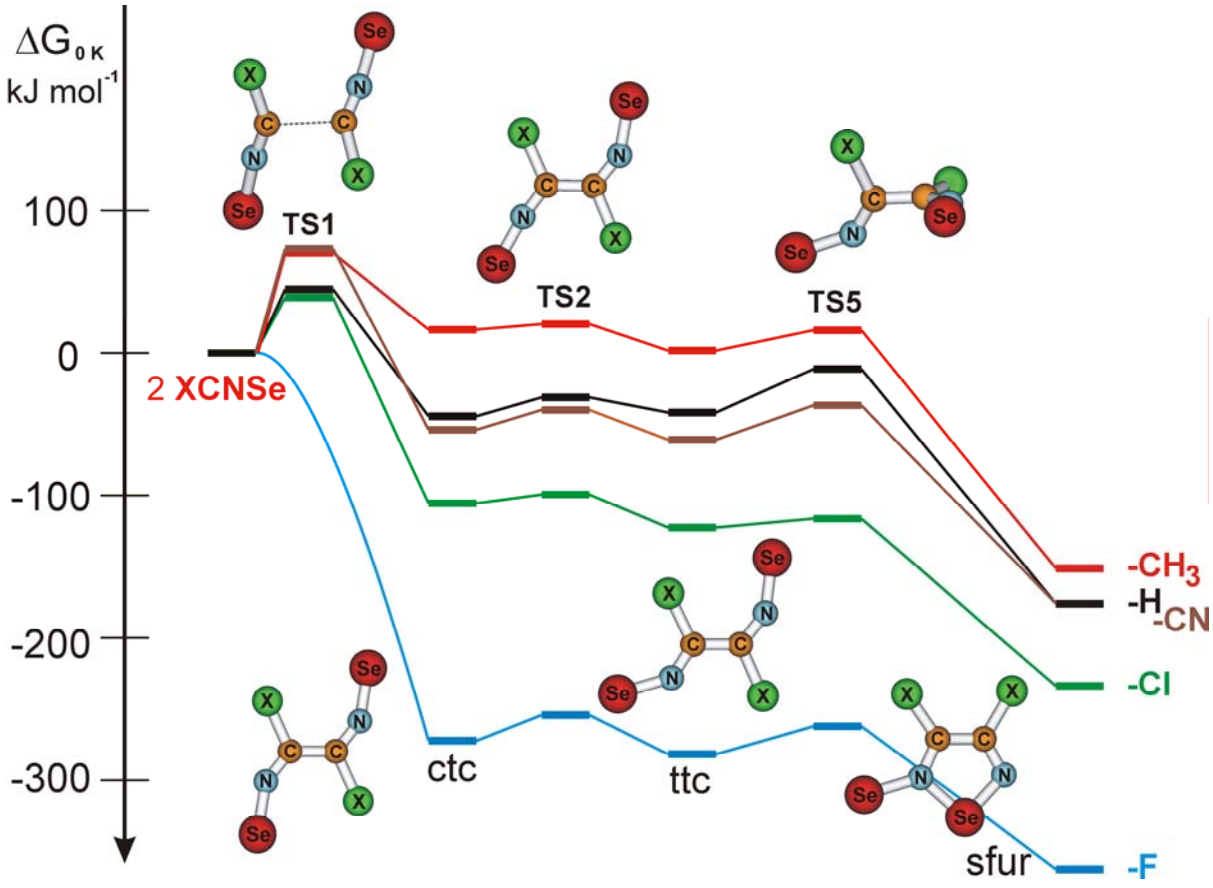


Figure S2

Multistep cyclodimerisation of nitrile selenides to 1,2,5-selenadiazole-2-selenide (**sfur**). Gibbs free energies are relative to that of the two monomers. Calculated at the MR-AQCC(2,2)//(U)B3LYP/cc-pVTZ level.

