Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Substituent effect in theoretical VCD spectra

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Spectral parameters of selected modes

TABLE S1. Spectral parameters of ν(CN) mode in CN-IND with energetics of the conformers. **R/D** is robustness parameter by Gabor (Góbi, S.; Magyarfalvi, G. *Phys. Chem. Chem. Phys.* **2011**, *13*, 16130). **% of population** was calculated at T=298.15K.

Substituent-Conformer	**Frequency** [cm^{-1}]	**IR intensity** [km/mol]	**dipole strength** [10^{-40} esu^2cm^2]	**rotational strength** [10^{-44} esu^2cm^2]	**R/D** [ppm]	**Sum of electronic and thermal Free Energies** [Hartree]	**% of population**
BF_2	2341.1	16.61	28.31	-2.483	8.8	-664.044660	100.00
Br	2340.4	18.12	30.89	-2.647	8.6	-3013.509236	100.00
CHO-1	2341.3	16.73	28.50	-2.212	7.8	-553.275490	61.90
CHO-2	2341.6	16.45	28.03	-2.704	9.6	-553.275032	38.10
Cl	2340.3	17.77	30.29	-2.674	8.8	-899.571723	100.00
$COCH_3$-1	2340.8	17.78	30.30	-2.570	8.5	-592.574952	38.55
$COCH_3$-2	2340.3	18.07	30.80	-2.608	8.5	-592.575392	61.45
$CONH_2$-1	2340.5	18.01	30.70	-2.472	8.1	-608.652785	33.72
$CONH_2$-2	2340.3	18.23	31.07	-2.991	9.6	-608.653423	66.28
$COOCH_3$-1	2340.6	18.3	31.18	-2.488	8.0	-667.815360	43.65
$COOCH_3$-2	2340.3	18.42	31.39	-2.659	8.5	-667.815601	56.35
COOH-1	2341.1	17.11	29.16	-2.549	8.7	-628.538830	45.85
COOH-2	2340.9	17.28	29.44	-2.442	8.3	-628.538987	54.15
Et-1	2337.9	21.39	36.50	-3.746	10.3	-518.527153	42.61
Et-2	2337.7	21.20	36.18	-3.403	9.4	-518.525732	9.46

Et-3	2338.0	20.87	35.62	-2.341	6.6	-518.527264	47.93
F	2339.8	17.24	29.40	-2.907	9.9	-539.200550	100.00
H	2338.8	18.95	32.32	-3.162	9.8	-439.940965	100.00
iPr-1	2337.8	21.45	36.61	-3.323	9.1	-557.817476	52.36
iPr-2	2337.7	21.56	36.80	-2.646	7.2	-557.817387	47.64
Me	2337.9	20.65	35.24	-2.977	8.4	-479.237175	100.00
MeS-1	2337.9	21.35	36.43	-3.941	10.8	-877.442501	53.81
MeS-2	2338.2	21.75	37.11	-2.259	6.1	-877.442357	46.19
$MeSO_2$-1	2342.7	15.81	26.92	-2.646	9.8	-1027.836697	36.03
$MeSO_2$-2	2341.8	16.29	27.75	-1.662	6.0	-1027.837239	63.97
NH_2	2336.2	22.19	37.89	-3.591	9.5	-495.295515	100.00
$NHNH_2$-1	2335.8	23.26	39.73	-4.438	11.2	-550.604154	35.86
$NHNH_2$-2	2335.3	24.08	41.14	-3.018	7.3	-550.604703	64.14
NMe_2	2334.9	24.92	42.57	-4.122	9.7	-573.855889	100.00
NO-1	2342.5	15.33	26.12	-2.815	10.8	-569.259127	40.07
NO-2	2342.4	15.31	26.07	-2.002	7.7	-569.259507	59.93
NO_2	2343.0	14.50	24.69	-2.142	8.7	-644.479658	100.00
OCF_3-1	2340.5	17.26	29.42	-2.581	8.8	-852.256190	23.70
OCF_3-2	2340.4	16.84	28.71	-2.897	10.1	-852.256087	21.25
OCF_3-3	2341.2	16.07	27.38	-2.203	8.0	-852.256986	55.06
OH-1	2337.6	19.87	33.91	-3.446	10.2	-515.175261	57.80
OH-2	2337.9	19.72	33.64	-3.105	9.2	-515.174964	42.20
OMe-1	2337.4	21.33	36.41	-2.853	7.8	-554.449898	46.64

OMe-2	2337.1	20.91	35.69	-3.829	10.7	-554.450025	53.36
SH	2338.7	20.03	34.16	-3.103	9.1	-838.154955	48.89
SiH_3	2339.4	19.33	32.97	-2.676	8.1	-730.638443	100.00
$SiMe_3$	2338.2	21.64	36.93	-2.774	7.5	-848.551657	100.00
tBu-1	2337.6	21.89	37.35	-2.929	7.8	-597.104273	33.27
tBu-2	2337.6	21.88	37.34	-2.937	7.9	-597.104270	33.17
tBu-3	2337.6	21.87	37.33	-3.250	8.7	-597.104281	33.56
Vin-1	2338.6	21.18	36.14	-1.487	4.1	-517.319332	53.54
Vin-2	2338.6	20.97	35.77	-4.385	12.3	-517.319198	46.46

TABLE S2. Spectral parameters of ν(NC) mode in NC-IND with energetics of the conformers.

