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SUPPORTING INFORMATION

Robust Fluorine Effects on Molecular Conformations of 2-Amino-2-Fluorotetrahydro-*2H*-Pyrans: Fluorine-Perlin-like vs Perlin Effects

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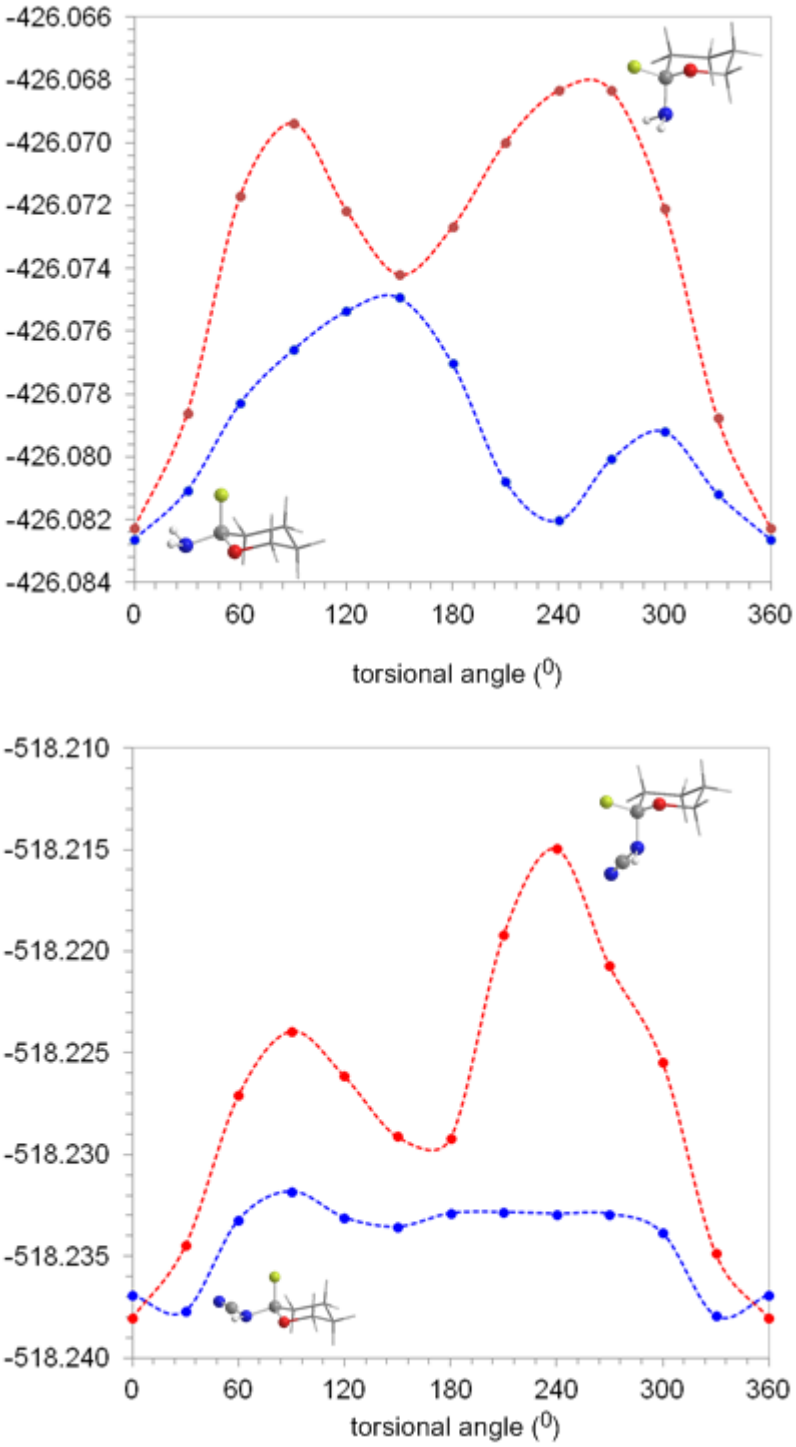


Figure S1. Representative rotational potential energy profiles for the 2-amino-2-fluorotetrahydro-*2H*-pyran conformers (amino- = -NH_2 and NHCN) calculated at the PBE0/Def2-TZVP level of theory in the gas phase.

Table S1. Free Energies, G (in Hartrees) of the more stable axial and equatorial rotamers of the 2-amino-2-fluorotetrahydro-*2H*-pyran (2-N-2-FTHP) conformers and their differences $\Delta G_{ax \rightarrow eq}$ (in kcal/mol) calculated at the PBE1PBE/Def2-TZVP level of theory in the gas phase.

Amino group	G_{ax}	G_{eq}	$\Delta G_{ax \rightarrow eq}$
NH_2	-425.957241	-425.959719	-1.55
NF_2	-624.220272	-624.221906	-1.03
NCl_2	-1344.819525	-1344.818975	0.35
NHMe	-465.198006	-465.200090	-1.31[a]
NH^{t}Bu	-582.953249	-582.956401	-1.97
$NHCF_3$	-762.832395	-762.833353	-0.60
NHPh	-656.732634	-656.734443	-1.14
NHF	-525.082482	-525.082042	0.28
NHCl	-885.390432	-885.390326	0.07
NHBr	-2999.193719	-2.999.194471	-0.47
NHCN	-518.117802	-518.120185	-1.50
$NHNH_2$	-481.218493	-481.218537	-0.03
NHOH	-501.072444	-501.073361	-0.58
NMeF	-564.330919	-564.330507	0.26
NMe_2	-504.437431	-504.439992	-1.61

[a] Experimental $\Delta G_{ax \rightarrow eq}$ value of -1.57 kcal/mol [5] and Calculated $\Delta H_{ax \rightarrow eq}$ value of -1.90 kcal/mol (expt -2.11 kcal/mol [4], -1.75 kcal/mol [5])

Table S2. Free Energies, *G* (in Hartrees) of the more stable axial and equatorial rotamers of the 2-amino-tetrahydropyran (2-N-THP) conformers and their differences $\Delta G_{ax \rightarrow eq}$ (*A*-values in kcal/mol) calculated at the PBE1PBE/Def2-TZVP level of theory in the gas phase.

Amino group	G_{ax}	G_{eq}	$\Delta G_{ax \rightarrow eq}$(*A*-values)
NH_2	-326.73423	-326.74020	-3.74
NF_2	-525.011542	-525.009108	1.53
NCl_2	-1245.607368	-1245.608632	-0.79
NHMe	-365,97706	-365,97875	-1,06
NH^tBu	-483.72972	-483.73264	-1.83
$NHCF_3$	-663.61560	-663.61727	-1.05
NHPh	-557.51744	-557.51341	2.53
NHF	-425.86482	-425.86860	-2.37
NHCl	-786.17288	-786.17543	-1.60
NHBr	-2899.97608	-2899.97609	-0.01
NHCN	-418.90139	-418.90138	0.00
$NHNH_2$	-381.99602	-382.00059	-2.87
NHOH	-401.85385	-401.85656	-1.70
NMeF	-465.11522	-465.11654	-0.83
NMe_2	-405,21780	-405,22201	-2,64

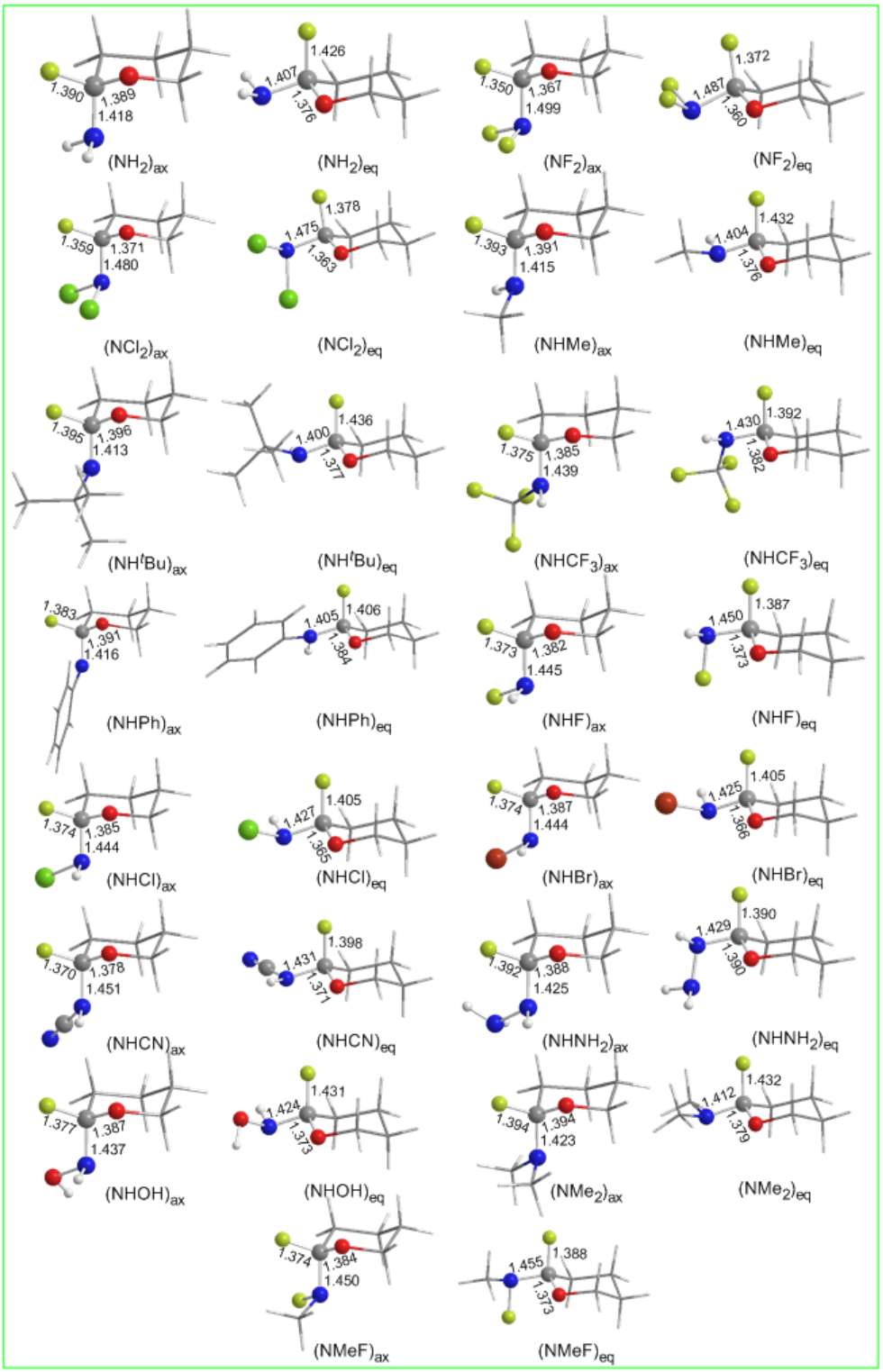


Figure S2 Equilibrium geometries of the stable rotamers of 2-N-2-FTHP conformers along with the *R*(C-F), *R*(C-N) and *R*(C-O) bond lengths (in Å) calculated at the PBE0/Def2-TZVP level of theory in the gas phase

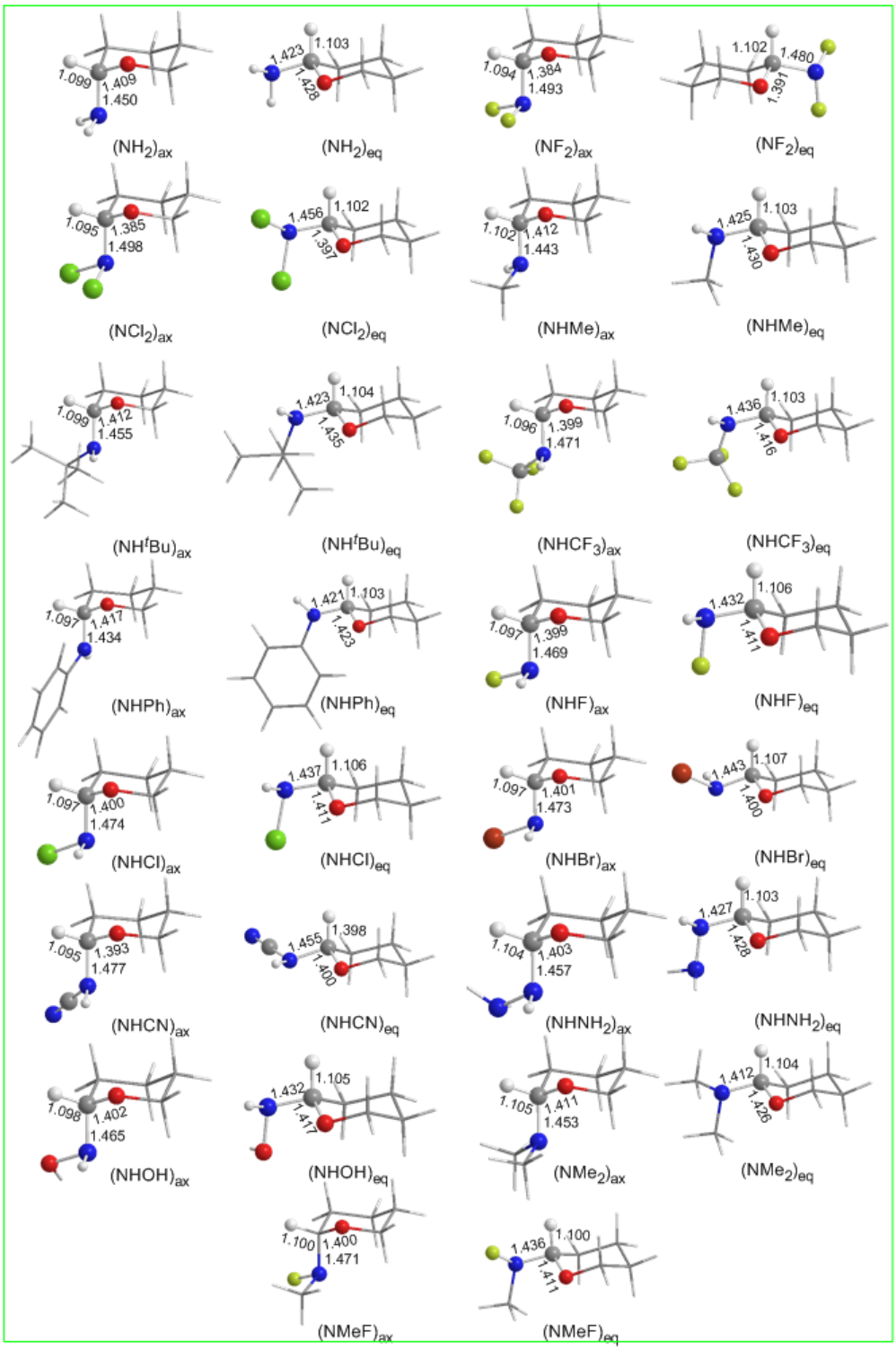


Figure S3 Equilibrium geometries of the stable rotamers of 2-N-THP conformers along with the *R*(C-H), *R*(C-N) and *R*(C-O) bond lengths (in Å) calculated at the PBE0/Def2-TZVP level of theory in the gas phase

Table S3. Total energies, E_{tot}, Lewis energies, E_{Lewis} (in Hartrees) and electronic delocalization contribution to the AE, $\Delta\Delta E_{deloc}$ (in kcal/mol) of the axial (equatorial) 2-amino-2-fluorotetrahydro-*2H*-pyran conformers calculated at the PBE1PBE/Def2-TZVP level of theory.