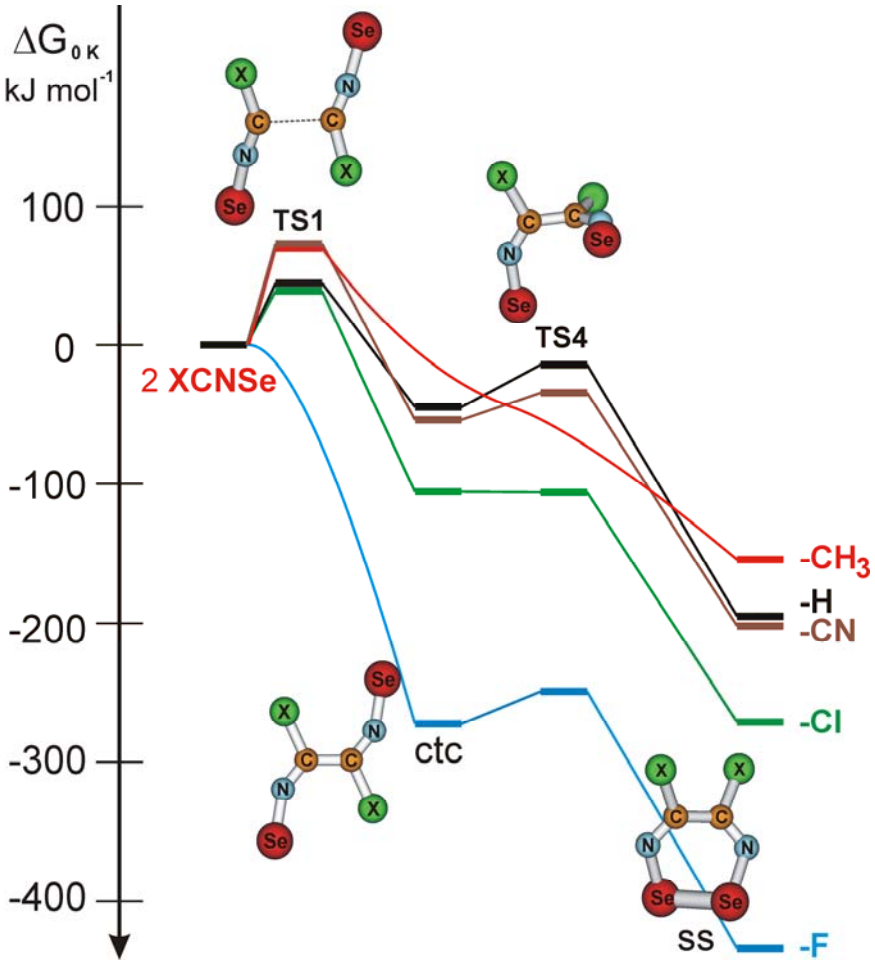


Figure S3

Multistep cyclodimerisation of nitrile selenides to 1,2,3,6-diselenadiazines (**ss**). Gibbs free energies are relative to that of the two monomers. Calculated at the MR-AQCC(2,2)//(U)B3LYP/cc-pVTZ level.

Cartesian coordinates (in Å) of calculated structures
Calculated at the (U)B3LYP/cc-pVTZ level.

HCNSe
H, 0.000000, 0.000000, -3.285228
C, 0.000000, 0.000000, -2.222756
N, 0.000000, 0.000000, -1.066383
Se, 0.000000, 0.000000, 0.708425

FCNSe
F, 0.517909, 2.868715, 0.000000
C, -0.107439, 1.743937, 0.000000
N, 0.000000, 0.573730, 0.000000
Se, -0.118134, -1.185240, 0.000000

ClCNSe
Cl, 0.000000, 0.000000, -2.882168
C, 0.000000, 0.000000, -1.258801
N, 0.000000, 0.000000, -0.098896
Se, 0.000000, 0.000000, 1.683586

BrCNSe
Br, 0.000000, 0.000000, 2.338041
C, 0.000000, 0.000000, 0.558977
N, 0.000000, 0.000000, -0.602173
Se, 0.000000, 0.000000, -2.381474

NCCNSe
C, 0.000000, 0.000000, -2.707544
C, 0.000000, 0.000000, -1.357596
N, 0.000000, 0.000000, -0.188312
Se, 0.000000, 0.000000, 1.552601
N, 0.000000, 0.000000, -3.868487

CH_3CNSe
C, 0.000000, 0.000000, -3.129228
C, 0.000000, 0.000000, -1.681324
N, 0.000000, 0.000000, -0.525378
Se, 0.000000, 0.000000, 1.266744
H, 0.000000, 1.022922, -3.509451
H, -0.885877, -0.511461, -3.509451
H, 0.885877, -0.511461, -3.509451

open-shell singlet Se_2
Se, 0.000000, 0.000000, 1.094407
Se, 0.000000, 0.000000, -1.094407

HCN
H, 0.000000, 0.000000, -1.562314
C, 0.000000, 0.000000, -0.497044
N, 0.000000, 0.000000, 0.649225

FCN
F, 0.000000, 0.000000, 1.114223
C, 0.000000, 0.000000, -0.151734
N, 0.000000, 0.000000, -1.302514

ClCN
Cl, 0.000000, 0.000000, 0.978410
C, 0.000000, 0.000000, -0.658470
N, 0.000000, 0.000000, -1.811734

BrCN
Br, 0.000000, 0.000000, 0.654428
C, 0.000000, 0.000000, -1.140835
N, 0.000000, 0.000000, -2.294282

NCCN
C, 0.000000, 0.000000, 0.687614
C, 0.000000, 0.000000, -0.687614
N, 0.000000, 0.000000, -1.840122
N, 0.000000, 0.000000, 1.840122

CH_3CN
C, 0.000000, 0.000000, -1.173902
C, 0.000000, 0.000000, 0.280614
N, 0.000000, 0.000000, 1.430247
H, 0.000000, 1.022343, -1.550667
H, -0.885375, -0.511171, -1.550667
H, 0.885375, -0.511171, -1.550667