Substituent-Conformer	**Frequency** [cm^{-1}]	**IR intensity** [km/mol]	**dipole strength** [10^{-40} esu^2cm^2]	**rotational strength** [10^{-44} esu^2cm^2]	**R/D**	**Sum of electronic and thermal Free Energies** [Hartree]	**% of population**
BF_2	2210.6	190.60	343.99	-32.507	9.5	-664.010806	100.00
Br	2210.8	193.34	348.88	-31.410	9.0	-3013.475412	100.00
CHO-1	2210.6	195.41	352.65	-29.919	8.5	-553.241701	63.46
CHO-2	2210.6	193.58	349.34	-33.817	9.7	-553.241180	36.54
Cl	2210.8	190.31	343.42	-31.123	9.1	-899.537904	100.00
$COCH_3$-1	2210.0	194.92	351.85	-32.003	9.1	-592.541058	37.53
$COCH_3$-2	2209.9	192.25	347.06	-32.756	9.4	-592.541539	62.47
$CONH_2$-1	2211.0	191.91	346.28	-30.572	8.8	-608.618933	34.10
$CONH_2$-2	2211.2	190.47	343.65	-34.083	9.9	-608.619555	65.90
$COOCH_3$-1	2211.1	193.88	349.82	-30.563	8.7	-667.781509	44.88
$COOCH_3$-2	2210.4	191.81	346.19	-33.291	9.6	-667.781703	55.12
COOH-1	2210.7	193.43	349.06	-32.307	9.3	-628.504963	45.54
COOH-2	2210.7	192.63	347.61	-32.303	9.3	-628.505132	54.46
Et-1	2211.5	182.92	329.98	-34.156	10.4	-518.493242	44.20
Et-2	2211.7	180.44	325.48	-32.728	10.1	-518.491868	10.31
Et-3	2211.4	179.88	324.51	-25.065	7.7	-518.493269	45.48
F	2211.0	181.88	328.18	-30.585	9.3	-539.166739	100.00

H	2211.8	177.02	319.29	-31.134	9.8	-439.907080	100.00
iPr-1	2211.5	181.49	327.40	-32.435	9.9	-557.783547	43.70
iPr-2	2211.5	183.38	330.80	-26.738	8.1	-557.783786	56.30
Me	2211.5	179.95	324.61	-29.666	9.1	-479.203348	100.00
MeS	2211.0	188.87	340.79	-38.066	11.2	-877.408711	100.00
$MeSO_2$	2210.4	203.76	367.75	-37.343	10.2	-1027.802896	100.00
NH_2	2211.0	177.87	320.95	-27.447	8.6	-495.261729	100.00
$NHNH_2$	2211.2	179.34	323.56	-32.820	10.1	-550.570357	100.00
NMe_2	2210.8	181.47	327.45	-29.851	9.1	-573.822075	100.00
NO-1	2210.5	199.70	360.41	-39.114	10.9	-569.225270	37.18
NO-2	2210.0	203.34	367.05	-25.942	7.1	-569.225765	62.82
NO_2	2209.8	202.39	365.38	-33.724	9.2	-644.445853	100.00
OCF_3-1	2211.2	188.29	339.71	-28.243	8.3	-852.222424	26.18
OCF_3-2	2210.4	187.86	339.06	-32.961	9.7	-852.222247	21.70
OCF_3-3	2210.6	188.82	340.76	-28.632	8.4	-852.223074	52.12
OH-1	2211.0	177.93	321.04	-30.162	9.4	-515.141485	59.09
OH-2	2211.1	179.24	323.40	-27.266	8.4	-515.141138	40.91
OMe-1	2211.5	180.49	325.59	-23.750	7.3	-554.416020	43.13
OMe-2	2211.1	178.92	322.81	-33.895	10.5	-554.416281	56.87
SH-1	2210.8	189.61	342.16	-31.421	9.2	-838.121079	47.57
SH-2	2210.8	190.57	343.89	-28.398	8.3	-838.121171	52.43
SiH_3	2211.3	183.86	331.70	80.327	24.2	-730.604573	100.00
$SiMe_3$	2211.2	187.33	337.97	-30.182	8.9	-848.518066	100.00

tBu	2211.5	184.27	332.42	-29.753	9.0	-597.070541	100.00
Vin-1	2211.1	194.10	350.21	-19.258	5.5	-517.285522	54.23
Vin-2	2211.3	189.61	342.06	-41.357	12.1	-517.285362	45.77

TABLE S3. Spectral parameters of ν(CH) mode in CN-IND with energetics of the conformers.