Amino group	E_{tot}	E_{Lewis}	ΔE_{tot} [a]	ΔE_{Lewis} [b]	$\Delta\Delta E_{deloc}$
NH_2	-426.082278 (-426.084571)	-425.310243 (-425.318590)	-1.439	-5.238	3.799
NF_2	-624.324853 (-624.326471)	-623.348364 (-623.363461)	-1.015	-9.474	8.459
NCl_2	-1344.919869 (-1344.919254)	-1343.983498 (-1343.991413)	0.386	-4.967	5.353
NHMe	-465.348817 (-465.350875)	-464.487147 (-464.492323)	-1.291	-3.248	1.957
NH^{t}Bu	-583.183507 (-583.186441)	-582.095257 (-582.097986)	-1.841	-1.712	-0.129
$NHCF_3$	-762.956971 (-762.957503)	-761.480950 (-761.484217)	-0.334	-2.050	1.716
NHPh	-656.930856 (-656.931702)	-655.379810 (-655.376995)	-0.531	1.766	-2.297
NHF	-525.197544 (-525.196889)	-524.361018 (-524.378198)	0.411	-10.781	11.192
NHCl	-885.503318 (-885.503092)	-884.673080 (-884.666173)	0.142	4.335	-4.193
NHBr	-2999.304910 (-2999.305532)	-2998.477013 (-2998.476366)	-0.390	0.406	-0.796
NHCN	-518.238018 (-518.240199)	-517.175640 (-517.181899)	-1.369	-3.928	2.559
$NHNH_2$	-481.359280 (-481.359181)	-480.503387 (-480.508412)	0.062	-3.153	3.215
NHOH	-501.200235 (-501.200928)	-500.364896 (-500.366828)	-0.435	-1.212	0.777
NMeF	-564.471846 (-564.471298)	-563.536136 (-563.543929)	0.345	-4.890	5.235
NMe_2	-504.614741 (-504.616899)	-503.653067 (-503.651522)	-1.354	0.970	-2.324

[a] $\Delta E_{total} = (E_{tot})_{eq}-(E_{tot})_{ax}$. [b] $\Delta E_{Lewis} = (E_{Lewis})_{eq}- (E_{Lewis})_{ax}$. [c] $\Delta\Delta E_{deloc} = \Delta E_{total} - \Delta E_{Lewis}$

Table S4. Total energies. E_{tot}. Lewis energies. E_{Lewis} (in Hartrees) and electronic delocalization contribution to the AE. $\Delta\Delta E_{deloc}$ (in kcal/mol) of the axial (equatorial) 2-amino-tetrahydro-*2H*-pyran conformers calculated at the PBE1PBE/Def2-TZVP level of theory.

Amino group	E_{tot}	E_{Lewis}	ΔE_{tot} [a]	ΔE_{Lewis} [b]	$\Delta\Delta E_{deloc}$ [c]
NH_2	-326.868173 (-326.873995)	-326.301484 (-326.298759)	-3.65	1.71	-5.36
NF_2	-525.125181 (-525.122555)	-524.379643 (-524.373060)	1.65	4.13	-2.48
NCl_2	-1245.716713 (-1245.717724)	-1245.015518 (-1245.006894)	-0.63	5.41	-6.05
NHMe	-366.136827 (-366.138541)	-365.480949 (-365.471945)	-1.08	5.65	-6.73
NH^{t}Bu	-483.969197 (-483.97199)	-483.110098 (-483.085945)	-1.75	15.16	-16.91
$NHCF_3$	-663.749233 (-663.750632)	-662.492253 (-662.473424)	-0.88	11.82	-12.69
NHPh	-557.724795 (-557.720530)	-556.372629 (-556.359216)	2.68	8.42	-5.74
NHF	-425.988931 (-425.992458)	-425.366808 (-425.347308)	-2.21	12.24	-14.45
NHCl	-786.294908 (-786.297054)	-785.684336 (-785.669159)	-1.35	9.52	-10.87
NHBr	-2900.096398 (-2900.095827)	-2899.489750 (-2899.482377)	0.36	4.63	-4.27
NHCN	-419.030638 (-419.029999)	-418.168638 (-418.179634)	0.40	-6.90	7.30
$NHNH_2$	-382.145763 (-382.150172)	-381.489587 (-381.490142)	-2.77	-0.35	-2.42
NHOH	-401.990644 (-401.993139)	-401.369253 -401.348174)	-1.57	13.23	-14.79
NMeF	-465.264970 (-465.266252)	-464.546613 (-464.535002)	-0.80	7.29	-8.09
NMe_2	-405.404057 (-405.407646)	-404.653691 (-404.646839)	-2.25	4.30	-6.55

[a] $\Delta E_{total} = (E_{tot})_{eq}-(E_{tot})_{ax}$. [b] $\Delta E_{Lewis} = (E_{Lewis})_{eq}-(E_{Lewis})_{ax}$. [c] $\Delta\Delta E_{deloc} = \Delta E_{total} - \Delta E_{Lewis}$

Table S5. Predominant hyperconjugative interactions, Δ*E*(2) (in kcal/mol) contributing to the AE in the 2-amino-2-fluorotetrahydro-*2H*-pyran conformers calculated by the NBO/PBE0/Def2-TZVP computational protocol.

Amino group	$n_O \rightarrow \sigma^*$(C-F)		$n_O \rightarrow \sigma^*$(C-N)		$n_N \rightarrow \sigma^*$(C-F)		$n_N \rightarrow \sigma^*$(C-O)		$n_F \rightarrow \sigma^*$(C-O)		$n_F \rightarrow \sigma^*$(C-N)	
	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$
NH_2	5.35	20.83	12.35	2.15	18.42	20.83	1.98	1.13	10.85	11.70	10.12	8.66
NF_2	6.13	23.01	16.97	3.79	6.29	7.05	0.53	-	12.88	12.65	15.44	11.46
NCl_2	6.07	22.65	16.77	2.61	9.92	1.58	0.81	8.69	12.55	12.64	13.82	10.71
NHF	6.15	22.00	12.35	3.03	11.74	1.62	0.93	9.39	11.82	11.75	11.93	8.87
NHCl	6.14	21.91	12.39	2.35	13.48	15.86	1.07	1.49	11.82	11.70	11.77	8.68
NHBr	6.18	21.73	12.21	2.12	13.89	15.81	0.94	1.39	11.87	11.41	11.59	9.88
NHOH	5.87	20.69	11.82	2.48	13.72	16.15	1.06	1.88	11.59	11.68	11.32	8.59
$NHNH_2$	5.81	19.91	12.17	2.36	17.89	2.02	1.25	13.48	10.45	11.91	9.82	8.48
NHCN	6.03	21.20	14.67	2.71	15.27	19.37	2.72	1.69	11.80	11.69	12.04	10.58
$NHCF_3$	6.02	20.20	13.37	2.68	16.88	8.13	2.43	11.50	11.14	11.69	11.59	9.22
MHMe	5.27	20.81	12.59	2.03	20.81	24.15	3.19	2.45	10.73	11.78	9.93	8.09
NMeF	5.92	21.99	12.58	2.85	14.00	1.82	1.30	11.06	11.85	11.87	12.03	9.06
NMe_2	5.18	20.58	12.20	1.99	20.57	24.82	3.26	2.57	10.87	10.35	9.74	8.22

Table S6. Predominant hyperconjugative interactions, Δ*E*(2) (in kcal/mol) contributing to the AE in the 2-amino-tetrahydro-*2H*-pyran conformers calculated by the NBO/PBE0/Def2-TZVP computational protocol.

Amino group	$n_O \rightarrow \sigma^*$(C-H)		$n_O \rightarrow \sigma^*$(C-N)		$n_N \rightarrow \sigma^*$(C-H)		$n_N \rightarrow \sigma^*$(C-O)	
	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$	$\Delta E(2)_{ax}$	$\Delta E(2)_{eq}$
NH_2	3.03	8.08	11.57	1.93	7.81	1.57	3.87	14.85
NF_2	3.06	10.19	15.38	3.69	2.90	-	0.70	1.13
NCl_2	3.13	9.63	16.10	2.32	4.16	0.67	0.85	9.44
NHF	2.99	9.36	11.84	2.59	5.05	0.83	-	11.15
NHCl	2.99	9.12	12.59	2.23	5.52	0.93	-	11.82
NHBr	2.96	8.78	12.46	2.06	5.48	6.65	-	3.64
NHOH	3.00	8.83	11.97	2.36	5.77	0.99	-	12.32
$NHNH_2$	2.95	8.30	11.80	2.18	7.93	0.13	0.57	14.43
NHCN	3.22	7.54	14.10	2.79	6.52	8.22	3.39	1.75
$NHCF_3$	3.16	8.36	12.78	2.33	6.97	2.48	1.55	13.78
MHMe	2.85	7.88	11.47	1.85	8.67	1.29	5.25	16.36
NMeF	2.85	8.54	12.60	2.42	6.00	0.77	0.98	12.31
NMe_2	2.78	7.78	11.43	1.81	8.70	1.23	3.42	16.87

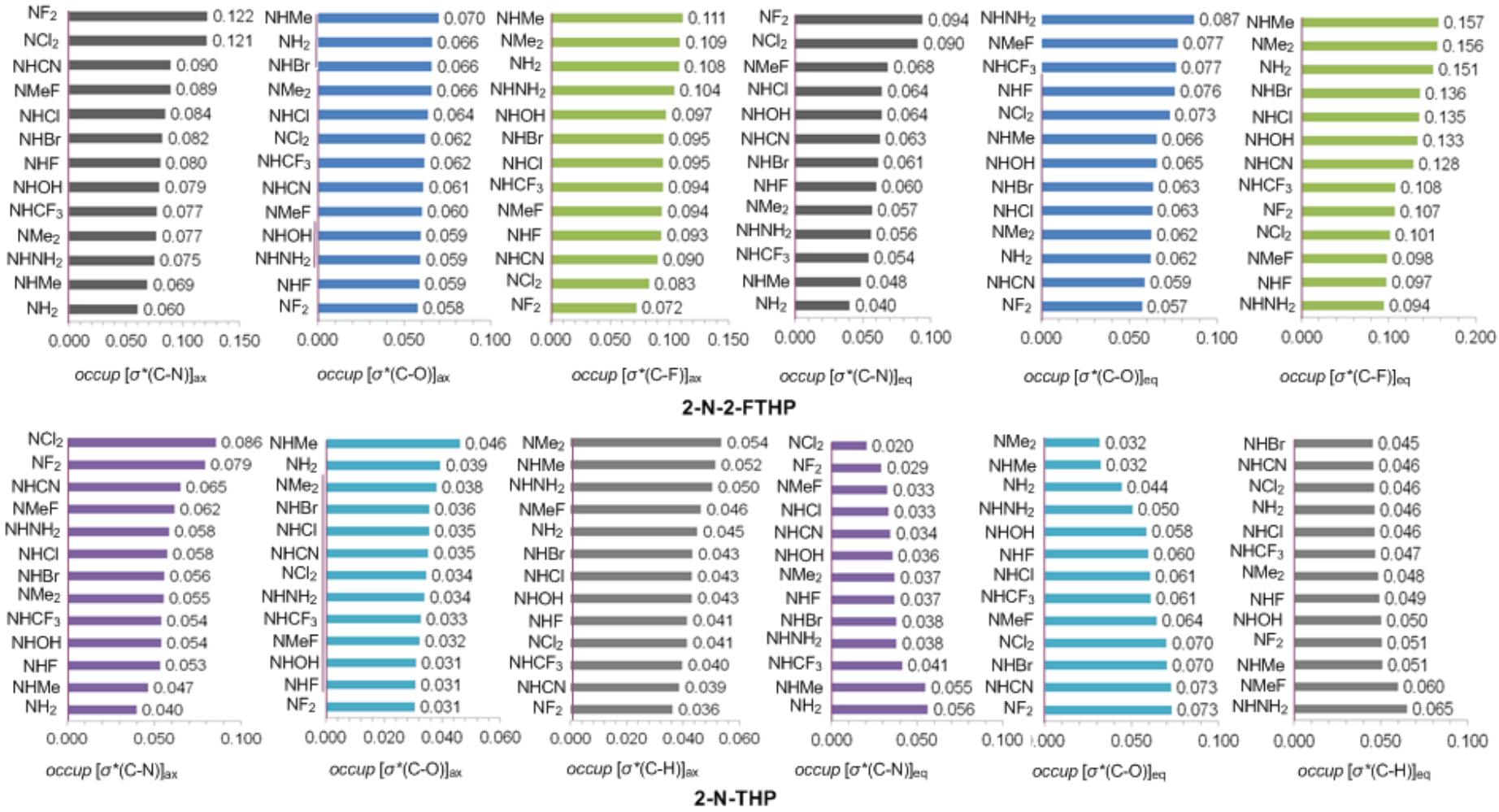
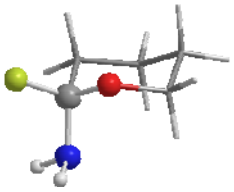


Chart S1. Acceptor capacity ladders of the σ^*(C-N), σ^*(C-O), σ^*(C-F) and σ^*(C-H) acceptor NBOs for the axial and equatorial 2-N-2-FTHP and 2-N-THP conformers calculated at the NBO/PBE0/Def2-TZVP level of theory in the gas phase

Table S7. Isotropic shielding constants, $\sigma^{iso\ 13}C$ (in ppm) for the anomeric carbon atom and their differences $\Delta\sigma^{iso} = (\sigma^{iso})_{ax}-(\sigma^{iso})_{eq}$ of 2-amino-2-fluoro-tetrahydro-*2H*-pyran (2-N-2-FTHP) and 2-amino-tetrahydro-*2H*-pyran (2-N-THP) conformers calculated at the PBE1PBE/Def2-TZVP level of theory.