HCCH
H, 0.000000, 0.000000, 1.659598
C, 0.000000, 0.000000, 0.597998
C, 0.000000, 0.000000, -0.597998
H, 0.000000, 0.000000, -1.659598

FCCF
F, 0.000000, 0.000000, 1.877146
C, 0.000000, 0.000000, 0.591778
C, 0.000000, 0.000000, -0.591778
F, 0.000000, 0.000000, -1.877146

H_2CCH_2
C, 0.000000, 0.000000, 0.662025
C, 0.000000, 0.000000, -0.662025
H, 0.000000, 0.920761, 1.231349
H, 0.000000, -0.920761, -1.231349
H, 0.000000, -0.920761, 1.231349
H, 0.000000, 0.920761, -1.231349

H_3CCCCH_3
C, 0.000000, 0.000000, 2.057181
C, 0.000000, 0.000000, 0.600477
C, 0.000000, 0.000000, -0.600477
C, 0.000000, 0.000000, -2.057181
H, 0.000000, 1.017851, 2.451866
H, -0.881485, -0.508926, 2.451866
H, 0.881485, -0.508926, 2.451866
H, 0.000000, 1.017851, -2.451866
H, 0.881485, -0.508926, -2.451866
H, -0.881485, -0.508926, -2.451866

FHCCHF
C, -0.331439, 0.570498, 0.000000
C, 0.331439, -0.570498, 0.000000
F, 0.331439, 1.740376, 0.000000
F, -0.331439, -1.740376, 0.000000
H, -1.407181, 0.665092, 0.000000
H, 1.407181, -0.665092, 0.000000

$H_3CHCCHCH_3$
C, -0.541988, 1.881828, 0.000000
C, -0.541988, 0.383982, 0.000000
C, 0.541988, -0.383982, 0.000000
C, 0.541988, -1.881828, 0.000000
H, -1.518421, -0.094500, 0.000000
H, 1.518421, 0.094500, 0.000000
H, -0.472868, -2.280704, 0.000000
H, 1.062141, -2.277841, 0.876470
H, 1.062141, -2.277841, -0.876470
H, 0.472868, 2.280704, 0.000000
H, -1.062141, 2.277841, 0.876470
H, -1.062141, 2.277841, -0.876470

ctc-H
C, -0.316589, 0.659626, 0.000000
C, 0.316589, -0.659626, 0.000000
H, 1.406923, -0.679288, 0.000000
H, -1.406923, 0.679288, 0.000000
N, 0.316589, 1.758584, 0.000000
Se, 1.942386, 2.391855, 0.000000
N, -0.316589, -1.758584, 0.000000
Se, -1.942386, -2.391855, 0.000000

ctc-F
C, 0.073824, 0.729751, 0.000000
C, -0.073824, -0.729751, 0.000000
F, 1.117569, -1.359885, 0.000000
F, -1.117569, 1.359885, 0.000000
N, 1.117569, 1.420429, 0.000000
Se, 2.861551, 1.259974, 0.000000
N, -1.117569, -1.420429, 0.000000
Se, -2.861551, -1.259974, 0.000000

ctc-Cl
C, 0.155480, 0.724645, 0.000000
C, -0.155480, -0.724645, 0.000000
Cl, 1.275430, -1.777179, 0.000000
Cl, -1.275430, 1.777179, 0.000000
N, 1.275430, 1.279416, 0.000000
Se, 3.006182, 1.184319, 0.000000
N, -1.275430, -1.279416, 0.000000
Se, -3.006182, -1.184319, 0.000000

ctc-NC
C, 0.061089, 0.740799, 0.000000
C, -0.061089, -0.740799, 0.000000
C, 1.158666, -1.502672, 0.000000
C, -1.158666, 1.502672, 0.000000
N, 1.158666, 1.400502, 0.000000
Se, 2.879927, 1.291740, 0.000000
N, -1.158666, -1.400502, 0.000000
Se, -2.879927, -1.291740, 0.000000
N, 2.129537, -2.123489, 0.000000
N, -2.129537, 2.123489, 0.000000

ctc-CH_3
C, -0.062584, 0.745455, 0.000000
C, 0.062584, -0.745455, 0.000000
C, -1.188486, -1.587529, 0.000000
C, 1.188486, 1.587529, 0.000000
N, -1.188486, 1.334733, 0.000000
Se, -2.925811, 1.348136, 0.000000
N, 1.188486, -1.334733, 0.000000
Se, 2.925811, -1.348136, 0.000000
H, -0.915162, -2.638579, 0.000000
H, -1.799931, -1.376767, 0.878257
H, -1.799931, -1.376767, -0.878257
H, 0.915162, 2.638579, 0.000000
H, 1.799931, 1.376767, 0.878257
H, 1.799931, 1.376767, -0.878257