Substituent-Conformer	**Frequency** [cm^{-1}]	**IR intensity** [km/mol]	**dipole strength** [10^{-40} esu^2cm^2]	**rotational strength** [10^{-44} esu^2cm^2]	**R/D**	**Sum of electronic and thermal Free Energies** [Hartree]	**% of population**
BF_2	3010.8	0.55	0.73	1.061	144.9	-664.044660	100.00
Br	3010.8	0.24	0.32	0.680	212.2	-3013.509236	100.00
CHO-1	3010.2	0.50	0.66	1.056	160.4	-553.275490	61.90
CHO-2	3010.5	0.67	0.89	1.032	116.4	-553.275032	38.10
Cl	3010.7	0.24	0.32	0.655	206.7	-899.571723	100.00
$COCH_3$-1	3010.7	0.49	0.65	1.023	157.7	-592.574952	38.55
$COCH_3$-2	3010.1	0.41	0.54	1.118	206.4	-592.575392	61.45
$CONH_2$-1	3012.4	0.37	0.50	0.953	192.3	-608.652785	33.72
$CONH_2$-2	3009.6	0.36	0.48	1.083	225.0	-608.653423	66.28
$COOCH_3$-1	3010.8	0.44	0.58	1.047	181.4	-667.815360	43.65
$COOCH_3$-2	3010.3	0.41	0.55	1.086	199.3	-667.815601	56.35
COOH-1	3010.7	0.51	0.68	1.025	150.7	-628.538830	45.85
COOH-2	3010.5	0.49	0.64	1.054	163.6	-628.538987	54.15
Et-1	3010.3	0.33	0.44	0.801	180.8	-518.527153	42.61
Et-2	3010.2	0.38	0.50	0.845	168.8	-518.525732	9.46
Et-3	3010.4	0.34	0.45	0.796	177.0	-518.527264	47.93
F	3011.0	0.26	0.34	0.590	174.2	-539.200550	100.00

H	3011.1	0.31	0.41	1.007	247.7	-439.940965	100.00
iPr-1	3010.2	0.34	0.45	0.798	177.4	-557.817476	52.36
iPr-2	3010.4	0.35	0.47	0.750	159.9	-557.817387	47.64
Me	3010.2	0.35	0.47	0.803	171.0	-479.237175	100.00
MeS-1	3008.2	0.49	0.65	0.222	34.2	-877.442501	53.81
MeS-2	3008.8	0.39	0.52	0.036	7.0	-877.442357	46.19
$MeSO_2$-1	3009.7	0.66	0.87	1.037	118.8	-1027.836697	36.03
$MeSO_2$-2	3013.3	0.71	0.94	0.905	95.8	-1027.837239	63.97
NH_2	3005.9	1.18	1.57	-0.551	35.2	-495.295515	100.00
$NHNH_2$-1	3006.2	1.30	1.73	-0.407	23.5	-550.604154	35.86
$NHNH_2$-2	3006.6	1.19	1.58	-0.599	38.0	-550.604703	64.14
NMe_2-1	3004.5	1.91	2.54	-0.777	30.6	-573.855889	50.82
NMe_2-2	3004.6	1.62	2.15	-0.948	44.0	-573.855858	49.18
NO-1	3009.5	1.09	1.45	0.767	52.8	-569.259127	40.07
NO-2	3010.1	0.72	0.95	1.448	152.6	-569.259507	59.93
NO_2-1	3011.1	0.92	1.22	1.008	82.3	-644.479658	49.97
NO_2-2	3011.1	0.92	1.22	1.009	82.4	-644.479659	50.03
OCF_3-1	3011.3	0.24	0.32	0.552	173.6	-852.256190	23.70
OCF_3-2	3011.1	0.23	0.30	0.537	179.2	-852.256087	21.25
OCF_3-3	3011.9	0.32	0.42	0.801	191.5	-852.256986	55.06
OH-1	3008.6	0.55	0.73	0.183	25.1	-515.175261	57.80
OH-2	3009.0	0.48	0.64	0.107	16.7	-515.174964	42.20
OMe-1	3008.8	3.70	4.91	-8.624	175.6	-554.449898	46.64

OMe-2	3008.3	0.92	1.21	0.935	77.0	-554.450025	53.36
SH-1	3008.9	0.31	0.41	0.269	66.5	-838.154955	48.89
SH-2	3009.3	0.30	0.39	0.249	63.5	-838.154997	51.11
SiH_3-1	3010.8	0.29	0.39	0.968	248.1	-730.638443	49.97
SiH_3-2	3010.8	0.29	0.39	0.968	248.1	-730.638444	50.03
$SiMe_3$	3010.4	0.31	0.41	1.030	254.0	-848.551657	100.00
tBu-1	3010.4	0.35	0.47	0.825	175.4	-597.104273	33.27
tBu-2	3010.4	0.36	0.48	0.838	173.6	-597.104270	33.17
tBu-3	3010.4	0.35	0.47	0.863	183.4	-597.104281	33.56
Vin-1	3009.0	0.27	0.36	0.566	158.1	-517.319332	53.54
Vin-2	3009.0	0.27	0.36	0.713	198.2	-517.319198	46.46

T**ABLE S4.** Spectral parameters of ν(CH) mode in NC-IND with energetics of the conformers.