Amino substituent	**2-N-2-FTHP**		$\Delta\sigma^{iso\ 13}C$	**2-N-THP**		$\Delta\sigma^{iso\ 13}C$
	$(\sigma^{iso\ 13}C)_{ax}$	$(\sigma^{iso\ 13}C)_{eq}$		$(\sigma^{iso\ 13}C)_{ax}$	$(\sigma^{iso\ 13}C)_{eq}$	
NH_2	68.62	70.24	-1.62	106.65	100.40	6.10
NF_2	66.08	64.96	1.12	91.52	87.00	4.52
NCl_2	63.95	63.49	0.46	86.99	83.54	3.45
NHMe	67.66	67.06	0.60	99.74	96.76	2.98
$NHCF_3$	71.10	71.30	-0.20	105.92	101.05	4.87
NHF	67.31	67.45	-0.14	100.63	94.47	6.16
NHCl	66.36	68.40	-2.04	97.24	95.32	1.92
NHBr	66.26	68.76	-2.50	96.89	90.30	6.59
NHCN	68.76	69.54	-0.78	103.46	98.57	4.89
$NHNH_2$	65.14	66.49	-1.35	95.94	94.74	1.20
NHOH	66.56	66.72	-0.16	100.13	94.42	5.71
NMeF	65.98	66.92	-0.94	93.26	92.44	0.82
NMe_2	65.45	65.38	0.07	95.49	90.99	4.50

Table S8. Cartesian coordinates and energies of the 2-amino-2-fluorotetrahydro-*2H*-pyran conformers



C	-1.168090000	1.193453000	1.095857000
O	-2.517061000	1.158045000	0.648550000
H	0.789507000	1.705153000	0.395010000
H	-0.855245000	0.187891000	1.402245000
C	-2.719467000	0.391245000	-0.492192000
H	-1.177077000	1.836405000	1.977145000
N	-2.552328000	-0.983422000	-0.188475000
C	-1.846080000	0.834667000	-1.653234000
C	-0.381014000	0.898150000	-1.243765000
C	-0.239632000	1.727063000	0.024552000
F	-4.039152000	0.667918000	-0.830541000
H	-2.000644000	0.161696000	-2.500873000
H	-2.203045000	1.823920000	-1.950086000
H	0.216481000	1.320937000	-2.055574000
H	-0.008090000	-0.114651000	-1.061790000
H	-0.491139000	2.773072000	-0.181624000
H	-3.170511000	-1.246955000	0.569148000
H	-2.738726000	-1.566184000	-0.993244000

Sum of electronic and zero-point Energies= -425.926208
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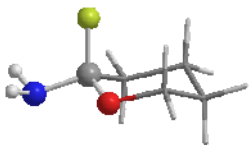
Sum of electronic and thermal Enthalpies= -425.918005
Sum of electronic and thermal Free Energies= -425.957241



C	-0.802731000	2.271178000	1.077517000
C	-2.298702000	2.545893000	1.060141000
H	-0.591469000	1.439448000	1.756650000
H	-0.266222000	3.142746000	1.460656000
C	-3.052617000	1.415515000	0.381211000
H	-2.515601000	3.455290000	0.494142000
H	-2.692629000	2.676745000	2.071106000
N	-4.418676000	1.702289000	0.208213000
O	-2.554258000	1.087050000	-0.858669000
C	-1.164784000	0.780131000	-0.879003000
C	-0.332072000	1.917537000	-0.326089000
H	0.721897000	1.624743000	-0.326213000
F	-2.881134000	0.271819000	1.215430000
H	-0.933403000	0.583950000	-1.926576000
H	-0.987939000	-0.139195000	-0.309193000
H	-0.429597000	2.788186000	-0.983775000
H	-4.873345000	0.944472000	-0.285693000
H	-4.871716000	1.847702000	1.099646000

Sum of electronic and zero-point Energies= -425.928621
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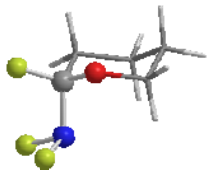

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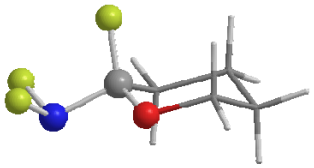
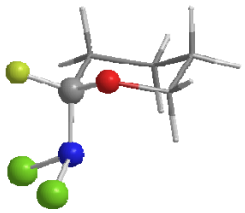
H	-0.514484000	0.533576000	1.448557000
C	-2.418274000	0.747066000	-0.471644000
H	-0.872865000	2.181090000	1.990927000
N	-2.188629000	-0.698563000	-0.150285000
C	-1.530205000	1.152194000	-1.630463000
C	-0.065741000	1.221607000	-1.219059000
C	0.072072000	2.061702000	0.041440000
F	-3.716531000	0.932854000	-0.790778000
H	-1.694561000	0.475118000	-2.468541000
H	-1.888848000	2.141964000	-1.926267000
H	0.524444000	1.642138000	-2.036309000
H	0.317378000	0.212894000	-1.035770000
H	-0.189222000	3.103622000	-0.171484000
F	-3.142744000	-1.028937000	0.779750000
F	-2.596236000	-1.400028000	-1.269724000

Sum of electronic and zero-point Energies= -624.186450
Sum of electronic and thermal Energies= -624.177661
Sum of electronic and thermal Enthalpies= -624.176717
Sum of electronic and thermal Free Energies= -624.220272



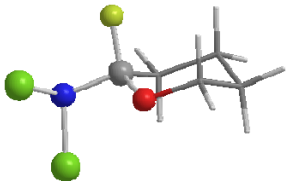
C	-0.840573000	2.228641000	1.092200000
C	-2.344204000	2.469330000	1.051329000
H	-0.622128000	1.373348000	1.739510000
H	-0.342000000	3.095484000	1.531090000
C	-3.021638000	1.334158000	0.313334000
H	-2.565490000	3.394677000	0.515569000
H	-2.776828000	2.541871000	2.050152000
N	-4.479969000	1.627050000	0.203887000
O	-2.510732000	1.060987000	-0.912990000
C	-1.101832000	0.813847000	-0.932209000
C	-0.325994000	1.955358000	-0.313668000
H	0.736945000	1.699094000	-0.300703000
F	-2.996655000	0.208903000	1.100798000
H	-0.858185000	0.675515000	-1.985155000
H	-0.900474000	-0.125673000	-0.405345000
H	-0.439237000	2.849709000	-0.935272000
F	-4.565584000	2.698576000	-0.665415000
F	-5.015921000	0.596723000	-0.529012000

Sum of electronic and zero-point Energies= -624.188084
Sum of electronic and thermal Energies= -624.179275
Sum of electronic and thermal Enthalpies= -624.178331
Sum of electronic and thermal Free Energies= -624.221906



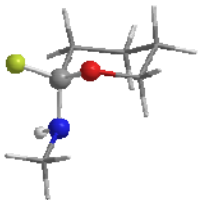
C	1.777885000	-1.288257000	-0.444727000
O	0.896368000	-1.115499000	0.667532000
H	3.374141000	-0.289136000	-1.453377000
H	1.187780000	-1.389524000	-1.362062000
C	0.179148000	0.052322000	0.677960000
H	2.278405000	-2.237250000	-0.252736000
N	-0.785951000	0.000500000	-0.443124000
C	1.064190000	1.283430000	0.568555000
C	2.015184000	1.180517000	-0.614653000
C	2.760783000	-0.144335000	-0.559693000
F	-0.470648000	0.066203000	1.871186000
H	0.454535000	2.184564000	0.531492000
H	1.624411000	1.301532000	1.507582000
H	2.713152000	2.020832000	-0.598237000
H	1.450166000	1.251876000	-1.549267000
H	3.433919000	-0.157831000	0.304042000
Cl	-1.748847000	-1.432279000	-0.359167000
Cl	-1.823689000	1.381547000	-0.462665000

Sum of electronic and zero-point Energies= -1344.784119
Sum of electronic and thermal Energies= -1344.774666
Sum of electronic and thermal Enthalpies= -1344.773722
Sum of electronic and thermal Free Energies= -1344.819522



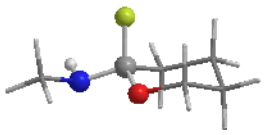
C	-0.866209000	1.988965000	1.170003000
C	-2.364993000	2.256951000	1.102801000
H	-0.674725000	1.123825000	1.812402000
H	-0.363522000	2.843862000	1.627839000
C	-3.048919000	1.129454000	0.348219000
H	-2.553744000	3.191877000	0.574236000
H	-2.814104000	2.327806000	2.094227000
N	-4.497275000	1.386866000	0.237634000
O	-2.509545000	0.865512000	-0.875797000
C	-1.106032000	0.598426000	-0.873236000
C	-0.326703000	1.722652000	-0.227464000
H	0.732257000	1.451670000	-0.195670000
F	-2.977642000	-0.000036000	1.133567000
H	-0.843836000	0.468896000	-1.923138000
H	-0.925796000	-0.349351000	-0.353598000
H	-0.415283000	2.624853000	-0.841855000
Cl	-4.791004000	2.783187000	-0.740669000
Cl	-5.298507000	0.024532000	-0.471893000

Sum of electronic and zero-point Energies= -1344.783565
Sum of electronic and thermal Energies= -1344.774075
Sum of electronic and thermal Enthalpies= -1344.773131
Sum of electronic and thermal Free Energies= -1344.818975



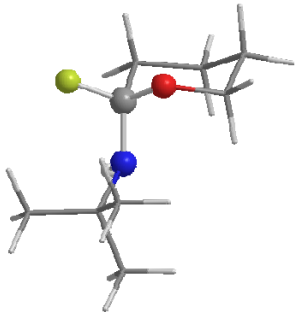
C	-1.165111000	1.240866000	1.088754000
O	-2.512306000	1.246570000	0.638436000
H	0.811209000	1.671974000	0.382328000
H	-0.888056000	0.230143000	1.414083000
C	-2.737237000	0.449787000	-0.479148000
H	-1.151418000	1.899773000	1.958269000
N	-2.606683000	-0.922809000	-0.159604000
C	-1.851296000	0.843070000	-1.649191000
C	-0.383798000	0.874847000	-1.243527000
C	-0.216278000	1.721358000	0.009850000
F	-4.050550000	0.762069000	-0.824125000
H	-2.025999000	0.159562000	-2.484687000
H	-2.181420000	1.835675000	-1.965244000
H	0.222788000	1.267654000	-2.063759000
H	-0.036414000	-0.143917000	-1.045025000
H	-0.432413000	2.771178000	-0.215879000
C	-3.478023000	-1.430264000	0.884847000
H	-2.656601000	-1.483647000	-0.998192000
H	-4.543510000	-1.362617000	0.637242000
H	-3.309018000	-0.866441000	1.802259000
H	-3.225565000	-2.473932000	1.077914000

Sum of electronic and zero-point Energies= -465.164729
Sum of electronic and thermal Energies= -465.155925
Sum of electronic and thermal Enthalpies= -465.154981
Sum of electronic and thermal Free Energies= -465.197993



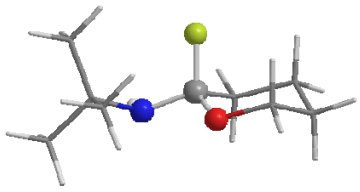
C	-0.654717000	2.341449000	0.991630000
C	-2.132193000	2.663013000	1.158153000
H	-0.363116000	1.578968000	1.720339000
H	-0.052933000	3.229992000	1.198319000
C	-2.998509000	1.494266000	0.719926000
H	-2.411294000	3.516661000	0.535065000
H	-2.369297000	2.909796000	2.196274000
N	-4.365449000	1.813517000	0.740613000
O	-2.688085000	1.026434000	-0.537128000
C	-1.323883000	0.667866000	-0.719764000
C	-0.397228000	1.826539000	-0.417302000
H	0.640039000	1.499073000	-0.533408000
F	-2.714110000	0.431601000	1.635064000
H	-1.249842000	0.355116000	-1.762085000
H	-1.085531000	-0.192471000	-0.084321000
H	-0.571223000	2.626238000	-1.145579000
C	-5.294551000	0.749526000	0.402948000
H	-4.596877000	2.251183000	1.620767000
H	-5.223044000	-0.120937000	1.065596000
H	-5.111770000	0.421559000	-0.619341000
H	-6.308887000	1.147510000	0.452832000

Sum of electronic and zero-point Energies= -465.166811
Sum of electronic and thermal Energies= -465.157959
Sum of electronic and thermal Enthalpies= -465.157015
Sum of electronic and thermal Free Energies= -465.200083



C	-1.295704000	1.078682000	1.176075000
O	-2.620485000	1.058883000	0.672119000
C	-2.747143000	0.424469000	-0.564606000
N	-2.493718000	-0.963650000	-0.494352000
C	-1.861853000	1.089972000	-1.610436000
C	-0.413660000	1.173413000	-1.146413000
C	-0.354611000	1.805535000	0.236603000
F	-4.069978000	0.704440000	-0.905531000
C	-3.384596000	-1.938623000	0.159973000
C	-4.608842000	-2.256498000	-0.704699000
H	-0.947026000	0.051176000	1.340157000
H	-1.362977000	1.579175000	2.143414000
H	-2.209560000	-1.314777000	-1.397894000
H	-1.955862000	0.561834000	-2.563245000
H	-2.270457000	2.093314000	-1.753115000
H	0.175815000	1.749496000	-1.864720000
H	0.022069000	0.169675000	-1.108197000
H	0.661662000	1.772165000	0.640331000
H	-0.649373000	2.858825000	0.178153000
C	-3.839597000	-1.453842000	1.530676000
C	-2.553822000	-3.208990000	0.327612000
H	-4.301247000	-2.607385000	-1.694679000
H	-5.238306000	-1.377074000	-0.834934000
H	-5.206115000	-3.047628000	-0.243427000
H	-1.684049000	-3.019578000	0.959861000
H	-2.197935000	-3.575491000	-0.640451000
H	-3.151798000	-4.001950000	0.782499000
H	-4.453258000	-0.556603000	1.459722000
H	-2.987508000	-1.233962000	2.176111000
H	-4.431865000	-2.241404000	2.002893000

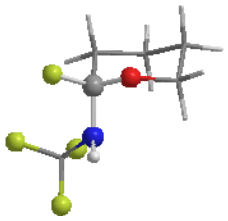
Sum of electronic and zero-point Energies= -582.915449
Sum of electronic and thermal Energies= -582.902850
Sum of electronic and thermal Enthalpies= -582.901906
Sum of electronic and thermal Free Energies= -582.953249



C	-0.410828000	2.093688000	0.760424000
C	-1.822106000	2.629738000	0.944100000
C	-2.863084000	1.540427000	0.718868000
N	-4.159306000	2.070674000	0.761933000
O	-2.679640000	0.871896000	-0.477061000
C	-1.387684000	0.306881000	-0.658451000
C	-0.303759000	1.359597000	-0.567986000
F	-2.644794000	0.575262000	1.751293000
C	-5.389585000	1.278173000	0.928270000
C	-5.592991000	0.843656000	2.383357000

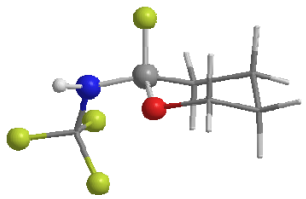
H	-0.174284000	1.406878000	1.578890000
H	0.308908000	2.914553000	0.813095000
H	-2.025918000	3.422162000	0.218540000
H	-1.956705000	3.042228000	1.947396000
H	-4.182911000	2.876580000	1.369930000
H	-1.416872000	-0.156157000	-1.645815000
H	-1.222110000	-0.481001000	0.085227000
H	0.675418000	0.884146000	-0.676591000
H	-0.418564000	2.066237000	-1.397239000
C	-5.398359000	0.054750000	0.021366000
C	-6.530778000	2.208694000	0.523353000
H	-5.598610000	1.712744000	3.048635000
H	-4.799074000	0.171660000	2.707347000
H	-6.552553000	0.332234000	2.498232000
H	-6.423683000	2.513702000	-0.519179000
H	-6.539556000	3.110741000	1.143453000
H	-7.495090000	1.710925000	0.648671000
H	-4.627613000	-0.661450000	0.305485000
H	-5.233951000	0.336523000	-1.019006000
H	-6.370719000	-0.437143000	0.103562000