ttc-H
C, -1.407385, 0.009391, 0.000000
C, 0.000000, 0.390888, 0.000000
H, 0.727513, -0.423999, 0.000000
H, -2.141885, 0.810771, 0.000000
N, -1.825271, -1.194229, 0.000000
Se, -1.153737, -2.812012, 0.000000
N, 0.343456, 1.613809, 0.000000
Se, 1.748778, 2.643614, 0.000000

ttc-F

C,	1.279871	-0.236564	0.000000
C,	0.000000	0.478376	0.000000
F,	-1.067348	-0.347405	0.000000
F,	2.330382	0.598026	0.000000
N,	1.489417	-1.470805	0.000000
Se,	0.634665	-3.000867	0.000000
N,	-0.110701	1.726772	0.000000
Se,	-1.478710	2.839154	0.000000

ttc-Cl

C,	0.911354	-0.683608	0.000000
C,	0.000000	0.478810	0.000000
Cl,	-1.728449	0.096867	0.000000
Cl,	2.625125	-0.239706	0.000000
N,	0.625559	-1.901729	0.000000
Se,	-0.600123	-3.132652	0.000000
N,	0.415918	1.664611	0.000000
Se,	-0.223464	3.289031	0.000000

ttc-NC

C,	1.006476	-0.667883	0.000000
C,	0.000000	0.414402	0.000000
C,	-1.393998	0.074602	0.000000
C,	2.384114	-0.251286	0.000000
N,	0.770030	-1.926943	0.000000
Se,	-0.514895	-3.087177	0.000000
N,	0.391113	1.637313	0.000000
Se,	-0.274371	3.234862	0.000000
N,	-2.528806	-0.129400	0.000000
N,	3.489875	0.070415	0.000000

ttt-H

C,	0.000000	0.724716	0.000000
C,	-0.001394	-0.724882	0.000000
H,	-0.972349	-1.220563	0.000000
H,	0.970098	1.221724	0.000000
N,	-1.101945	1.368908	0.000000
Se,	-1.650138	3.028403	0.000000
N,	1.099802	-1.370382	0.000000
Se,	1.650892	-3.028104	0.000000

ttt-F

C,	0.000000	0.731976	0.000000
C,	-0.000031	-0.731982	0.000000
F,	-1.233568	-1.263147	0.000000
F,	1.233536	1.263142	0.000000
N,	-1.043709	1.428867	0.000000
Se,	-1.331911	3.170968	0.000000
N,	1.043676	-1.428874	0.000000
Se,	1.331932	-3.170965	0.000000

ttc-CH_3

C,	-0.050971	-1.496887	0.001652
C,	-0.431025	-0.042276	0.000730
N,	-1.638568	0.365644	-0.000016
Se,	-3.274233	-0.260604	-0.000397
C,	0.619396	1.012660	0.000533
N,	1.867249	0.767087	0.000158
Se,	3.164820	-0.395637	-0.000433
C,	0.168004	2.452264	0.000503
H,	-0.949227	-2.109229	0.004064
H,	0.546817	-1.744388	-0.876745
H,	0.550353	-1.742445	0.878143
H,	1.032733	3.109743	0.001977
H,	-0.445562	2.657755	-0.877494
H,	-0.448248	2.657062	0.876743

ttt-Cl

C,	0.000000	0.736026	0.000000
C,	-0.000009	-0.736029	0.000000
Cl,	-1.601702	-1.478109	0.000000
Cl,	1.601691	1.478110	0.000000
N,	-1.059579	1.414456	0.000000
Se,	-1.526688	3.099276	0.000000
N,	1.059568	-1.414463	0.000000
Se,	1.526697	-3.099275	0.000000

ttt-NC

C,	-1.272560	-1.402804	0.000000
N,	-2.262577	-1.991957	0.000000
C,	-0.000532	-0.734805	0.000000
N,	1.113834	-1.373729	0.000000
Se,	1.671340	-3.016574	0.000000
C,	0.000000	0.734601	0.000000
N,	-1.114419	1.373481	0.000000
Se,	-1.670930	3.016766	0.000000
C,	1.272043	1.402537	0.000000
N,	2.262071	1.991674	0.000000

ttt-CH_3

C,	0.000000	0.738979	0.000000
N,	-1.131797	1.335908	0.000000
Se,	-1.694490	2.998037	0.000000
C,	-0.000006	-0.738983	0.000000
N,	1.131789	-1.335914	0.000000
Se,	1.694494	-2.998034	0.000000
C,	1.299235	1.496939	0.000000
C,	-1.299242	-1.496943	0.000000
H,	-2.152537	-0.826303	0.000000
H,	-1.343846	-2.142344	0.879879
H,	-1.343846	-2.142344	-0.879879
H,	2.152531	0.826299	0.000000
H,	1.343839	2.142340	0.879879
H,	1.343839	2.142340	-0.879879