Substituent-Conformer	**Frequency** [cm^{-1}]	**IR intensity** [km/mol]	**dipole strength** [10^{-40} esu^2cm^2]	**rotational strength** [10^{-44} esu^2cm^2]	**R/D**	**Sum of electronic and thermal Free Energies** [Hartree]	**% of population**
BF_2	3015.9	3.49	4.61	3.145	68.2	-664.010806	100.00
Br	3017.2	3.30	4.36	2.103	48.2	-3013.475412	100.00
CHO-1	3015.8	3.37	4.46	3.153	70.8	-553.241701	63.46
CHO-2	3015.4	4.02	5.31	2.801	52.7	-553.241180	36.54
Cl	3017.2	3.33	4.40	2.034	46.2	-899.537904	100.00
$COCH_3$-1	3015.0	3.48	4.61	2.785	60.5	-592.541058	37.53
$COCH_3$-2	3015.4	3.43	4.53	3.381	74.6	-592.541539	62.47
$CONH_2$-1	3017.8	3.29	4.35	2.889	66.4	-608.618933	34.10
$CONH_2$-2	3015.4	3.53	4.67	3.105	66.5	-608.619555	65.90
$COOCH_3$-1	3016.0	3.46	4.58	2.991	65.3	-667.781509	44.88
$COOCH_3$-2	3015.3	3.46	4.57	3.246	71.0	-667.781703	55.12
COOH-1	3015.9	3.46	4.57	2.965	64.9	-628.504963	45.54
COOH-2	3016.0	3.44	4.55	3.125	68.7	-628.505132	54.46
Et-1	3016.5	3.70	4.90	2.493	50.9	-518.493242	44.20
Et-2	3017.2	3.79	5.02	2.261	45.1	-518.491868	10.31
Et-3	3016.7	3.73	4.94	2.497	50.6	-518.493269	45.48
F	3017.7	3.46	4.58	1.988	43.4	-539.166739	100.00

H	3017.6	3.70	4.89	2.959	60.6	-439.907080	100.00
iPr-1	3016.1	3.73	4.94	2.562	51.9	-557.783547	43.70
iPr-2	3016.6	3.73	4.94	2.421	49.0	-557.783786	56.30
Me	3017.0	3.81	5.04	2.439	48.4	-479.203348	100.00
MeS	3016.2	3.82	5.06	1.265	25.0	-877.408711	100.00
$MeSO_2$	3014.3	3.64	4.82	2.913	60.5	-1027.802896	100.00
NH_2	3014.5	4.89	6.47	-0.220	3.4	-495.261729	100.00
$NHNH_2$	3015.0	5.04	6.67	0.115	1.7	-550.570357	100.00
NMe_2	3013.7	5.76	7.62	-0.380	5.0	-573.822075	100.00
NO-1	3014.2	3.80	5.03	2.374	47.2	-569.225270	37.18
NO-2	3015.8	3.33	4.41	3.960	89.9	-569.225765	62.82
NO_2	3015.9	3.51	4.64	2.957	63.7	-644.445853	100.00
OCF_3-1	3017.5	3.33	4.40	1.607	36.6	-852.222424	26.18
OCF_3-2	3017.6	3.28	4.34	1.736	40.0	-852.222247	21.70
OCF_3-3	3017.5	3.28	4.34	2.399	55.3	-852.223074	52.12
OH-1	3016.7	4.04	5.35	1.219	22.8	-515.141485	59.09
OH-2	3016.6	3.95	5.22	0.925	17.7	-515.141138	40.91
OMe-1	3016.0	4.09	5.41	1.400	25.9	-554.416020	43.13
OMe-2	3017.0	4.17	5.52	0.675	12.2	-554.416281	56.87
SH-1	3016.3	3.56	4.71	1.202	25.5	-838.121079	47.57
SH-2	3016.5	3.54	4.68	1.072	22.9	-838.121171	52.43
SiH_3	3017.2	3.51	4.64	2.808	60.5	-730.604573	100.00
$SiMe_3$	3016.3	3.61	4.78	3.064	64.1	-848.518066	100.00

tBu	3017.0	3.69	4.88	2.816	57.7	-597.070541	100.00
Vin-1	3016.0	3.53	4.67	1.726	37.0	-517.285522	54.23
Vin-2	3015.4	3.58	4.74	2.003	42.2	-517.285362	45.77

TABLE S5. EDTM, MDTM and cos(ξ) of the examined modes in CN-IND with energetics of the conformers.