Sum of electronic and zero-point Energies= -582.917629
Sum of electronic and thermal Energies= -582.904916
Sum of electronic and thermal Enthalpies= -582.903972
Sum of electronic and thermal Free Energies= -582.955695



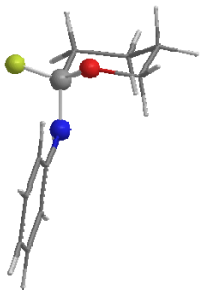
C	-1.090042000	1.499931000	0.968770000
O	-2.395561000	1.255588000	0.451703000
H	0.826706000	2.210457000	0.341238000
H	-0.674235000	0.566944000	1.368841000
C	-2.438401000	0.407124000	-0.641618000
H	-1.242218000	2.191795000	1.797642000
N	-2.168561000	-0.923722000	-0.165786000
C	-1.543343000	0.868159000	-1.776338000
C	-0.127395000	1.150082000	-1.293134000
C	-0.170814000	2.075455000	-0.086408000
F	-3.745064000	0.486817000	-1.063703000
H	-1.562721000	0.142895000	-2.590371000
H	-2.006248000	1.786145000	-2.146896000
H	0.455344000	1.592940000	-2.104217000
H	0.365661000	0.211622000	-1.023125000
H	-0.536394000	3.064220000	-0.382876000
C	-2.052212000	-2.025542000	-1.019767000
H	-2.749057000	-1.139637000	0.633825000
F	-0.868283000	-2.051116000	-1.647607000
F	-2.980192000	-2.098153000	-1.988568000
F	-2.152870000	-3.140004000	-0.290306000

Sum of electronic and zero-point Energies= -762.795819
Sum of electronic and thermal Energies= -762.785364
Sum of electronic and thermal Enthalpies= -762.784419
Sum of electronic and thermal Free Energies= -762.832395



C	-0.735847000	2.098098000	1.140165000
C	-2.215702000	2.429628000	1.002931000
H	-0.607529000	1.276134000	1.850938000
H	-0.206235000	2.960641000	1.550924000
C	-2.942890000	1.287434000	0.318759000
H	-2.335850000	3.329383000	0.396176000
H	-2.682691000	2.610718000	1.971522000
N	-4.336252000	1.508573000	0.086142000
O	-2.365317000	0.908903000	-0.878314000
C	-0.980044000	0.572590000	-0.802580000
C	-0.165106000	1.702806000	-0.213487000
H	0.877763000	1.386051000	-0.123929000
F	-2.890708000	0.186887000	1.169954000
H	-0.686947000	0.351850000	-1.829262000
H	-0.864211000	-0.340138000	-0.207436000
H	-0.189353000	2.559995000	-0.894795000
C	-4.845959000	2.743219000	-0.319194000
H	-4.730130000	0.756987000	-0.464511000
F	-4.189065000	3.332003000	-1.339773000
F	-4.848176000	3.638432000	0.674742000
F	-6.106579000	2.565949000	-0.721367000

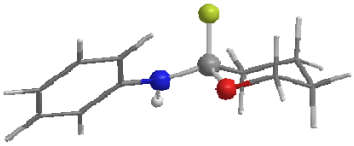
Sum of electronic and zero-point Energies= -762.796461
Sum of electronic and thermal Energies= -762.785900
Sum of electronic and thermal Enthalpies= -762.784956
Sum of electronic and thermal Free Energies= -762.833353



C	-1.992294000	1.794595000	0.721442000
O	-2.996381000	1.230017000	-0.110301000
H	0.000009000	2.575260000	0.590389000
H	-1.728477000	1.084299000	1.514854000
C	-2.592929000	0.077004000	-0.776854000
H	-2.459316000	2.665362000	1.182940000
N	-2.352699000	-1.001951000	0.108736000
C	-1.374560000	0.336970000	-1.648828000
C	-0.244052000	0.969173000	-0.846413000
C	-0.765787000	2.177355000	-0.081626000
F	-3.664232000	-0.196212000	-1.607114000
H	-1.063925000	-0.592530000	-2.133997000
H	-1.709668000	1.017263000	-2.435067000
H	0.572677000	1.253079000	-1.514960000
H	0.165190000	0.239345000	-0.139709000
H	-1.032408000	2.975315000	-0.782730000
C	-3.283492000	-1.553121000	0.991601000
H	-1.672944000	-1.661520000	-0.230516000
C	-4.509212000	-0.956924000	1.288907000

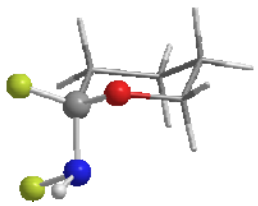
C	-5.364692000	-1.556371000	2.200693000
C	-5.031764000	-2.746870000	2.827865000
C	-3.814928000	-3.342539000	2.528329000
C	-2.950119000	-2.753473000	1.624096000
H	-4.791831000	-0.032923000	0.805603000
H	-6.314368000	-1.079162000	2.416523000
H	-5.710410000	-3.206043000	3.536475000
H	-3.532413000	-4.275903000	3.002564000
H	-1.997575000	-3.225895000	1.402199000

Sum of electronic and zero-point Energies= -656.694104
Sum of electronic and thermal Energies= -656.682280
Sum of electronic and thermal Enthalpies= -656.681336
Sum of electronic and thermal Free Energies= -656.732558



C	-0.375372000	2.245666000	0.061102000
C	-1.594118000	3.021483000	0.536877000
H	0.172699000	1.866507000	0.928988000
H	0.302016000	2.912633000	-0.477626000
C	-2.617583000	2.087810000	1.165151000
H	-2.076107000	3.515824000	-0.313078000
H	-1.323153000	3.784517000	1.269535000
N	-3.778715000	2.789002000	1.531872000
O	-2.941122000	1.021801000	0.344251000
C	-1.833600000	0.238917000	-0.088812000
C	-0.810424000	1.082806000	-0.819027000
H	0.044322000	0.458735000	-1.094949000
F	-2.022711000	1.550095000	2.320338000
H	-2.262902000	-0.525942000	-0.736975000
H	-1.377850000	-0.258916000	0.774635000
H	-1.251908000	1.460783000	-1.747697000
C	-4.964590000	2.231785000	1.998103000
H	-3.864053000	3.700554000	1.119187000
C	-5.035154000	0.954363000	2.555181000
C	-6.242819000	0.475670000	3.035605000
C	-7.395503000	1.245685000	2.983312000
C	-7.324704000	2.517771000	2.435365000
C	-6.126080000	3.005182000	1.945346000
H	-4.146591000	0.342245000	2.614378000
H	-6.277623000	-0.520356000	3.463389000
H	-8.333625000	0.861161000	3.364829000
H	-8.211573000	3.139568000	2.382676000
H	-6.084456000	4.001249000	1.514144000

Sum of electronic and zero-point Energies= -656.695422
Sum of electronic and thermal Energies= -656.683333
Sum of electronic and thermal Enthalpies= -656.682388
Sum of electronic and thermal Free Energies= -656.734443



C	1.546695000	-0.937334000	-0.697337000
O	0.388228000	-1.327118000	0.044402000
H	3.105341000	0.520163000	-0.692337000
H	1.255314000	-0.694862000	-1.725134000

C	-0.524579000	-0.320330000	0.296548000
H	2.174051000	-1.828999000	-0.716899000
N	-1.188367000	-0.082599000	-0.964602000
C	0.072886000	0.932735000	0.897139000
C	1.288484000	1.397154000	0.108775000
C	2.257301000	0.237197000	-0.062224000
F	-1.404358000	-0.864531000	1.198925000
H	-0.699988000	1.699931000	0.952555000
H	0.358050000	0.669152000	1.918855000
H	1.766028000	2.233631000	0.624295000
H	0.972781000	1.763149000	-0.873271000
H	2.659191000	-0.062931000	0.911436000
H	-1.705667000	-0.932677000	-1.187528000
F	-2.208651000	0.861425000	-0.762524000

Sum of electronic and zero-point Energies= -525.049832
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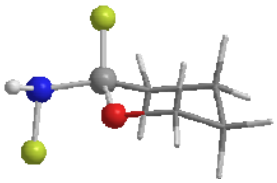
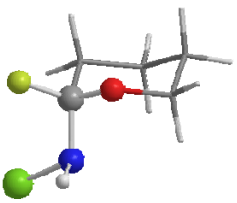
Sum of electronic and thermal Enthalpies= -525.040842
Sum of electronic and thermal Free Energies= -525.082482



C	-0.989148000	1.956564000	0.868909000
C	-2.492329000	2.191859000	0.839595000
H	-0.762151000	1.102786000	1.515905000
H	-0.486681000	2.824638000	1.301628000
C	-3.201519000	1.075075000	0.107625000
H	-2.723641000	3.120162000	0.312130000
H	-2.918504000	2.261423000	1.841382000
N	-4.623698000	1.325392000	-0.025002000
O	-2.670256000	0.775792000	-1.122498000
C	-1.263399000	0.529816000	-1.140890000
C	-0.485230000	1.678375000	-0.539044000
H	0.579064000	1.426655000	-0.535397000
F	-3.179791000	-0.070990000	0.887993000
H	-1.017067000	0.376552000	-2.191812000
H	-1.057142000	-0.401734000	-0.600614000
H	-0.609222000	2.568015000	-1.165582000
F	-4.766620000	2.458764000	-0.842432000
H	-4.987466000	0.580957000	-0.621895000

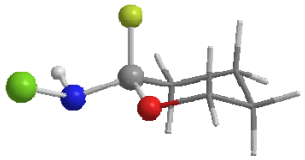
Sum of electronic and zero-point Energies= -525.049228
Sum of electronic and thermal Energies= -525.041116
Sum of electronic and thermal Enthalpies= -525.040172
Sum of electronic and thermal Free Energies= -525.082042



C	**1.883271000**	**-0.548961000**	**-0.971660000**
O	**0.919232000**	**-1.291815000**	**-0.224287000**
H	**3.160191000**	**1.153469000**	**-0.796101000**
H	**1.418487000**	**-0.167171000**	**-1.887562000**
C	**-0.118441000**	**-0.547320000**	**0.311139000**
H	**2.642488000**	**-1.281137000**	**-1.248638000**
N	**-0.958109000**	**-0.188030000**	**-0.807728000**
C	**0.345847000**	**0.638308000**	**1.129670000**

C	**1.350382000**	**1.480459000**	**0.357351000**
C	**2.467292000**	**0.589728000**	**-0.164881000**
F	**-0.770138000**	**-1.425971000**	**1.142412000**
H	**-0.520323000**	**1.220666000**	**1.445483000**
H	**0.808164000**	**0.218391000**	**2.026565000**
H	**1.747417000**	**2.267469000**	**1.002825000**
H	**0.848597000**	**1.975163000**	**-0.480397000**
H	**3.044606000**	**0.183314000**	**0.672454000**
H	**-1.237980000**	**-1.051635000**	**-1.264752000**
Cl	**-2.423388000**	**0.605450000**	**-0.368994000**

Sum of electronic and zero-point Energies= -885.356949
Sum of electronic and thermal Energies= -885.348649
Sum of electronic and thermal Enthalpies= -885.347704
Sum of electronic and thermal Free Energies= -885.390432



C	-0.897091000	1.856026000	0.948429000
C	-2.393241000	2.137342000	0.989492000
H	-0.660058000	1.041899000	1.640094000
H	-0.347428000	2.736695000	1.288984000
C	-3.162065000	0.977917000	0.369447000
H	-2.631725000	3.031617000	0.409115000
H	-2.739029000	2.291925000	2.014488000
N	-4.540119000	1.335767000	0.273810000
O	-2.726813000	0.636470000	-0.878787000
C	-1.339438000	0.320815000	-0.955946000
C	-0.482852000	1.467677000	-0.463640000
H	0.569427000	1.171560000	-0.495667000
F	-2.987317000	-0.128339000	1.217717000
H	-1.159424000	0.102884000	-2.008648000
H	-1.142985000	-0.588454000	-0.377222000
H	-0.602818000	2.322544000	-1.137725000
Cl	-5.543906000	0.069299000	-0.325433000
H	-4.887318000	1.537257000	1.204993000

Sum of electronic and zero-point Energies= -885.356822
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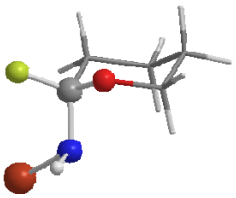
Sum of electronic and thermal Enthalpies= -885.347518
Sum of electronic and thermal Free Energies= -885.390326



C	2.046978000	-0.640189000	-1.022854000
O	1.083328000	-1.380827000	-0.273190000
H	3.327062000	1.060403000	-0.850782000
H	1.581296000	-0.258046000	-1.938130000
C	0.045785000	-0.633971000	0.264027000
H	2.804003000	-1.374231000	-1.300948000
N	-0.789848000	-0.271226000	-0.856013000
C	0.518719000	0.547692000	1.083879000
C	1.521742000	1.389309000	0.309063000
C	2.635445000	0.497310000	-0.217572000
F	-0.603743000	-1.514083000	1.095510000
H	-0.342845000	1.133012000	1.407646000
H	0.984605000	0.123566000	1.976963000

H	1.922132000	2.175253000	0.953808000
H	1.017829000	1.885413000	-0.526606000
H	3.214968000	0.089809000	0.617736000
H	-1.064925000	-1.136045000	-1.314373000
Br	-2.404231000	0.571752000	-0.400964000

Sum of electronic and zero-point Energies= -2999.159156
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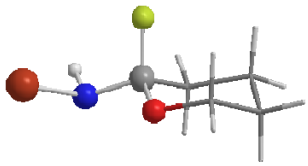
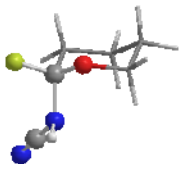
Sum of electronic and thermal Enthalpies= -2999.149720
Sum of electronic and thermal Free Energies= -2999.193719



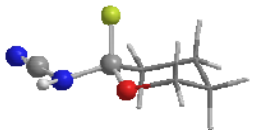
C	-0.887707000	1.860713000	0.942487000
C	-2.382845000	2.146565000	0.995614000
H	-0.646633000	1.049308000	1.635867000
H	-0.332980000	2.741769000	1.274072000
C	-3.162172000	0.985399000	0.388054000
H	-2.624177000	3.038485000	0.413071000
H	-2.719708000	2.307040000	2.022539000
N	-4.538002000	1.346054000	0.302787000
O	-2.736505000	0.638612000	-0.862975000
C	-1.350975000	0.318382000	-0.950799000
C	-0.486914000	1.465116000	-0.471264000
H	0.564197000	1.165871000	-0.511284000
F	-2.976522000	-0.117018000	1.239898000
H	-1.180627000	0.094820000	-2.003962000
H	-1.152038000	-0.588608000	-0.369371000
H	-0.610641000	2.317298000	-1.148042000
Br	-5.648751000	-0.020787000	-0.350915000
H	-4.880703000	1.529681000	1.239525000