tct-H

C,	1.350977	-0.551860	0.000000
C,	1.155015	0.890844	0.000000
H,	2.063022	1.495880	0.000000
H,	2.387449	-0.892944	0.000000
N,	0.381923	-1.380505	0.000000
Se,	0.086398	-3.094745	0.000000
N,	0.000000	1.431251	0.000000
Se,	-0.738159	3.006743	0.000000

tct-F

C,	0.000000	1.053439	0.000000
C,	-1.053389	0.028753	0.000000
F,	-2.299179	0.539724	0.000000
F,	-0.476248	2.312857	0.000000
N,	1.225709	0.791208	0.000000
Se,	2.687893	1.777306	0.000000
N,	-0.824695	-1.203696	0.000000
Se,	-1.849890	-2.638452	0.000000

tct-Cl

C,	0.000000	0.953397	0.000000
N,	1.242425	0.753577	0.000000
Se,	2.732608	1.661035	0.000000
C,	-0.932330	-0.199595	0.000000
N,	-0.476796	-1.372633	0.000000
Se,	-1.052160	-3.019819	0.000000
Cl,	-0.683126	2.578072	0.000000
Cl,	-2.663970	0.128354	0.000000

tct-NC

C,	-1.017656	-0.050571	0.000000
N,	-0.647281	-1.281056	0.000000
Se,	-1.353830	-2.860307	0.000000
C,	0.000000	1.018719	0.000000
N,	1.247337	0.709736	0.000000
Se,	2.789330	1.494337	0.000000
C,	-2.405455	0.316699	0.000000
C,	-0.435460	2.386653	0.000000
N,	-3.532370	0.558763	0.000000
N,	-0.732765	3.500270	0.000000

sfur-H

C,	1.071486	1.251711	0.000000
C,	2.310865	0.567367	0.000000
N,	2.310886	-0.742193	0.000000
Se,	0.598729	-1.298305	0.000000
N,	0.000000	0.470174	0.000000
Se,	-1.794840	0.932907	0.000000
H,	0.937944	2.322218	0.000000
H,	3.259521	1.090970	0.000000

tct-CH_3

C,	-1.487678	2.293309	0.158697
C,	-0.742229	0.987189	0.031362
C,	0.742240	0.987138	-0.031364
C,	1.487770	2.293207	-0.158702
N,	-1.344833	-0.135317	-0.037288
Se,	-2.966475	-0.782500	-0.020485
N,	1.344754	-0.135423	0.037295
Se,	2.966463	-0.782498	0.020485
H,	-2.461163	2.114438	0.610609
H,	-0.943292	3.015105	0.765198
H,	-1.651796	2.740654	-0.825615
H,	2.461184	2.114293	-0.610752
H,	0.943366	3.015087	-0.765084
H,	1.652052	2.740466	0.825622

sfur-F

C,	1.203973	-0.144448	0.000000
C,	1.252985	-1.570702	0.000000
N,	0.161412	-2.247102	0.000000
Se,	-1.210601	-1.060465	0.000000
N,	0.000000	0.383086	0.000000
Se,	-0.503880	2.160980	0.000000
F,	2.278675	0.606222	0.000000
F,	2.434738	-2.170497	0.000000

sfur-Cl

C,	0.669713	-0.550835	0.000000
C,	-0.167458	-1.721232	0.000000
N,	-1.450075	-1.577928	0.000000
Se,	-1.821313	0.193698	0.000000
N,	0.000000	0.595096	0.000000
Se,	0.581904	2.350192	0.000000
Cl,	2.369085	-0.574684	0.000000
Cl,	0.529555	-3.306493	0.000000

sfur-NC

C,	0.763138	-0.585517	0.000000
C,	0.015451	-1.811432	0.000000
N,	-1.292729	-1.750856	0.000000
Se,	-1.786993	-0.028843	0.000000
N,	0.000000	0.522987	0.000000
Se,	0.486446	2.286689	0.000000
C,	2.173761	-0.508968	0.000000
C,	0.661437	-3.089795	0.000000
N,	3.326414	-0.485640	0.000000
N,	1.185727	-4.113988	0.000000

sfur-CH_3

C,	-1.196177	-0.215205	0.000000
C,	-1.146613	-1.655385	0.000000
N,	0.029991	-2.227025	0.000000
Se,	1.309072	-0.959288	0.000000
N,	0.000000	0.361069	0.000000
Se,	0.424505	2.173669	0.000000
C,	-2.426731	0.619569	0.000000
C,	-2.378030	-2.513195	0.000000
H,	-3.321827	0.003574	0.000000
H,	-2.436049	1.277007	0.872421
H,	-2.436049	1.277007	-0.872421
H,	-2.086741	-3.560077	0.000000
H,	-2.992788	-2.319724	-0.880758
H,	-2.992788	-2.319724	0.880758