Substituent-Conformer	ν(CN) EDTM	ν(CN) MDTM	ν(CN) cos(ξ)	ν(CH) EDTM	ν(CH) MDTM	ν(CH) cos(ξ)	% of population
BF_2	5.314	8.285	-0.056	0.858	1.447	0.857	100.00
Br	5.558	9.173	-0.052	0.566	1.422	0.845	100.00
CHO-1	5.376	7.043	-0.063	0.788	1.551	0.832	61.90
CHO-2	5.294	7.455	-0.069	0.940	1.309	0.838	38.10
Cl	5.504	7.532	-0.064	0.563	1.377	0.845	100.00
$COCH_3$-1	5.504	8.291	-0.056	0.805	1.342	0.947	38.55
$COCH_3$-2	5.552	8.494	-0.056	0.734	1.596	0.951	61.45
$CONH_2$-1	5.540	8.386	-0.053	0.705	1.397	0.969	33.72
$CONH_2$-2	5.575	8.449	-0.064	0.694	1.578	0.990	66.28
$COOCH_3$-1	5.585	9.197	-0.048	0.759	1.439	0.957	43.65
$COOCH_3$-2	5.338	8.048	-0.062	0.749	1.256	0.979	56.35
COOH-1	5.603	9.716	-0.049	0.739	1.508	0.976	45.85
COOH-2	5.433	9.700	-0.037	0.707	1.254	0.986	54.15
Et-1	5.399	8.192	-0.057	0.825	1.389	0.895	42.61
Et-2	5.426	8.272	-0.055	0.803	1.455	0.902	9.46
Et-3	5.207	7.929	-0.058	0.852	1.352	0.872	47.93
F	6.042	7.805	-0.080	0.666	1.965	0.614	100.00
H	6.008	8.665	-0.066	0.707	2.106	0.567	100.00
iPr-1	5.968	8.838	-0.044	0.671	1.850	0.642	52.36

iPr-2	5.418	6.566	-0.081	0.581	1.449	0.699	47.64
Me	5.685	5.895	-0.094	0.638	1.669	0.946	100.00
MeS-1	6.051	9.654	-0.057	0.671	2.049	0.581	53.81
MeS-2	6.066	9.016	-0.048	0.685	1.963	0.558	46.19
$MeSO_2$-1	5.936	7.105	-0.071	0.685	1.812	0.646	36.03
$MeSO_2$-2	6.036	9.410	-0.069	0.806	2.257	0.122	63.97
NH_2	6.092	8.592	-0.043	0.718	1.959	0.026	100.00
$NHNH_2$-1	5.188	8.993	-0.057	0.934	1.220	0.910	35.86
$NHNH_2$-2	5.268	9.694	-0.033	0.972	1.233	0.755	64.14
NMe_2-1	6.155	7.058	-0.083	1.251	2.328	-0.189	50.82
NMe_2-2	6.303	8.447	-0.083	1.316	2.864	-0.108	49.18
NO-1	6.414	8.473	-0.056	1.255	2.579	-0.185	40.07
NO-2	6.525	9.348	-0.068	1.593	3.114	-0.157	59.93
NO_2-1	6.501	9.707	-0.052	1.468	3.485	-0.185	49.97
NO_2-2	5.112	7.233	-0.076	1.203	0.907	0.701	50.03
OCF_3-1	5.106	6.543	-0.060	0.974	1.864	0.798	23.70
OCF_3-2	4.970	7.536	-0.057	1.110	1.458	0.624	21.25
OCF_3-3	4.969	7.536	-0.057	1.107	1.456	0.625	55.06
OH-1	5.424	9.235	-0.052	0.564	1.363	0.718	57.80
OH-2	5.358	10.612	-0.051	0.548	1.638	0.599	42.20
OMe-1	5.233	10.584	-0.040	0.647	1.288	0.962	46.64
OMe-2	5.821	6.905	-0.085	0.857	1.883	0.118	53.36
SH-1	5.800	6.825	-0.079	0.799	1.794	0.076	48.89

SH-2	2.263	6.927	-0.563	6.034	7.924	-0.060	51.11
SiH_3-1	1.102	2.719	1.253	5.974	8.410	-0.076	49.97
SiH_3-2	5.844	7.842	-0.069	0.637	1.733	0.245	50.03
$SiMe_3$	5.834	7.763	-0.060	0.626	1.696	0.234	100.00
tBu-1	5.742	8.016	-0.058	0.625	1.580	0.981	33.27
tBu-2	5.742	8.016	-0.058	0.625	1.580	0.981	33.17
tBu-3	6.077	10.949	-0.042	0.637	2.153	0.751	33.56
Vin-1	6.109	10.008	-0.046	0.683	2.265	0.541	53.54
Vin-2	6.193	10.073	-0.003	0.682	2.444	0.484	46.46

TABLE S6. EDTM, MDTM and cos(ξ) of the examined modes in NC-IND with energetics of the conformers.