Sum of electronic and zero-point Energies= -2999.159875
Sum of electronic and thermal Energies= -2999.151321
Sum of electronic and thermal Enthalpies= -2999.150377
Sum of electronic and thermal Free Energies= -2999.194471



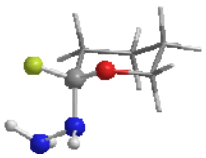
C	-1.794587000	0.283999000	-1.022740000
O	-0.956332000	1.221331000	-0.346950000
H	-2.851301000	-1.539583000	-0.674504000
H	-1.256785000	-0.129458000	-1.885051000
C	0.156018000	0.673906000	0.253532000
H	-2.632142000	0.875533000	-1.392493000
N	1.090591000	0.301209000	-0.792173000
C	-0.153106000	-0.473367000	1.191624000
C	-1.039749000	-1.512162000	0.519325000
C	-2.247907000	-0.828636000	-0.103350000
F	0.694873000	1.706314000	0.974580000
H	0.779939000	-0.905566000	1.558610000
H	-0.667665000	-0.023375000	2.043956000
H	-1.347486000	-2.261678000	1.251579000
H	-0.472090000	-2.041164000	-0.253214000
H	-2.888981000	-0.411227000	0.680138000
H	1.230119000	1.035281000	-1.474393000
C	2.158487000	-0.449167000	-0.525849000
N	3.056303000	-1.143163000	-0.311469000

Sum of electronic and zero-point Energies= -518.083606
Sum of electronic and thermal Energies= -518.074662
Sum of electronic and thermal Enthalpies= -518.073718
Sum of electronic and thermal Free Energies= -518.117802



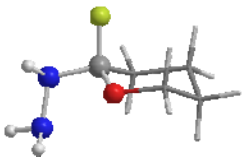
C	-1.011889000	2.047773000	0.787042000
C	-2.439749000	2.426902000	0.420739000
H	-1.024908000	1.318669000	1.602806000
H	-0.480889000	2.928453000	1.154490000
C	-3.135482000	1.252591000	-0.236444000
H	-2.446067000	3.250651000	-0.297803000
H	-3.014148000	2.738373000	1.295058000
N	-4.418608000	1.589484000	-0.772762000
O	-2.452064000	0.709328000	-1.293146000
C	-1.116363000	0.304750000	-0.984299000
C	-0.306719000	1.453842000	-0.424197000
H	0.690657000	1.091905000	-0.159871000
F	-3.293532000	0.259606000	0.735254000
H	-0.710348000	-0.059004000	-1.927959000
H	-1.150607000	-0.530764000	-0.276907000
H	-0.181756000	2.218678000	-1.198066000
C	-5.295261000	2.284556000	-0.052717000
H	-4.795107000	0.894073000	-1.402381000
N	-6.044958000	2.925336000	0.547762000

Sum of electronic and zero-point Energies= -518.085877
Sum of electronic and thermal Energies= -518.076825
Sum of electronic and thermal Enthalpies= -518.075881
Sum of electronic and thermal Free Energies= -518.120166



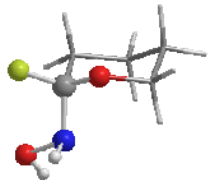
C	1.553332000	-0.905188000	-0.738425000
O	0.429767000	-1.321080000	0.032239000
H	3.102449000	0.569786000	-0.738875000
H	1.226433000	-0.634920000	-1.749477000
C	-0.501842000	-0.326442000	0.280369000
H	2.190845000	-1.787659000	-0.806246000
N	-1.201542000	-0.049192000	-0.930463000
C	0.103435000	0.902013000	0.932411000
C	1.302042000	1.404646000	0.140194000
C	2.275249000	0.259010000	-0.094050000
F	-1.366949000	-0.902452000	1.208533000
H	-0.663522000	1.671623000	1.041142000
H	0.408401000	0.600840000	1.937543000
H	1.785960000	2.226006000	0.674630000
H	0.965679000	1.800733000	-0.823664000
H	2.706817000	-0.065575000	0.858852000
H	-1.441691000	-0.928306000	-1.372907000
N	-2.352137000	0.750501000	-0.840368000
H	-2.094465000	1.724166000	-0.920332000
H	-2.840039000	0.600626000	0.037446000

Sum of electronic and zero-point Energies= -481.185607
Sum of electronic and thermal Energies= -481.177185
Sum of electronic and thermal Enthalpies= -481.176241
Sum of electronic and thermal Free Energies= -481.218340



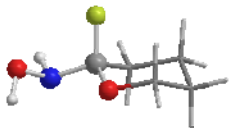
C	-0.889403000	1.912160000	0.851747000
C	-2.379035000	2.215611000	0.913317000
H	-0.666674000	1.030701000	1.462617000
H	-0.322200000	2.743660000	1.277583000
C	-3.193220000	1.161405000	0.195115000
H	-2.604712000	3.167597000	0.428233000
H	-2.740555000	2.269888000	1.941532000
N	-4.582787000	1.486348000	0.119550000
O	-2.724749000	0.876006000	-1.081728000
C	-1.340346000	0.555391000	-1.172109000
C	-0.473112000	1.648240000	-0.587002000
H	0.576826000	1.346656000	-0.646722000
F	-3.146482000	-0.017783000	0.928752000
H	-1.146852000	0.409750000	-2.236036000
H	-1.155912000	-0.396346000	-0.658818000
H	-0.587452000	2.559216000	-1.184485000
N	-4.809927000	2.638032000	-0.655941000
H	-5.063046000	0.665622000	-0.241954000
H	-5.684936000	3.051537000	-0.368610000
H	-4.837624000	2.430710000	-1.648542000

Sum of electronic and zero-point Energies= -481.185660
Sum of electronic and thermal Energies= -481.177164
Sum of electronic and thermal Enthalpies= -481.176219
Sum of electronic and thermal Free Energies= -481.218537



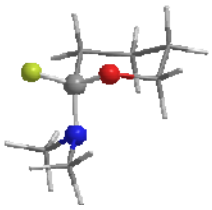
C	1.541761000	-0.864643000	-0.784172000
O	0.418301000	-1.328996000	-0.041196000
H	3.083083000	0.614743000	-0.705456000
H	1.215590000	-0.545225000	-1.780858000
C	-0.514563000	-0.355845000	0.283272000
H	2.184930000	-1.738555000	-0.895678000
N	-1.211403000	-0.028082000	-0.930109000
C	0.080782000	0.849933000	0.978157000
C	1.275462000	1.396240000	0.209810000
C	2.255386000	0.269048000	-0.079241000
F	-1.363410000	-0.985674000	1.166590000
H	-0.701971000	1.596715000	1.115316000
H	0.391650000	0.506841000	1.968088000
H	1.754191000	2.194253000	0.782741000
H	0.939215000	1.838332000	-0.734229000
H	2.686007000	-0.100392000	0.857609000
H	-1.637031000	-0.888830000	-1.265623000
O	-2.279586000	0.857498000	-0.672628000
H	-2.107836000	1.593350000	-1.266814000

Sum of electronic and zero-point Energies= -501.039719
Sum of electronic and thermal Energies= -501.031372
Sum of electronic and thermal Enthalpies= -501.030428
Sum of electronic and thermal Free Energies= -501.072444



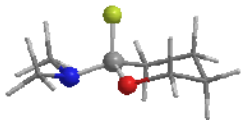
C	-0.990253000	2.073533000	0.790640000
C	-2.497133000	2.286686000	0.832017000
H	-0.710107000	1.312930000	1.525876000
H	-0.476449000	2.995832000	1.072189000
C	-3.219199000	1.062169000	0.293279000
H	-2.781768000	3.134888000	0.204522000
H	-2.840015000	2.486091000	1.850428000
N	-4.612659000	1.331813000	0.177619000
O	-2.776748000	0.666282000	-0.945004000
C	-1.378884000	0.408198000	-1.014524000
C	-0.570189000	1.619536000	-0.600382000
H	0.494396000	1.369899000	-0.626555000
F	-2.981414000	0.013051000	1.195435000
H	-1.191702000	0.134001000	-2.053230000
H	-1.137240000	-0.453931000	-0.382779000
H	-0.734643000	2.426396000	-1.322850000
O	-5.329787000	0.170709000	-0.171346000
H	-4.969320000	1.595163000	1.089453000
H	-5.519087000	0.303252000	-1.104486000

Sum of electronic and zero-point Energies= -501.040566
Sum of electronic and thermal Energies= -501.032097
Sum of electronic and thermal Enthalpies= -501.031153
Sum of electronic and thermal Free Energies= -501.073361



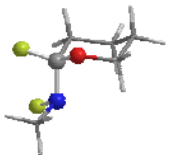
C	-1.138986000	1.228658000	1.108656000
O	-2.490751000	1.287921000	0.675005000
H	0.844787000	1.582904000	0.380588000
H	-0.894856000	0.203497000	1.413680000
C	-2.755342000	0.507451000	-0.448775000
H	-1.092240000	1.871788000	1.988890000
N	-2.651829000	-0.874924000	-0.128167000
C	-1.893059000	0.954165000	-1.617662000
C	-0.416172000	0.905357000	-1.252689000
C	-0.184698000	1.695343000	0.027882000
F	-4.073148000	0.840997000	-0.759741000
H	-2.119790000	0.374659000	-2.512506000
H	-2.195832000	1.984683000	-1.819335000
H	0.186324000	1.307737000	-2.071280000
H	-0.104560000	-0.134148000	-1.105117000
H	-0.350911000	2.761313000	-0.161094000
C	-3.494663000	-1.283773000	0.982263000
C	-2.742121000	-1.803579000	-1.234874000
H	-4.549794000	-1.385941000	0.693167000
H	-3.431343000	-0.552543000	1.785484000
H	-3.144433000	-2.248094000	1.357002000
H	-1.941114000	-1.640538000	-1.955752000
H	-3.707226000	-1.756685000	-1.761081000
H	-2.623743000	-2.815748000	-0.843343000

Sum of electronic and zero-point Energies= -504.402782
Sum of electronic and thermal Energies= -504.392735
Sum of electronic and thermal Enthalpies= -504.391791
Sum of electronic and thermal Free Energies= -504.437431



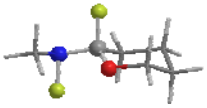
C	-0.642699000	2.451994000	0.897091000
C	-2.117595000	2.824698000	0.826289000
H	-0.471095000	1.828382000	1.779993000
H	-0.042329000	3.356419000	1.024208000
C	-2.977742000	1.617886000	0.479361000
H	-2.287936000	3.574906000	0.048664000
H	-2.441763000	3.242729000	1.779345000
N	-4.334958000	1.921466000	0.235746000
O	-2.508333000	0.932252000	-0.621066000
C	-1.152391000	0.513204000	-0.549647000
C	-0.223957000	1.689890000	-0.349495000
H	0.806606000	1.332759000	-0.265933000
F	-2.862485000	0.730786000	1.597934000
H	-0.963914000	0.003735000	-1.495625000
H	-1.035798000	-0.213674000	0.262116000
H	-0.275045000	2.343211000	-1.227331000
C	-5.157738000	0.775592000	-0.110889000
C	-4.979013000	2.762595000	1.221410000
H	-5.372189000	0.133158000	0.754943000
H	-4.664473000	0.180224000	-0.874814000
H	-6.105544000	1.138588000	-0.513470000
H	-4.476758000	3.725393000	1.308993000
H	-5.033166000	2.298303000	2.217601000
H	-5.998986000	2.958905000	0.886574000

Sum of electronic and zero-point Energies= -504.405096
Sum of electronic and thermal Energies= -504.394907
Sum of electronic and thermal Enthalpies= -504.393962
Sum of electronic and thermal Free Energies= -504.439992



C	-0.795048000	1.576041000	1.113105000
O	-2.160815000	1.521215000	0.700002000
H	1.147067000	2.043369000	0.358114000
H	-0.476096000	0.583466000	1.450894000
C	-2.404091000	0.770498000	-0.436659000
H	-0.792214000	2.250712000	1.970023000
N	-2.228058000	-0.620146000	-0.066779000
C	-1.543696000	1.175090000	-1.616020000
C	-0.070999000	1.212911000	-1.236146000
C	0.111460000	2.070201000	0.007027000
F	-3.717078000	1.031133000	-0.746867000
H	-1.736204000	0.504467000	-2.452192000
H	-1.888460000	2.173471000	-1.898194000
H	0.516245000	1.605182000	-2.069882000
H	0.284741000	0.196280000	-1.042386000
H	-0.129677000	3.114178000	-0.220086000
C	-3.215029000	-1.123569000	0.863280000
F	-2.396120000	-1.386118000	-1.243880000
H	-4.227262000	-1.095190000	0.451104000
H	-3.168790000	-0.496671000	1.753333000
H	-2.944976000	-2.144820000	1.128807000

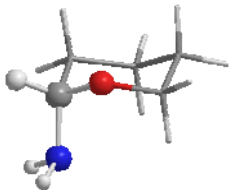
Sum of electronic and zero-point Energies= -564.296708
Sum of electronic and thermal Energies= -564.287277
Sum of electronic and thermal Enthalpies= -564.286333
Sum of electronic and thermal Free Energies= -564.330919



C	2.081153000	0.898667000	0.421305000
C	0.614517000	1.290153000	0.310833000
H	2.281927000	0.492597000	1.418164000
H	2.710132000	1.784570000	0.307007000
C	-0.271244000	0.061987000	0.324925000
H	0.431087000	1.816216000	-0.627552000
H	0.299334000	1.941032000	1.127554000
N	-1.672956000	0.410654000	0.148747000
O	0.100553000	-0.904857000	-0.575878000
C	1.464545000	-1.317382000	-0.504771000
C	2.413405000	-0.146580000	-0.632809000
H	3.441198000	-0.504946000	-0.525431000
F	-0.239264000	-0.487147000	1.599587000
H	1.587175000	-2.032165000	-1.319136000
H	1.629123000	-1.844926000	0.442226000
H	2.320480000	0.287325000	-1.634071000
F	-1.745508000	1.051432000	-1.110365000
C	-2.561727000	-0.727293000	0.050726000
H	-2.477128000	-1.280245000	0.986123000
H	-2.319300000	-1.382356000	-0.789764000
H	-3.578707000	-0.348690000	-0.043568000

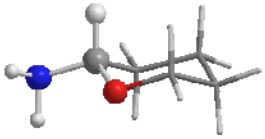
Sum of electronic and zero-point Energies= -564.296233
Sum of electronic and thermal Energies= -564.286761
Sum of electronic and thermal Enthalpies= -564.285817
Sum of electronic and thermal Free Energies= -564.330507

Table S9. Cartesian coordinates and energies of the 2-amino-tetrahydro-*2H*-pyran conformers