ss-H

C,	0.664643	1.978458	-0.332247
N,	1.536387	1.064196	-0.480025
Se,	1.168060	-0.655325	0.180418
Se,	-1.168060	-0.655325	-0.180418
N,	-1.536386	1.064198	0.480026
C,	-0.664642	1.978458	0.332246
H,	-0.958614	2.960918	0.706898
H,	0.958617	2.960917	-0.706898

ss-F

C,	-1.507693	0.698392	-0.267705
C,	-1.507692	-0.698392	0.267705
N,	-0.589543	-1.547588	0.343498
Se,	1.108772	-1.148389	-0.294082
Se,	1.108771	1.148389	0.294082
N,	-0.589544	1.547588	-0.343499
F,	-2.725029	-1.055941	0.698646
F,	-2.725030	1.055940	-0.698646

ss-CH_3

C,	1.486610	-0.696807	-0.295059
C,	2.788014	-1.146705	-0.922318
C,	1.486610	0.696807	0.295059
C,	2.788014	1.146705	0.922318
N,	0.545224	-1.558422	-0.303186
Se,	-1.141306	-1.106577	0.392620
Se,	-1.141306	1.106577	-0.392620
N,	0.545224	1.558422	0.303186
H,	2.643533	-2.125643	-1.370166
H,	3.108807	-0.443862	-1.694093
H,	3.587764	-1.207454	-0.182677
H,	2.643533	2.125644	1.370165
H,	3.108806	0.443863	1.694094
H,	3.587764	1.207453	0.182677

ss-Cl

C,	1.085450	-0.734939	-0.164621
C,	1.085445	0.734960	0.164571
N,	0.158015	1.575794	0.036578
Se,	-1.523884	1.033467	-0.569597
Se,	-1.523862	-1.033482	0.569603
N,	0.158036	-1.575787	-0.036601
Cl,	2.599561	1.340655	0.828637
Cl,	2.599593	-1.340636	-0.828621

ss-NC

C,	1.220828	0.739077	0.154810
C,	2.493610	1.279406	0.568828
C,	1.220839	-0.739037	-0.154860
C,	2.493643	-1.279359	-0.568824
N,	0.269980	1.588808	0.066903
Se,	-1.432004	1.103434	-0.449599
Se,	-1.431975	-1.103454	0.449607
N,	0.270016	-1.588790	-0.066927
N,	3.501546	1.705795	0.927148
N,	3.501568	-1.705792	-0.927123

SP1-H

H,	2.098287	0.778511	0.000000
C,	1.319405	0.028845	0.000000
N,	1.567917	-1.230218	0.000000
Se,	-0.022462	-2.136536	0.000000
C,	-0.875076	-0.491244	0.000000
N,	0.000000	0.494159	0.000000
Se,	-0.383520	2.355871	0.000000
H,	-1.936287	-0.309108	0.000000

SP1-F

F,	2.248651	0.917527	0.000000
C,	1.319612	0.003191	0.000000
N,	1.612006	-1.237722	0.000000
Se,	0.051332	-2.197711	0.000000
C,	-0.825340	-0.551534	0.000000
N,	0.000000	0.475421	0.000000
Se,	-0.505872	2.312958	0.000000
F,	-2.114798	-0.394441	0.000000

SP1-Cl

Cl,	2.601706	1.103081	0.000000
C,	1.341199	-0.050002	0.000000
N,	1.613374	-1.300840	0.000000
Se,	0.055912	-2.253578	0.000000
C,	-0.838625	-0.618837	0.000000
N,	0.000000	0.413932	0.000000
Se,	-0.518400	2.234759	0.000000
Cl,	-2.518440	-0.464184	0.000000

SP1-NC

C,	2.414644	0.866542	0.000000
C,	1.324095	-0.060263	0.000000
N,	1.557893	-1.329419	0.000000
Se,	-0.000730	-2.245137	0.000000
C,	-0.879793	-0.587579	0.000000
N,	0.000000	0.423212	0.000000
Se,	-0.410822	2.245129	0.000000
C,	-2.271630	-0.436126	0.000000
N,	3.364482	1.515886	0.000000
N,	-3.426826	-0.423279	0.000000

SP1-CH_3

C,	-2.416313	1.117017	0.000000
C,	-1.367265	0.061982	0.000000
N,	-1.670588	-1.191937	0.000000
Se,	-0.140203	-2.188525	0.000000
C,	0.829208	-0.602148	0.000000
N,	0.000000	0.431387	0.000000
Se,	0.598737	2.243155	0.000000
C,	2.301296	-0.480974	0.000000
H,	-3.393521	0.642612	0.000000
H,	-2.305531	1.759039	0.873951
H,	-2.305531	1.759039	-0.873951
H,	2.781621	-1.457580	0.000000
H,	2.622684	0.094041	0.872373
H,	2.622684	0.094041	-0.872373