Substituent-Conformer	ν(NC) EDTM	ν(NC) MDTM	ν(NC) cos(ξ)	ν(CH) EDTM	ν(CH) MDTM	ν(CH) cos(ξ)	% of population
BF_2	18.547	29.309	-0.060	2.149	3.592	0.408	100.00
Br	18.678	32.476	-0.052	2.088	4.854	0.207	100.00
CHO-1	18.775	25.411	-0.062	2.107	3.038	0.494	63.46
CHO-2	18.788	26.319	-0.070	2.163	2.998	0.417	36.54
Cl	18.532	26.192	-0.064	2.098	3.700	0.262	100.00
$COCH_3$-1	18.758	29.028	-0.059	2.147	3.782	0.343	37.53
$COCH_3$-2	18.629	29.315	-0.060	2.129	3.967	0.400	62.47
$CONH_2$-1	18.609	29.010	-0.058	2.119	3.838	0.362	34.10
$CONH_2$-2	18.538	28.850	-0.064	2.161	4.065	0.353	65.90
$COOCH_3$-1	18.703	32.260	-0.051	2.139	4.480	0.312	44.88
$COOCH_3$-2	18.607	33.340	-0.054	2.139	4.653	0.326	55.12
COOH-1	18.683	28.901	-0.060	2.138	3.597	0.385	45.54
COOH-2	18.644	29.059	-0.060	2.133	3.674	0.399	54.46
Et-1	18.165	24.814	-0.076	2.213	4.432	0.254	44.20
Et-2	18.041	26.979	-0.067	2.240	4.598	0.219	10.31
Et-3	18.014	27.320	-0.051	2.222	4.304	0.262	45.48
F	18.116	22.210	-0.076	2.140	3.124	0.297	100.00
H	17.871	18.357	-0.096	2.209	2.521	0.529	100.00
iPr-1	18.094	29.928	-0.060	2.222	5.115	0.225	43.70

iPr-2	18.188	28.722	-0.051	2.222	4.994	0.218	56.30
Me	18.017	22.349	-0.074	2.245	3.580	0.304	100.00
MeS	18.461	30.480	-0.068	2.249	5.368	0.105	100.00
$MeSO_2$	19.178	34.621	-0.056	2.195	4.510	0.294	100.00
NH_2	17.915	21.959	-0.070	2.545	4.330	-0.020	100.00
$NHNH_2$	17.988	25.879	-0.071	2.582	5.441	0.008	100.00
NMe_2	18.099	28.589	-0.058	2.765	6.207	-0.026	100.00
NO-1	18.982	26.405	-0.078	2.248	2.866	0.373	37.18
NO-2	19.159	25.137	-0.054	2.099	3.249	0.581	62.82
NO_2	19.115	29.162	-0.061	2.154	3.036	0.452	100.00
OCF_3-1	18.431	33.762	-0.045	2.096	5.249	0.146	26.18
OCF_3-2	18.414	37.313	-0.048	2.084	5.745	0.145	21.70
OCF_3-3	18.460	37.866	-0.041	2.084	5.150	0.224	52.12
OH-1	17.918	22.148	-0.076	2.313	3.776	0.140	59.09
OH-2	17.983	21.999	-0.069	2.286	3.716	0.109	40.91
OMe-1	18.044	25.213	-0.052	2.327	4.578	0.131	43.13
OMe-2	17.967	26.593	-0.071	2.349	4.872	0.059	56.87
SH-1	18.498	26.229	-0.065	2.170	4.297	0.129	47.57
SH-2	18.544	26.115	-0.059	2.163	4.275	0.116	52.43
SiH_3	18.213	22.578	0.195	2.154	3.836	0.340	100.00
$SiMe_3$	18.384	35.164	-0.047	2.186	6.047	0.232	100.00
tBu	18.233	31.865	-0.051	2.210	5.722	0.223	100.00
Vin-1	18.715	24.926	-0.041	2.161	3.944	0.203	54.23

Vin-2	18.495	26.490	-0.084	2.178	4.033	0.228	45.77

Correlations of spectral parameters of selected modes with substituent constants

Figure S1. A non-linear correlation is found for ν(NC) (NC-IND) frequency. Infrared intensity depends on σ_p. a) $\nu = -1.07\ (\pm 0.23)\ \sigma_p^2 - 0.61\ (\pm 0.12)\ \sigma_p + 2211.17\ (\pm 0.07)$, $r = 0.84$, $r^2 = 0.71$, $n = 27$. (SiH_3 excluded due to coupling of ν(NC) and ν(SiH).) b) $I_{IR} = 8.27\ (\pm 2.97)\ \sigma_p^2 + 14.44\ (\pm 1.58)\ \sigma_p + 185.07\ (\pm 0.86)$, $r = 0.90$, $r^2 = 0.82$, $n = 27$. (SiH_3 excluded). c) VCD intensities of ν(NC) in NC-IND follow the trend, however even after exclusion of apparent outliers, the correlation has low statistical parameters r^2=0.59, r=0.76.