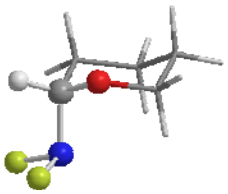
C	-0.778038000	-1.281612000	0.229778000
O	0.317620000	-1.149010000	-0.661512000
H	-2.550720000	-0.236245000	0.837444000
H	-0.412049000	-1.371368000	1.259560000
C	1.081162000	0.019398000	-0.466684000
H	-1.263886000	-2.219408000	-0.046846000
N	1.743175000	-0.042517000	0.821528000
C	0.218581000	1.273236000	-0.560494000
C	-0.985806000	1.193171000	0.368083000
C	-1.733729000	-0.109806000	0.120388000
H	1.786243000	0.002453000	-1.309170000
H	0.828420000	2.157571000	-0.348221000
H	-0.120827000	1.362199000	-1.597232000
H	-1.640750000	2.054990000	0.212136000
H	-0.651378000	1.226920000	1.409529000
H	-2.177726000	-0.099875000	-0.881669000
H	2.434138000	-0.782264000	0.826466000
H	2.212323000	0.828401000	1.032974000

Sum of electronic and zero-point Energies= -326.704059
Sum of electronic and thermal Energies= -326.697349
Sum of electronic and thermal Enthalpies= -326.696405
Sum of electronic and thermal Free Energies= -326.734232



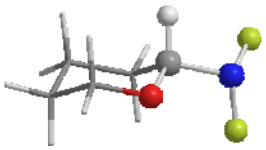
C	1.226296000	1.190964000	0.207128000
C	-0.254322000	1.269702000	-0.140958000
H	1.343109000	1.246275000	1.296629000
H	1.762921000	2.048960000	-0.206651000
C	-0.989666000	0.023748000	0.319390000
H	-0.379394000	1.353587000	-1.227638000
H	-0.723227000	2.146568000	0.311546000
N	-2.362784000	0.070100000	-0.051308000
O	-0.371064000	-1.144651000	-0.219743000
C	0.974573000	-1.282785000	0.180508000
C	1.821443000	-0.117149000	-0.293765000
H	2.850787000	-0.240354000	0.056881000
H	-0.932751000	-0.046225000	1.418513000
H	1.324712000	-2.229202000	-0.237151000
H	1.030883000	-1.360822000	1.279407000
H	1.846717000	-0.121789000	-1.388872000
H	-2.449760000	0.139127000	-1.058644000
H	-2.835942000	-0.776499000	0.239265000

Sum of electronic and zero-point Energies= -326.710050
Sum of electronic and thermal Energies= -326.703384
Sum of electronic and thermal Enthalpies= -326.702439
Sum of electronic and thermal Free Energies= -326.740196



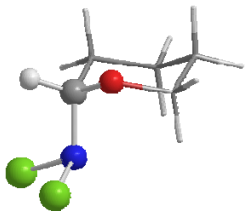
C	1.345467000	-1.283646000	-0.304480000
O	0.372118000	-1.155385000	0.730810000
H	3.018338000	-0.250307000	-1.146676000
H	0.841894000	-1.371492000	-1.274410000
C	-0.359096000	0.019815000	0.719953000
H	1.849103000	-2.228595000	-0.097606000
N	-1.266819000	-0.017606000	-0.465304000
C	0.501257000	1.271710000	0.657625000
C	1.551395000	1.187100000	-0.441408000
C	2.315970000	-0.122710000	-0.318046000
H	-0.992294000	0.006964000	1.612035000
H	-0.133241000	2.151970000	0.548286000
H	0.992800000	1.347425000	1.632528000
H	2.227965000	2.042624000	-0.374730000
H	1.067823000	1.239482000	-1.422208000
H	2.900452000	-0.128896000	0.608590000
F	-2.125533000	-1.069335000	-0.209477000
F	-2.098023000	1.083061000	-0.296860000

Sum of electronic and zero-point Energies= *-524.978468*
Sum of electronic and thermal Energies= *-524.970380*
Sum of electronic and thermal Enthalpies= *-524.969436*
Sum of electronic and thermal Free Energies= *-525.011542*



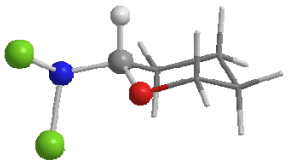
C	1.800861000	-1.116322000	-0.361197000
O	0.421627000	-1.237050000	-0.058702000
H	1.927434000	-1.026423000	-1.451692000
H	2.255106000	-2.056210000	-0.045566000
C	-0.296789000	-0.109599000	-0.442393000
N	-1.709087000	-0.494917000	-0.225022000
C	0.167012000	1.146553000	0.268740000
C	1.653900000	1.342406000	-0.007443000
C	2.424301000	0.075411000	0.337411000
H	3.474661000	0.160552000	0.043996000
H	-0.250547000	0.026379000	-1.535006000
H	2.032362000	2.195760000	0.560271000
H	1.801960000	1.582064000	-1.067707000
H	2.399439000	-0.093796000	1.418817000
F	-1.923234000	-0.435590000	1.139824000
F	-2.423891000	0.603853000	-0.686094000
H	-0.004753000	1.024298000	1.340339000
H	-0.416646000	2.003137000	-0.072974000

Sum of electronic and zero-point Energies= *-524.976107*
Sum of electronic and thermal Energies= *-524.968012*
Sum of electronic and thermal Enthalpies= *-524.967068*
Sum of electronic and thermal Free Energies= *-525.009108*



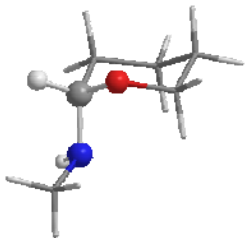
C	1.746284000	-1.277764000	-0.324245000
O	0.886693000	-1.116052000	0.802881000
H	3.328935000	-0.273678000	-1.356532000
H	1.143981000	-1.377394000	-1.234542000
C	0.151163000	0.057362000	0.829437000
H	2.257163000	-2.225551000	-0.150406000
N	-0.836372000	0.011531000	-0.296095000
C	1.037455000	1.290223000	0.694530000
C	1.968557000	1.189859000	-0.504536000
C	2.723702000	-0.130282000	-0.456783000
H	-0.387273000	0.057530000	1.783256000
H	0.433686000	2.196526000	0.664055000
H	1.625066000	1.327317000	1.617680000
H	2.661732000	2.034809000	-0.506973000
H	1.387410000	1.250597000	-1.430136000
H	3.406788000	-0.137339000	0.399803000
Cl	-1.799737000	-1.426192000	-0.141132000
Cl	-1.897874000	1.380222000	-0.186340000

Sum of electronic and zero-point Energies= -1245.572635
Sum of electronic and thermal Energies= -1245.563876
Sum of electronic and thermal Enthalpies= -1245.562932
Sum of electronic and thermal Free Energies= -1245.607368



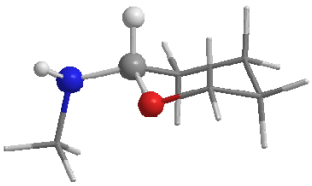
C	-0.859225000	1.758443000	1.333027000
C	-2.354225000	2.049825000	1.244691000
H	-0.693784000	0.888733000	1.980553000
H	-0.342557000	2.599524000	1.801550000
C	-3.032941000	0.921002000	0.489710000
H	-2.523674000	2.985138000	0.705606000
H	-2.802947000	2.144191000	2.235920000
N	-4.471105000	1.136733000	0.426798000
O	-2.483761000	0.738634000	-0.781295000
C	-1.111910000	0.394706000	-0.732301000
C	-0.293383000	1.473660000	-0.050976000
H	0.751792000	1.156619000	0.010042000
H	-2.944884000	-0.011321000	1.071267000
H	-0.804563000	0.245295000	-1.768252000
H	-0.992317000	-0.563661000	-0.202177000
H	-0.325207000	2.381868000	-0.661568000
Cl	-4.869269000	2.510969000	-0.556287000
Cl	-5.245342000	-0.270356000	-0.237309000

Sum of electronic and zero-point Energies= -1245.573993
Sum of electronic and thermal Energies= -1245.565196
Sum of electronic and thermal Enthalpies= -1245.564251
Sum of electronic and thermal Free Energies= -1245.608632



C	-0.781696000	1.409302000	-0.160229000
O	0.089530000	0.937368000	0.853315000
H	-2.651856000	0.917226000	-1.092975000
H	-0.250932000	1.450340000	-1.119635000
C	0.551315000	-0.380677000	0.642383000
H	-1.043694000	2.428052000	0.132498000
N	1.400692000	-0.433493000	-0.522407000
C	-0.611525000	-1.357194000	0.510510000
C	-1.603829000	-0.905683000	-0.553368000
C	-2.014860000	0.536382000	-0.288733000
H	1.114927000	-0.597645000	1.564741000
H	-0.229976000	-2.362059000	0.300752000
H	-1.111654000	-1.404705000	1.482665000
H	-2.476381000	-1.565023000	-0.559907000
H	-1.141838000	-0.974757000	-1.543261000
H	-2.593152000	0.593931000	0.640488000
C	2.676274000	0.228410000	-0.352234000
H	1.524032000	-1.391526000	-0.819444000
H	3.269632000	-0.167198000	0.488156000
H	2.510363000	1.290888000	-0.167414000
H	3.265371000	0.134743000	-1.266303000

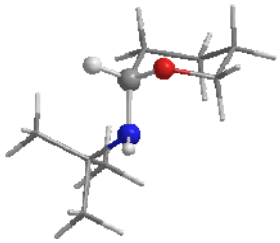
Sum of electronic and zero-point Energies= -365.944728
Sum of electronic and thermal Energies= -365.936628
Sum of electronic and thermal Enthalpies= -365.935684
Sum of electronic and thermal Free Energies= -365.977059



C	-1.610193000	1.199234000	-0.114496000
C	-0.089965000	1.263891000	-0.037620000
H	-1.921765000	1.228326000	-1.166160000
H	-2.055285000	2.074324000	0.366666000
C	0.523970000	0.001669000	-0.620416000
H	0.217579000	1.360115000	1.008073000
H	0.299358000	2.129745000	-0.579243000
N	1.948148000	0.000359000	-0.587455000
O	0.011094000	-1.151741000	0.051235000
C	-1.386947000	-1.277087000	-0.073560000
C	-2.115382000	-0.087364000	0.522348000
H	-3.193648000	-0.203017000	0.374974000
H	0.226385000	-0.073770000	-1.679871000
H	-1.660368000	-2.207344000	0.429466000
H	-1.657200000	-1.380690000	-1.138416000
H	-1.933779000	-0.065471000	1.602397000
C	2.575128000	0.052066000	0.721893000
H	2.284324000	-0.806037000	-1.096668000
H	2.200378000	-0.702248000	1.424825000
H	2.439324000	1.038397000	1.169899000
H	3.649240000	-0.095365000	0.597460000

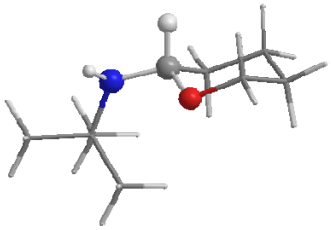
Sum of electronic and zero-point Energies= -365.946396
Sum of electronic and thermal Energies= -365.938294

Sum of electronic and thermal Enthalpies= *-365.937350*
Sum of electronic and thermal Free Energies= *-365.978747*



C	-1.284433000	1.098510000	1.108493000
O	-2.674444000	1.047682000	0.822959000
C	-2.994249000	0.503576000	-0.440062000
N	-2.667899000	-0.914101000	-0.398442000
C	-2.289870000	1.277310000	-1.547754000
C	-0.788564000	1.350470000	-1.315242000
C	-0.522869000	1.906512000	0.076923000
H	-4.076742000	0.675897000	-0.525393000
C	-3.161279000	-1.841843000	-1.430895000
C	-2.156832000	-1.951318000	-2.578674000
H	-0.874627000	0.082516000	1.161771000
H	-1.211712000	1.549834000	2.100184000
H	-3.001221000	-1.235156000	0.503444000
H	-2.526984000	0.848700000	-2.523092000
H	-2.710937000	2.288546000	-1.539613000
H	-0.315850000	1.973407000	-2.079720000
H	-0.354078000	0.349603000	-1.398528000
H	0.545099000	1.885494000	0.315105000
H	-0.847641000	2.952062000	0.126806000
C	-4.541561000	-1.470619000	-1.979647000
C	-3.250977000	-3.207651000	-0.754845000
H	-1.175297000	-2.230273000	-2.190464000
H	-2.049849000	-1.015339000	-3.127822000
H	-2.477816000	-2.715223000	-3.291981000
H	-3.999723000	-3.201197000	0.043350000
H	-2.286069000	-3.480394000	-0.320369000
H	-3.533992000	-3.978861000	-1.473991000
H	-4.527906000	-0.516592000	-2.512195000
H	-5.278950000	-1.399532000	-1.175300000
H	-4.885424000	-2.232519000	-2.683602000

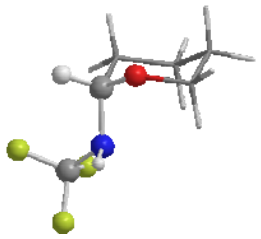
Sum of electronic and zero-point Energies= *-483.692787*
Sum of electronic and thermal Energies= *-483.680900*
Sum of electronic and thermal Enthalpies= *-483.679956*
Sum of electronic and thermal Free Energies= *-483.729722*



C	-0.571237000	1.863008000	1.239526000
C	-1.979247000	2.410675000	1.036222000
C	-2.891842000	1.311004000	0.517378000
N	-4.265329000	1.654818000	0.379163000
O	-2.361947000	0.778266000	-0.705190000
C	-1.093358000	0.191994000	-0.526673000
C	-0.070975000	1.199838000	-0.035578000
H	-2.864258000	0.487644000	1.252840000
C	-4.779894000	2.773177000	-0.429603000
C	-4.089320000	2.951011000	-1.784090000

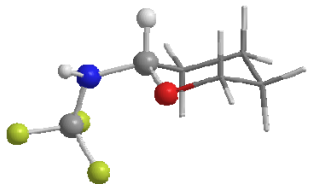
H	-0.585027000	1.124101000	2.050468000
H	0.105888000	2.661050000	1.555977000
H	-1.946349000	3.228759000	0.312021000
H	-2.386006000	2.806688000	1.969708000
H	-4.778738000	0.814875000	0.150369000
H	-0.807657000	-0.230421000	-1.492643000
H	-1.166600000	-0.640390000	0.194429000
H	0.889561000	0.702260000	0.130524000
H	0.083632000	1.955659000	-0.813329000
C	-4.716129000	4.078707000	0.365146000
C	-6.251697000	2.445425000	-0.672736000
H	-4.141598000	2.032648000	-2.371174000
H	-3.035069000	3.206331000	-1.672543000
H	-4.574609000	3.754148000	-2.346397000
H	-6.774419000	2.299866000	0.275937000
H	-6.354739000	1.533848000	-1.269636000
H	-6.741362000	3.256325000	-1.215090000
H	-3.691733000	4.409464000	0.535741000
H	-5.199108000	3.951445000	1.336168000
H	-5.232134000	4.874477000	-0.178636000