SP2-H

H,	1.098710	-2.284919	0.815283
C,	0.549961	-1.436965	0.408036
Se,	1.692147	-0.000089	-0.191797
N,	0.709766	1.460687	0.465368
C,	-0.549962	1.436964	0.408044
H,	-1.098712	2.284935	0.815255
N,	-0.709767	-1.460684	0.465371
Se,	-1.692147	0.000088	-0.191797

SP2-CH_3

Se,	1.372968	0.980100	-0.317092
N,	-0.275270	1.600330	0.313620
C,	-1.312566	0.880484	0.261960
Se,	-1.373013	-0.980192	-0.317106
N,	0.275321	-1.600343	0.314085
C,	1.312513	-0.880384	0.262072
C,	-2.632375	1.421645	0.739536
C,	2.632520	-1.421362	0.739391
H,	2.558490	-2.498811	0.871976
H,	-2.557986	2.499004	0.872633
H,	2.913642	-0.957068	1.685357
H,	3.421332	-1.199098	0.017830
H,	-3.421321	1.199941	0.017951
H,	-2.913555	0.956954	1.685294

SP2-F

C,	-1.083762	-1.076524	0.000009
N,	0.016605	-1.654548	0.000014
Se,	1.640587	-0.771094	-0.000010
C,	1.083762	1.076524	0.000009
F,	2.203616	1.825470	0.000022
F,	-2.203616	-1.825470	0.000022
Se,	-1.640587	0.771094	-0.000010
N,	-0.016605	1.654548	0.000013

SP2-Cl

C,	-0.105761	1.548943	0.000000
N,	-1.258965	1.081746	0.000000
Se,	-1.646117	-0.737061	0.000000
C,	0.105761	-1.548943	0.000000
Cl,	-0.105761	-3.306725	0.000000
Cl,	0.105761	3.306725	0.000000
Se,	1.646117	0.737061	0.000000
N,	1.258965	-1.081746	0.000000

SP2-NC

C,	-2.779017	0.790307	0.641136
C,	-1.440945	0.566219	0.177399
Se,	-1.136262	-1.271935	-0.392514
N,	0.596238	-1.510491	0.231754
C,	1.440871	-0.566073	0.177672
C,	2.778862	-0.790159	0.641643
N,	-0.596337	1.510690	0.231522
Se,	1.136310	1.272125	-0.392245
N,	-3.876112	0.912129	0.972659
N,	3.876174	-0.913499	0.971881

cycloadduct FCNSe-FCCF

F,	1.992868	-1.852707	0.000000
C,	0.942071	-1.036653	0.000000
N,	-0.246513	-1.523351	0.000000
Se,	-1.445792	-0.140278	0.000000
C,	0.000000	1.064454	0.000000
C,	1.164410	0.375188	0.000000
F,	2.381086	0.918728	0.000000
F,	-0.124661	2.380086	0.000000

cycloadduct CH_3CNSe-FCCF

C,	-2.057032	-2.041941	0.000000
C,	-0.923010	-1.063725	0.000000
N,	0.312697	-1.488007	0.000000
Se,	1.478043	-0.068422	0.000000
C,	0.000000	1.084471	0.000000
C,	-1.137392	0.350140	0.000000
F,	-2.368919	0.883801	0.000000
F,	0.069359	2.408070	0.000000
H,	-1.664137	-3.055367	0.000000
H,	-2.688780	-1.901373	0.878888
H,	-2.688780	-1.901373	-0.878888

cycloadduct CH_3CNSe-HCCH

C,	2.382869	1.558887	0.000000
C,	1.210201	0.618773	0.000000
N,	0.000000	1.112324	0.000000
Se,	-1.213846	-0.253847	0.000000
C,	0.185965	-1.482186	0.000000
C,	1.363085	-0.811039	0.000000
H,	2.328918	-1.296735	0.000000
H,	0.035817	-2.549610	0.000000
H,	2.036026	2.589030	0.000000
H,	3.008643	1.397623	0.880076
H,	3.008643	1.397623	-0.880076

cycloadduct CH_3CNSe-H_3CCCCH_3

C,	-1.956957	-2.148562	0.000000
C,	-0.862119	-1.118785	0.000000
N,	0.377126	-1.533103	0.000000
Se,	1.485316	-0.084235	0.000000
C,	0.000000	1.059872	0.000000
C,	0.122011	2.552454	0.000000
C,	-1.132663	0.300269	0.000000
C,	-2.530212	0.853404	0.000000
H,	-1.524590	-3.145701	0.000000
H,	-2.597069	-2.042878	0.878971
H,	-2.597069	-2.042878	-0.878971
H,	-2.531966	1.941845	0.000000
H,	-3.090744	0.522301	0.877518
H,	-3.090744	0.522301	-0.877518
H,	1.162310	2.873939	0.000000
H,	-0.355557	2.987437	0.880581
H,	-0.355557	2.987437	-0.880581