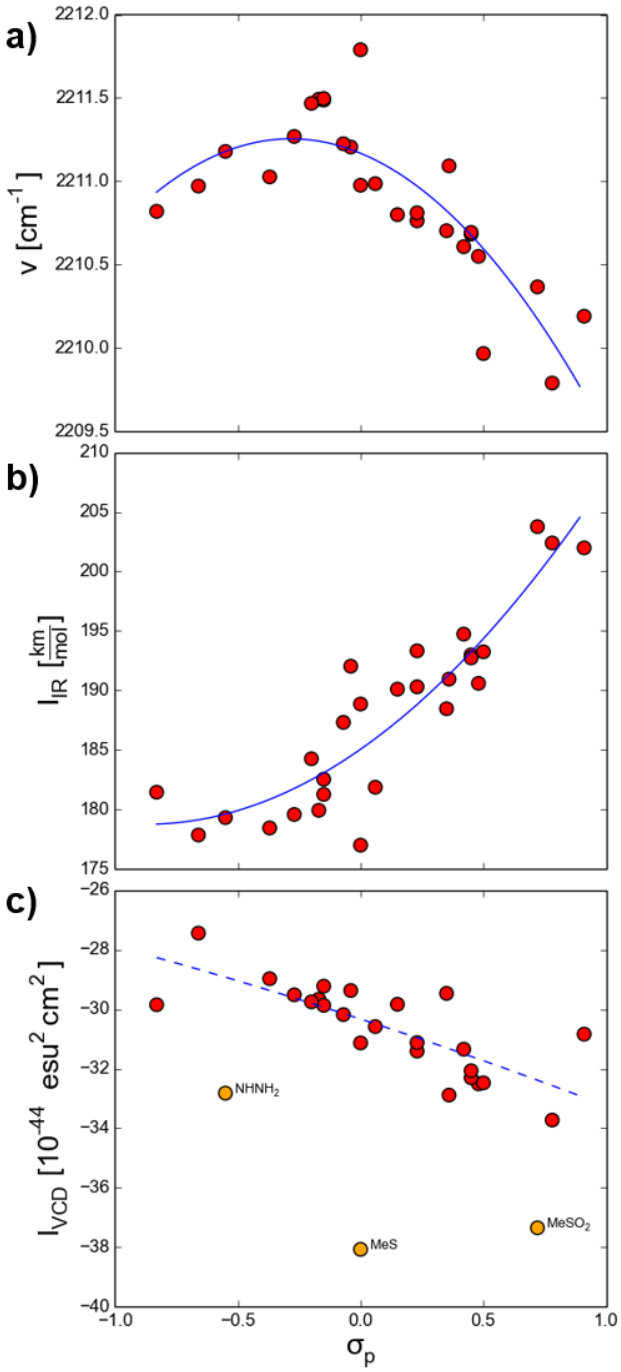


Figure S2. Correlations of ν(CH) (CN-IND) spectral parameters a) $\nu = -3.82\ (\pm 0.67)\sigma_p^2 + 3.49\ (\pm 0.36)\sigma_p + 3010.17\ (\pm 0.19)$, r=0.90, r^2=0.81, n=28 b) $I_{IR} = 1.45\ (\pm 0.09)\sigma_p^2 - 0.46\ (\pm 0.05)\sigma_p + 0.31\ (\pm 0.03)$, r=0.96, r^2=0.92, n=27 – OMe excluded due to coupling of νCH in the chiral center with the ν(CH) in OMe group.

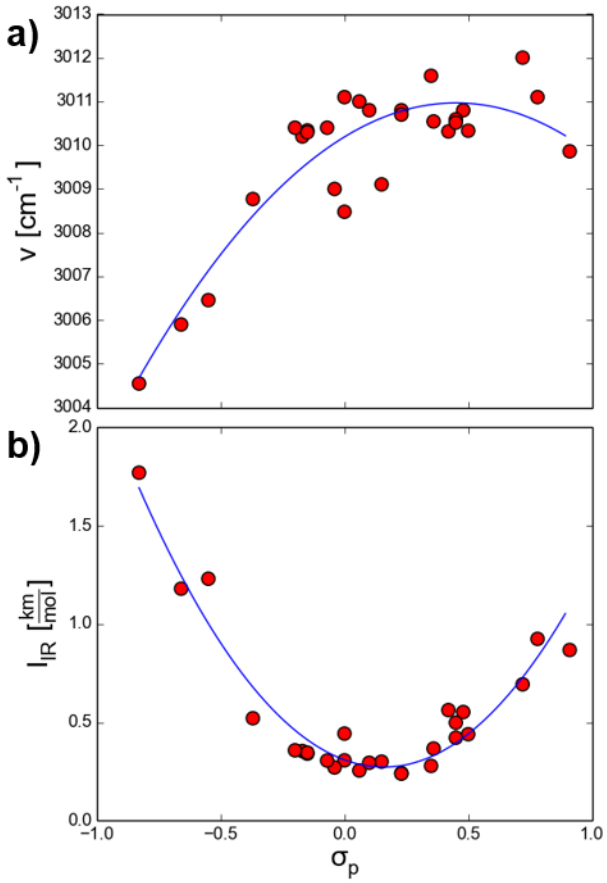


Figure S3. Correlations of ν(CH) (NC-IND) spectral parameters a) frequency has no significant correlation with σ_p b) $I_{IR} = 1.98\ (\pm 0.17)\sigma_p^2 - 1.59\ (\pm 0.09)\sigma_p + 4.77\ (\pm 0.05)$, $r=0.97$, $r^2=0.93$, $n=28$.