Sum of electronic and zero-point Energies= -483.695902
Sum of electronic and thermal Energies= -483.683974
Sum of electronic and thermal Enthalpies= -483.683030
Sum of electronic and thermal Free Energies= -483.732640



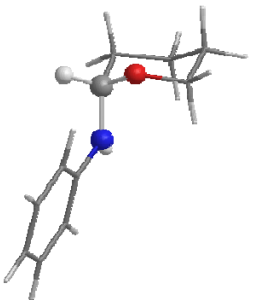
C	2.258900000	-1.017632000	-0.565176000
O	1.479971000	-1.330315000	0.584854000
H	3.387356000	0.588383000	-1.418909000
H	1.648892000	-1.133318000	-1.469721000
C	0.418584000	-0.452138000	0.830721000
H	3.046869000	-1.772071000	-0.586417000
N	-0.582158000	-0.682791000	-0.222456000
C	0.875367000	0.996450000	0.907734000
C	1.703712000	1.391144000	-0.305614000
C	2.828229000	0.384043000	-0.501082000
H	0.022411000	-0.763628000	1.803490000
H	0.018214000	1.657969000	1.044568000
H	1.485574000	1.075727000	1.813085000
H	2.102714000	2.400046000	-0.173904000
H	1.067857000	1.412952000	-1.195927000
H	3.536134000	0.447858000	0.332741000
H	-0.734071000	-1.677674000	-0.329637000
C	-1.808978000	-0.027913000	-0.166385000
F	-2.353753000	0.044163000	1.073067000
F	-2.691551000	-0.667930000	-0.939203000
F	-1.732640000	1.239555000	-0.594108000

Sum of electronic and zero-point Energies= -663.579616
Sum of electronic and thermal Energies= -663.569857
Sum of electronic and thermal Enthalpies= -663.568913
Sum of electronic and thermal Free Energies= -663.615602



C	-2.348974000	1.265760000	-0.125728000
C	-0.829428000	1.189547000	-0.214120000
H	-2.772230000	1.283656000	-1.137748000
H	-2.650542000	2.199532000	0.355083000
C	-0.426646000	-0.156786000	-0.790241000
H	-0.396697000	1.298887000	0.783722000
H	-0.427378000	1.989034000	-0.840172000
N	0.989797000	-0.336326000	-0.942771000
O	-0.947297000	-1.222548000	-0.016495000
C	-2.359868000	-1.216520000	0.019381000
C	-2.897485000	0.063247000	0.629036000
H	-3.991207000	0.050542000	0.605813000
H	-0.850068000	-0.239235000	-1.804897000
H	-2.651628000	-2.094317000	0.598391000
H	-2.755787000	-1.339271000	-1.002639000
H	-2.592664000	0.110644000	1.679618000
C	1.892177000	-0.000780000	0.069398000
H	1.216357000	-1.244478000	-1.322414000
F	2.080296000	1.323689000	0.153985000
F	3.072902000	-0.564593000	-0.209774000
F	1.551578000	-0.397666000	1.310261000

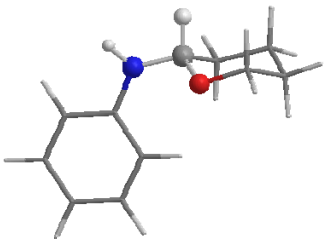
Sum of electronic and zero-point Energies= *-663.581429*
Sum of electronic and thermal Energies= *-663.571597*
Sum of electronic and thermal Enthalpies= *-663.570653*
Sum of electronic and thermal Free Energies= *-663.617269*



C	-2.153462000	1.104136000	-0.970351000
O	-1.450073000	1.267987000	0.246582000
H	-3.941611000	0.185184000	-1.730105000
H	-1.510266000	0.603331000	-1.706448000
C	-1.062668000	0.045260000	0.847858000
H	-2.358131000	2.113490000	-1.331478000
N	-0.108423000	-0.673924000	0.054801000
C	-2.284642000	-0.821692000	1.128117000
C	-3.123067000	-1.029716000	-0.128306000
C	-3.434012000	0.316319000	-0.769780000
H	-0.599836000	0.362094000	1.790072000
H	-1.972958000	-1.773123000	1.569797000
H	-2.883635000	-0.301069000	1.880334000
H	-4.042806000	-1.566357000	0.119735000
H	-2.583842000	-1.657340000	-0.847474000
H	-4.106399000	0.888030000	-0.120591000
C	1.232694000	-0.338143000	0.008907000
H	-0.310998000	-1.645002000	-0.108002000
C	2.168057000	-1.281846000	-0.429254000
C	3.512738000	-0.967128000	-0.491920000
C	3.963254000	0.292046000	-0.117554000

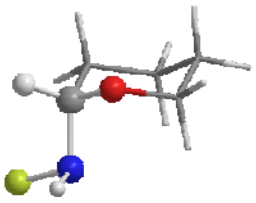
C	3.038639000	1.231412000	0.312018000
C	1.686039000	0.933078000	0.372613000
H	1.829735000	-2.272843000	-0.717857000
H	4.217568000	-1.717780000	-0.832543000
H	5.017345000	0.536852000	-0.165804000
H	3.369747000	2.223699000	0.598790000
H	0.974217000	1.692042000	0.671225000

Sum of electronic and zero-point Energies= *-557.479859*
Sum of electronic and thermal Energies= *-557.468688*
Sum of electronic and thermal Enthalpies= *-557.467744*
Sum of electronic and thermal Free Energies= *-557.517439*



C	3.004480000	0.120283000	1.243529000
C	1.536421000	-0.287328000	1.258152000
H	3.630596000	-0.780878000	1.221514000
H	3.260899000	0.654236000	2.162308000
C	1.149454000	-0.926504000	-0.070920000
H	0.904247000	0.583429000	1.445437000
H	1.337201000	-1.007398000	2.055807000
N	-0.207052000	-1.346665000	-0.134135000
O	1.458168000	-0.067860000	-1.162422000
C	2.831514000	0.248937000	-1.231327000
C	3.309464000	0.966216000	0.016270000
H	4.381541000	1.170229000	-0.064154000
H	1.751723000	-1.843281000	-0.184687000
H	2.957313000	0.865019000	-2.123898000
H	3.417341000	-0.674807000	-1.375750000
H	2.798763000	1.932532000	0.088783000
C	-1.333341000	-0.534060000	-0.072726000
H	-0.355217000	-2.215277000	-0.616792000
C	-1.285898000	0.861589000	-0.068223000
C	-2.455730000	1.600387000	0.027112000
C	-3.693381000	0.980760000	0.095460000
C	-3.747184000	-0.406421000	0.065432000
C	-2.586658000	-1.153494000	-0.009442000
H	-0.337464000	1.366601000	-0.184554000
H	-2.392704000	2.683294000	0.028068000
H	-4.601918000	1.566970000	0.162029000
H	-4.703828000	-0.915325000	0.111344000
H	-2.639325000	-2.238004000	-0.007049000

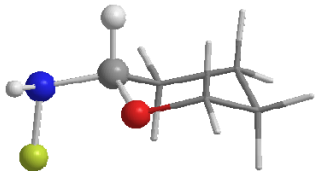
Sum of electronic and zero-point Energies= *-557.475880*
Sum of electronic and thermal Energies= *-557.464648*
Sum of electronic and thermal Enthalpies= *-557.463703*
Sum of electronic and thermal Free Energies= *-557.513409*



C	1.398009000	-1.095695000	-0.358291000
O	0.380826000	-1.263789000	0.627991000
H	2.820342000	0.341150000	-1.052058000

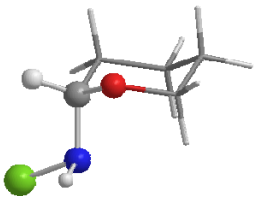
H	0.972347000	-1.229311000	-1.359801000
C	-0.600444000	-0.266825000	0.654559000
H	2.101141000	-1.909879000	-0.175055000
N	-1.418764000	-0.476634000	-0.547442000
C	-0.042978000	1.143527000	0.695335000
C	1.028425000	1.358624000	-0.362724000
C	2.071514000	0.255884000	-0.259027000
H	-1.196455000	-0.461556000	1.554326000
H	-0.869033000	1.849303000	0.583497000
H	0.381820000	1.296590000	1.692722000
H	1.486107000	2.343359000	-0.238981000
H	0.572065000	1.338644000	-1.357284000
H	2.600345000	0.327912000	0.698043000
H	-1.777181000	-1.428893000	-0.483700000
F	-2.592657000	0.289592000	-0.363628000

Sum of electronic and zero-point Energies= -425.832938
Sum of electronic and thermal Energies= -425.825516
Sum of electronic and thermal Enthalpies= -425.824572
Sum of electronic and thermal Free Energies= -425.864823



C	1.550886000	1.210537000	0.152829000
C	0.031040000	1.256630000	0.062335000
H	1.856164000	1.227363000	1.206658000
H	1.984234000	2.099832000	-0.311499000
C	-0.560771000	-0.034121000	0.594802000
H	-0.283761000	1.370386000	-0.977759000
H	-0.379673000	2.096160000	0.627983000
N	-1.991902000	-0.044061000	0.540470000
O	-0.032780000	-1.166293000	-0.062248000
C	1.370613000	-1.268318000	0.072222000
C	2.078753000	-0.057502000	-0.502764000
H	3.157650000	-0.158927000	-0.351984000
H	-0.352805000	-0.118503000	1.677529000
H	1.657895000	-2.186564000	-0.442966000
H	1.632229000	-1.383790000	1.137383000
H	1.900488000	-0.022241000	-1.582560000
F	-2.387889000	0.118958000	-0.807498000
H	-2.298992000	-0.998920000	0.722843000

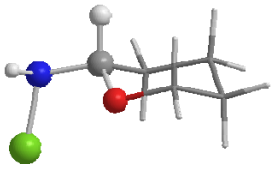
Sum of electronic and zero-point Energies= -425.836859
Sum of electronic and thermal Energies= -425.829492
Sum of electronic and thermal Enthalpies= -425.828548
Sum of electronic and thermal Free Energies= -425.868596



C	1.808091000	-1.021567000	-0.431386000
O	0.874269000	-1.271553000	0.616922000
H	3.079702000	0.520244000	-1.191657000
H	1.323531000	-1.166385000	-1.404233000
C	-0.173036000	-0.349107000	0.721887000
H	2.573309000	-1.790608000	-0.313579000
N	-1.046218000	-0.592056000	-0.439975000

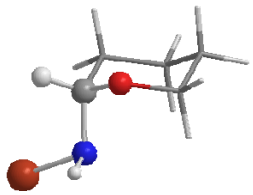
C	0.301574000	1.092653000	0.770319000
C	1.279938000	1.402079000	-0.352520000
C	2.397541000	0.369890000	-0.349636000
H	-0.689679000	-0.605524000	1.654821000
H	-0.564574000	1.757268000	0.744316000
H	0.789196000	1.237375000	1.739695000
H	1.680053000	2.412174000	-0.233396000
H	0.757024000	1.374512000	-1.313660000
H	2.988343000	0.459998000	0.568864000
H	-1.255318000	-1.587064000	-0.438792000
Cl	-2.590403000	0.161244000	-0.224701000

Sum of electronic and zero-point Energies= -786.140174
Sum of electronic and thermal Energies= -786.132525
Sum of electronic and thermal Enthalpies= -786.131581
Sum of electronic and thermal Free Energies= -786.172884



C	1.901441000	1.211225000	0.059301000
C	0.382559000	1.255572000	0.170028000
H	2.342933000	1.215773000	1.063765000
H	2.269535000	2.107064000	-0.446873000
C	-0.135063000	-0.039673000	0.762131000
H	-0.062600000	1.383170000	-0.820417000
H	0.050035000	2.088748000	0.793707000
N	-1.563531000	-0.059939000	0.914247000
O	0.303521000	-1.164233000	0.030662000
C	1.712305000	-1.265922000	-0.025509000
C	2.337882000	-0.047864000	-0.675664000
H	3.427278000	-0.149131000	-0.670769000
H	0.230543000	-0.132795000	1.801724000
H	1.926889000	-2.177810000	-0.585493000
H	2.114372000	-1.393830000	0.993332000
H	2.017601000	-0.000392000	-1.721678000
Cl	-2.421326000	0.063955000	-0.591686000
H	-1.832238000	-0.974631000	1.264618000

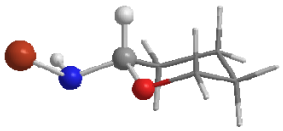
Sum of electronic and zero-point Energies= -786.142779
Sum of electronic and thermal Energies= -786.135136
Sum of electronic and thermal Enthalpies= -786.134192
Sum of electronic and thermal Free Energies= -786.175426



C	2.406308000	-0.979638000	-0.470327000
O	1.514602000	-1.275228000	0.602515000
H	3.595966000	0.616475000	-1.250837000
H	1.898212000	-1.131904000	-1.429779000
C	0.436366000	-0.392623000	0.751278000
H	3.202105000	-1.721402000	-0.384331000
N	-0.456578000	-0.653043000	-0.391264000
C	0.864905000	1.063622000	0.806985000
C	1.793632000	1.422171000	-0.342873000
C	2.947293000	0.431420000	-0.389493000
H	-0.037244000	-0.680862000	1.697360000
H	-0.021654000	1.701371000	0.821499000

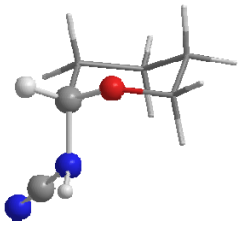
H	1.380728000	1.209673000	1.761425000
H	2.161006000	2.444584000	-0.223347000
H	1.240880000	1.387239000	-1.286929000
H	3.563875000	0.532416000	0.510782000
H	-0.631376000	-1.654981000	-0.391774000
Br	-2.170408000	0.080023000	-0.115393000

Sum of electronic and zero-point Energies= -2899.942248
Sum of electronic and thermal Energies= -2899.934418
Sum of electronic and thermal Enthalpies= -2899.933474
Sum of electronic and thermal Free Energies= -2899.976076



C	2.871247000	0.834573000	0.396804000
C	1.547244000	1.375619000	-0.133238000
H	2.836301000	0.804144000	1.492488000
H	3.687476000	1.510043000	0.128432000
C	0.442422000	0.360036000	0.128989000
H	1.603152000	1.542053000	-1.213243000
H	1.302448000	2.329315000	0.345179000
N	-0.769163000	0.823772000	-0.502699000
O	0.749255000	-0.879046000	-0.444968000
C	1.915690000	-1.446729000	0.111620000
C	3.126592000	-0.567747000	-0.138102000
H	4.008751000	-1.009980000	0.334256000
H	0.324566000	0.222622000	1.221019000
H	2.025779000	-2.426908000	-0.354749000
H	1.775990000	-1.600792000	1.193842000
H	3.317247000	-0.527906000	-1.215554000
Br	-2.284561000	-0.133776000	0.089643000
H	-0.951141000	1.771021000	-0.186994000