cycloadduct CH_3CNSe-$H_3CHCCHCH_3$

C,	-2.635119	-0.922002	-0.796019
C,	-1.260764	-0.521405	-0.340259
C,	-1.006353	0.913071	0.118119
C,	0.502326	1.191084	0.005564
Se,	1.294125	-0.628055	0.249431
N,	-0.330720	-1.389156	-0.295787
C,	-1.534892	1.095903	1.551814
C,	0.919399	1.806044	-1.324143
H,	-2.668186	-1.989372	-0.998101
H,	-3.387595	-0.677935	-0.042772
H,	-2.907005	-0.379692	-1.705487
H,	0.841319	1.807460	0.835952
H,	-1.543897	1.604911	-0.537864
H,	1.999357	1.938410	-1.379011
H,	-2.600084	0.874615	1.614680
H,	0.618806	1.175251	-2.161541
H,	0.452161	2.787455	-1.451770
H,	-1.009012	0.436071	2.242527
H,	-1.388657	2.124620	1.882801

cycloadduct FCNSe-FHCCHF

F,	-2.412618	-1.143786	-0.579312
C,	-1.195611	-0.681009	-0.283008
N,	-0.207604	-1.450210	-0.231822
Se,	1.341905	-0.502712	0.201164
C,	-1.126806	0.800830	0.004534
F,	-1.737819	1.041023	1.228234
C,	0.345261	1.210014	0.058768
F,	0.682121	1.883065	-1.099144
H,	0.548284	1.853757	0.910620
H,	-1.642025	1.388178	-0.757202

cycloadduct CH_3CNSe-FHCCHF

C,	-2.680655	-0.997513	-0.540149
C,	-1.274849	-0.565241	-0.255054
N,	-0.321499	-1.403208	-0.195061
Se,	1.326369	-0.601723	0.191209
C,	-1.006028	0.906779	0.022743
F,	-1.549280	1.212994	1.272847
C,	0.497100	1.178566	0.030155
F,	0.855186	1.792081	-1.160448
H,	-2.731428	-2.079087	-0.629448
H,	-3.345320	-0.667920	0.261061
H,	-3.040408	-0.544667	-1.467466
H,	0.782233	1.827968	0.853666
H,	-1.477681	1.563516	-0.711240

cycloadduct CH_3CNSe-H_2CCH_2

C,	2.828861	-0.521309	0.046836
C,	1.375048	-0.150976	0.006002
N,	0.479608	-1.051525	0.062194
Se,	-1.247843	-0.326658	-0.027602
C,	0.988611	1.308129	-0.183078
H,	1.151717	1.551660	-1.239155
C,	-0.479850	1.493542	0.195747
H,	-0.602287	1.792202	1.233940
H,	2.944150	-1.600427	0.102767
H,	3.343344	-0.150903	-0.844007
H,	3.318524	-0.063869	0.910221
H,	-1.002695	2.194945	-0.447278
H,	1.640623	1.967136	0.393580

cycloadduct FCNSe-FCN

F,	2.602417	-0.989398	0.000000
C,	1.364251	-0.527034	0.000000
N,	1.244261	0.836477	0.000000
C,	0.000000	1.133384	0.000000
F,	-0.438072	2.371626	0.000000
N,	0.382995	-1.360227	0.000000
Se,	-1.148689	-0.365056	0.000000

cycloadduct CH_3CNSe-FCN

C,	-2.724000	-1.159730	0.000000
C,	-1.347403	-0.575290	0.000000
N,	-0.301933	-1.352644	0.000000
Se,	1.199831	-0.305885	0.000000
N,	-1.229226	0.806624	0.000000
C,	0.000000	1.146756	0.000000
F,	0.396969	2.404152	0.000000
H,	-2.671459	-2.244662	0.000000
H,	-3.274486	-0.820446	0.878532
H,	-3.274486	-0.820446	-0.878532

cycloadduct CH_3CNSe-HCN

C,	2.408708	1.467490	0.000000
C,	1.196608	0.589302	0.000000
N,	0.000000	1.105858	0.000000
Se,	-1.212789	-0.253818	0.000000
N,	1.384698	-0.784229	0.000000
C,	0.261434	-1.416708	0.000000
H,	0.180274	-2.494526	0.000000
H,	2.118952	2.514298	0.000000
H,	3.021113	1.259065	0.878293
H,	3.021113	1.259065	-0.878293

cycloadduct CH_3CNSe-H_3CCN

C,	-2.726185	-1.214721	0.000000
C,	-1.348567	-0.628515	0.000000
N,	-1.229274	0.751554	0.000000
C,	0.000000	1.145902	0.000000
Se,	1.182923	-0.338342	0.000000
N,	-0.300363	-1.400043	0.000000
C,	0.427027	2.575782	0.000000
H,	-2.675993	-2.299816	0.000000
H,	-3.277641	-0.875802	0.878214
H,	-3.277641	-0.875802	-0.878214
H,	-0.454528	3.213389	0.000000
H,	1.030128	2.805200	0.879598
H,	1.030128	2.805200	-0.879598