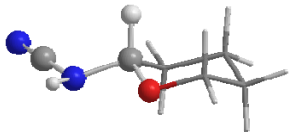
Sum of electronic and zero-point Energies= -2899.942197
Sum of electronic and thermal Energies= -2899.934331
Sum of electronic and thermal Enthalpies= -2899.933387
Sum of electronic and thermal Free Energies= -2899.976086



C	1.715783000	-0.767551000	-0.666520000
O	1.008677000	-1.306515000	0.446749000
H	2.597759000	1.060201000	-1.344338000
H	1.108369000	-0.872405000	-1.574395000
C	-0.147825000	-0.612082000	0.795791000
H	2.598952000	-1.398821000	-0.772680000
N	-1.152058000	-0.850079000	-0.260275000
C	0.082281000	0.873862000	1.009297000
C	0.833782000	1.499495000	-0.156875000
C	2.084869000	0.685093000	-0.454074000
H	-0.482460000	-1.079186000	1.728090000
H	-0.872542000	1.373963000	1.189054000
H	0.672268000	0.967175000	1.925812000
H	1.088153000	2.535610000	0.078519000
H	0.190709000	1.527021000	-1.042551000
H	2.788172000	0.759816000	0.382610000
H	-1.281958000	-1.829595000	-0.473106000

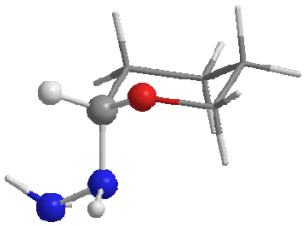
C	-2.252401000	-0.110726000	-0.337213000
N	-3.187338000	0.564335000	-0.427360000

Sum of electronic and zero-point Energies= -418.867830
Sum of electronic and thermal Energies= -418.859540
Sum of electronic and thermal Enthalpies= -418.858595
Sum of electronic and thermal Free Energies= -418.901385



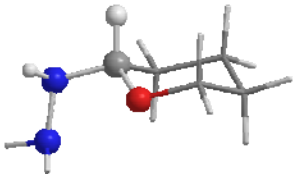
C	1.489113000	1.444258000	0.185553000
C	0.073255000	1.073585000	-0.237684000
H	1.525560000	1.562847000	1.275233000
H	1.769531000	2.409447000	-0.242103000
C	-0.245776000	-0.319159000	0.264796000
H	-0.014890000	1.064679000	-1.328446000
H	-0.657908000	1.786601000	0.151878000
N	-1.528240000	-0.796592000	-0.230431000
O	0.670534000	-1.270329000	-0.199381000
C	1.986937000	-0.996714000	0.247208000
C	2.467249000	0.356709000	-0.239054000
H	3.467731000	0.551538000	0.157855000
H	-0.231299000	-0.322623000	1.370865000
H	2.605420000	-1.808755000	-0.137176000
H	2.016815000	-1.037284000	1.347382000
H	2.547930000	0.332673000	-1.330684000
C	-2.621658000	-0.071553000	-0.021295000
H	-1.644098000	-1.797205000	-0.145603000
N	-3.563730000	0.582015000	0.127388000

Sum of electronic and zero-point Energies= -418.867685
Sum of electronic and thermal Energies= -418.859281
Sum of electronic and thermal Enthalpies= -418.858336
Sum of electronic and thermal Free Energies= -418.901383



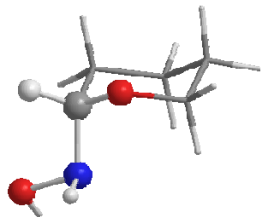
C	1.406000000	-1.081447000	-0.384937000
O	0.433463000	-1.262384000	0.636493000
H	2.791516000	0.378776000	-1.116947000
H	0.941047000	-1.204927000	-1.370682000
C	-0.578055000	-0.290923000	0.660549000
H	2.124248000	-1.890922000	-0.241665000
N	-1.423972000	-0.474937000	-0.511799000
C	-0.018867000	1.122892000	0.738095000
C	1.019985000	1.371677000	-0.345307000
C	2.074190000	0.275063000	-0.297209000
H	-1.145252000	-0.504977000	1.583687000
H	-0.839761000	1.843209000	0.678744000
H	0.436295000	1.244119000	1.726341000
H	1.474681000	2.357474000	-0.215492000
H	0.534902000	1.365526000	-1.326651000
H	2.638124000	0.339791000	0.640225000
H	-1.597089000	-1.467976000	-0.614400000
N	-2.669706000	0.175431000	-0.452895000
H	-2.571445000	1.115075000	-0.812625000
H	-3.018747000	0.236873000	0.503241000

Sum of electronic and zero-point Energies= *-381.964084*
Sum of electronic and thermal Energies= *-381.956304*
Sum of electronic and thermal Enthalpies= *-381.955360*
Sum of electronic and thermal Free Energies= *-381.996018*



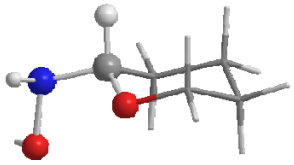
C	-1.603261000	1.197946000	-0.092267000
C	-0.083174000	1.274078000	-0.033812000
H	-1.934096000	1.240814000	-1.138009000
H	-2.046881000	2.062163000	0.409495000
C	0.538213000	0.023091000	-0.624057000
H	0.260839000	1.363867000	0.999026000
H	0.291134000	2.141946000	-0.582872000
N	1.962796000	0.021109000	-0.547492000
O	0.030349000	-1.149760000	0.012406000
C	-1.369439000	-1.275284000	-0.100665000
C	-2.091985000	-0.101376000	0.530974000
H	-3.172106000	-0.220684000	0.400300000
H	0.288723000	-0.041023000	-1.696806000
H	-1.634479000	-2.218254000	0.382815000
H	-1.650523000	-1.354440000	-1.164787000
H	-1.889855000	-0.098950000	1.607388000
N	2.435235000	0.090208000	0.780509000
H	2.310731000	-0.803109000	-1.028504000
H	3.377216000	0.453665000	0.767616000
H	2.428158000	-0.817871000	1.232931000

Sum of electronic and zero-point Energies= *-381.968677*
Sum of electronic and thermal Energies= *-381.960869*
Sum of electronic and thermal Enthalpies= *-381.959925*
Sum of electronic and thermal Free Energies= *-382.000588*



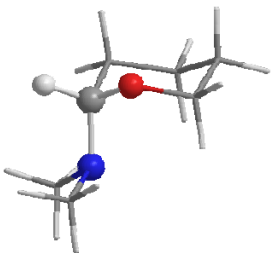
C	1.399387000	-1.085187000	-0.387441000
O	0.413695000	-1.268058000	0.622011000
H	2.803046000	0.367693000	-1.095773000
H	0.946788000	-1.202699000	-1.379841000
C	-0.583276000	-0.283164000	0.664055000
H	2.111526000	-1.899246000	-0.239706000
N	-1.428502000	-0.468522000	-0.517965000
C	-0.024419000	1.127736000	0.728612000
C	1.025768000	1.368800000	-0.345447000
C	2.073703000	0.266997000	-0.286266000
H	-1.159860000	-0.492731000	1.574340000
H	-0.853292000	1.835597000	0.654472000
H	0.421820000	1.259836000	1.719626000
H	1.484009000	2.352553000	-0.213084000
H	0.552052000	1.364915000	-1.332617000
H	2.625013000	0.325727000	0.658988000
H	-1.690834000	-1.451191000	-0.523965000
O	-2.647339000	0.223634000	-0.294596000
H	-2.718581000	0.803495000	-1.057085000

Sum of electronic and zero-point Energies= -401.821897
Sum of electronic and thermal Energies= -401.814162
Sum of electronic and thermal Enthalpies= -401.813218
Sum of electronic and thermal Free Energies= -401.853848



C	1.549327000	1.225905000	0.158230000
C	0.028254000	1.245501000	0.075342000
H	1.858526000	1.236877000	1.211050000
H	1.966684000	2.127151000	-0.298498000
C	-0.545357000	-0.057053000	0.598729000
H	-0.292168000	1.360342000	-0.963280000
H	-0.389155000	2.075835000	0.651345000
N	-1.975948000	-0.093629000	0.540407000
O	0.003716000	-1.171902000	-0.082656000
C	1.405459000	-1.253631000	0.051702000
C	2.096314000	-0.026537000	-0.511311000
H	3.177147000	-0.112162000	-0.363104000
H	-0.309154000	-0.157737000	1.673215000
H	1.710270000	-2.162118000	-0.471550000
H	1.670980000	-1.373960000	1.116030000
H	1.915316000	0.017169000	-1.590435000
O	-2.428755000	0.053453000	-0.797470000
H	-2.270900000	-1.030476000	0.801783000
H	-3.009590000	0.816963000	-0.744548000

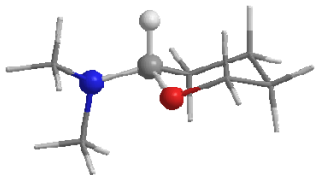
Sum of electronic and zero-point Energies= -401.824718
Sum of electronic and thermal Energies= -401.817024
Sum of electronic and thermal Enthalpies= -401.816080
Sum of electronic and thermal Free Energies= -401.856561



C	1.290334000	-1.283990000	-0.400862000
O	0.448494000	-1.192051000	0.737374000
H	2.880875000	-0.223474000	-1.375266000
H	0.681254000	-1.301231000	-1.313346000
C	-0.313801000	-0.006062000	0.787282000
H	1.799024000	-2.245697000	-0.308132000
N	-1.277718000	0.004672000	-0.300370000
C	0.613609000	1.203614000	0.794742000
C	1.546634000	1.193324000	-0.407693000
C	2.282421000	-0.138966000	-0.462957000
H	-0.835980000	-0.067836000	1.759596000
H	0.047650000	2.134274000	0.864662000
H	1.203701000	1.129113000	1.713542000
H	2.254208000	2.024933000	-0.346256000
H	0.968507000	1.329984000	-1.327735000
H	2.970698000	-0.214600000	0.386422000
C	-2.180567000	-1.123616000	-0.201392000
C	-2.016887000	1.239331000	-0.424149000
H	-2.844334000	-1.055603000	0.679582000
H	-1.612594000	-2.049389000	-0.123921000
H	-2.806217000	-1.170953000	-1.095214000

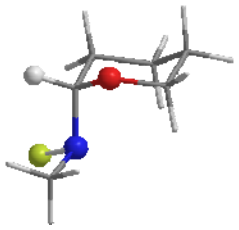
H	-1.365293000	2.066233000	-0.707761000
H	-2.552980000	1.520704000	0.500892000
H	-2.762904000	1.125439000	-1.213279000

Sum of electronic and zero-point Energies= -405.184067
Sum of electronic and thermal Energies= -405.174814
Sum of electronic and thermal Enthalpies= -405.173870
Sum of electronic and thermal Free Energies= -405.217800



C	-2.053425000	0.950638000	-0.510247000
C	-0.590437000	1.304846000	-0.269974000
H	-2.191014000	0.669247000	-1.561788000
H	-2.691182000	1.821170000	-0.334685000
C	0.277324000	0.067466000	-0.431590000
H	-0.478043000	1.698950000	0.743985000
H	-0.247265000	2.073411000	-0.967232000
N	1.673499000	0.305587000	-0.268116000
O	-0.162084000	-0.956813000	0.463855000
C	-1.488044000	-1.361368000	0.215178000
C	-2.466532000	-0.213445000	0.379400000
H	-3.478595000	-0.553411000	0.138710000
H	0.141675000	-0.312119000	-1.458997000
H	-1.701591000	-2.172792000	0.914728000
H	-1.566058000	-1.771146000	-0.806346000
H	-2.468991000	0.102180000	1.428353000
C	2.083170000	0.807954000	1.027009000
C	2.488257000	-0.817665000	-0.680384000
H	1.925912000	0.084787000	1.840766000
H	1.550233000	1.726398000	1.272907000
H	3.148051000	1.048908000	0.987487000
H	2.185889000	-1.144839000	-1.678005000
H	2.416471000	-1.679204000	-0.000215000
H	3.534815000	-0.506708000	-0.730036000

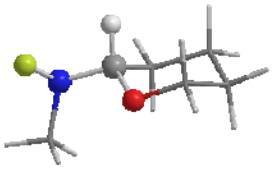
Sum of electronic and zero-point Energies= -405.187998
Sum of electronic and thermal Energies= -405.178539
Sum of electronic and thermal Enthalpies= -405.177595
Sum of electronic and thermal Free Energies= -405.222014



C	1.312864000	-1.318439000	-0.311774000
O	0.375557000	-1.161353000	0.750220000
H	2.986521000	-0.336196000	-1.211491000
H	0.782298000	-1.390187000	-1.268909000
C	-0.332168000	0.046304000	0.744636000
H	1.798769000	-2.276150000	-0.117138000
N	-1.260138000	0.001391000	-0.396011000
C	0.580047000	1.259405000	0.675598000
C	1.585063000	1.145346000	-0.460461000
C	2.315586000	-0.185489000	-0.360487000
H	-0.903963000	0.053360000	1.684118000
H	-0.022794000	2.164042000	0.592350000

H	1.108610000	1.306486000	1.633378000
H	2.289474000	1.980378000	-0.423201000
H	1.062702000	1.207722000	-1.420180000
H	2.929758000	-0.207446000	0.546755000
C	-2.271120000	-1.015895000	-0.234417000
F	-1.978529000	1.227216000	-0.328188000
H	-2.832904000	-0.899342000	0.702189000
H	-1.763247000	-1.980057000	-0.229768000
H	-2.953585000	-0.973863000	-1.082675000

Sum of electronic and zero-point Energies= -465.081707
Sum of electronic and thermal Energies= -465.072956
Sum of electronic and thermal Enthalpies= -465.072012
Sum of electronic and thermal Free Energies= -465.115222



C	-2.044819000	1.002510000	-0.371489000
C	-0.579175000	1.343699000	-0.126679000
H	-2.203577000	0.849498000	-1.445931000
H	-2.682476000	1.840210000	-0.077823000
C	0.281954000	0.126938000	-0.431762000
H	-0.437542000	1.632201000	0.919567000
H	-0.254551000	2.179118000	-0.750415000
N	1.670828000	0.430743000	-0.230947000
O	-0.120249000	-0.985283000	0.337766000
C	-1.448565000	-1.375247000	0.060870000
C	-2.430739000	-0.264367000	0.379498000
H	-3.444329000	-0.581811000	0.116963000
H	0.188561000	-0.120521000	-1.499452000
H	-1.637290000	-2.265475000	0.663664000
H	-1.535550000	-1.662373000	-0.999589000
H	-2.416538000	-0.078120000	1.458732000
C	2.129970000	0.399717000	1.140192000
F	2.388020000	-0.620094000	-0.870048000
H	1.955976000	-0.565315000	1.623110000
H	1.597158000	1.180594000	1.684956000
H	3.192416000	0.640400000	1.147376000

Sum of electronic and zero-point Energies= -465.083172
Sum of electronic and thermal Energies= -465.074416
Sum of electronic and thermal Enthalpies= -465.073471
Sum of electronic and thermal Free Energies= -465.116544