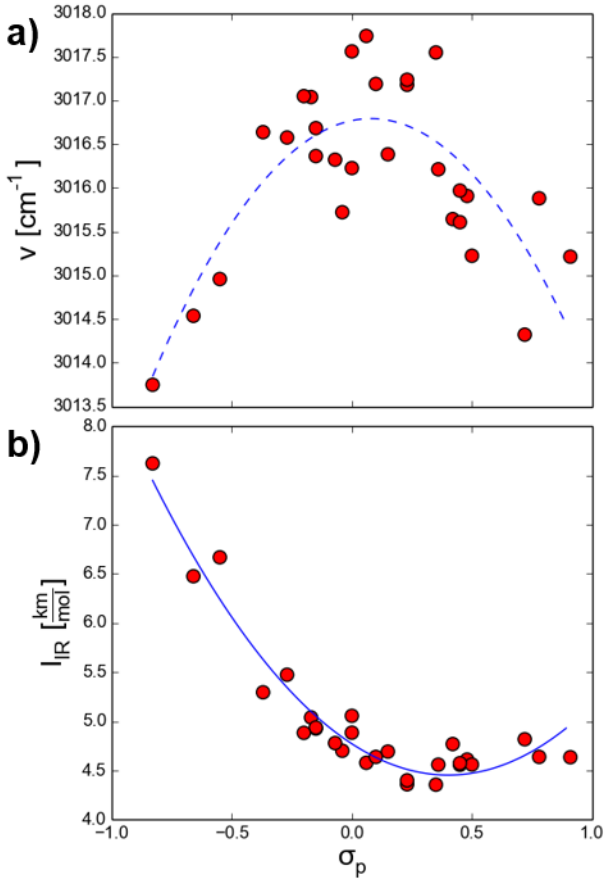


Figure S4. In ν(CN) (CN-IND) EDTM correlates well with σ_p while other factors do not. a) EDTM = - 0.83 (± 0.07) σ_p + 5.80 (± 0.03), r = 0.92, r^2 = 0.84, n = 28

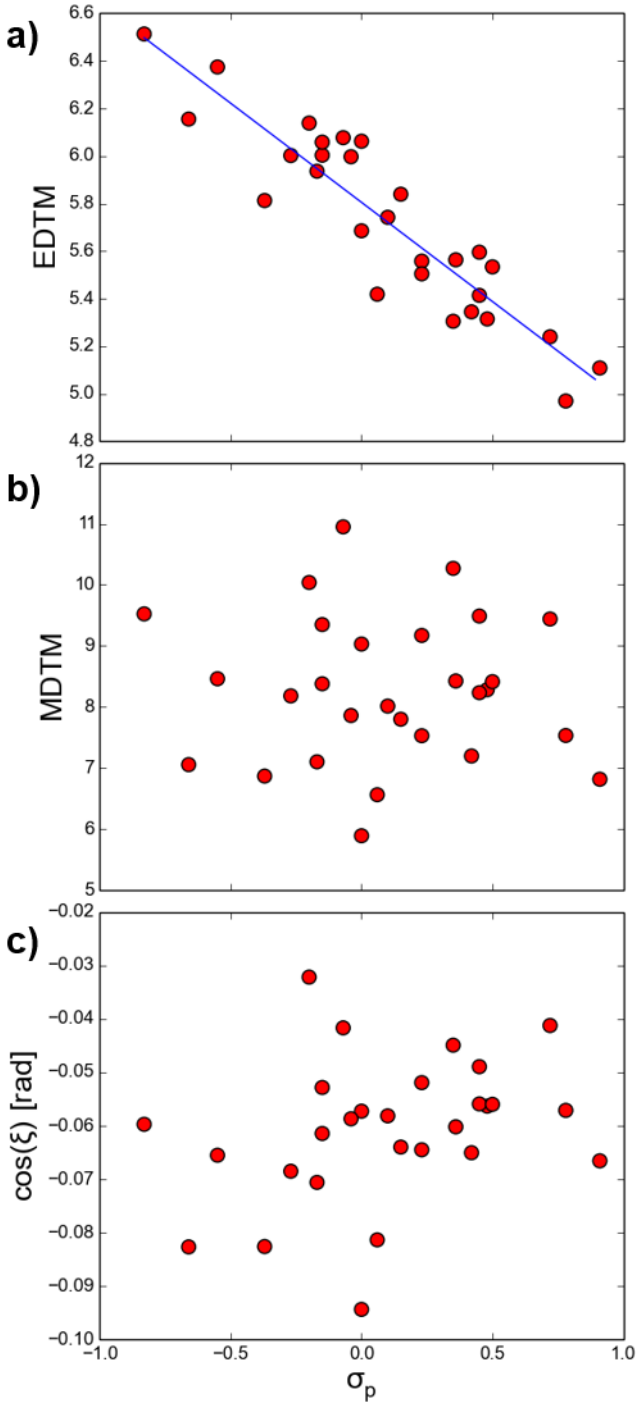


Figure S5. In ν(NC) (NC-IND) EDTM also correlates well with σ_p while other factors do not. a) EDTM = 0.42 (± 0.14) σ_p^2 + 0.71 (± 0.08) σ_p + 18.27 (± 0.04), r = 0.90, r^2 = 0.81, n = 28

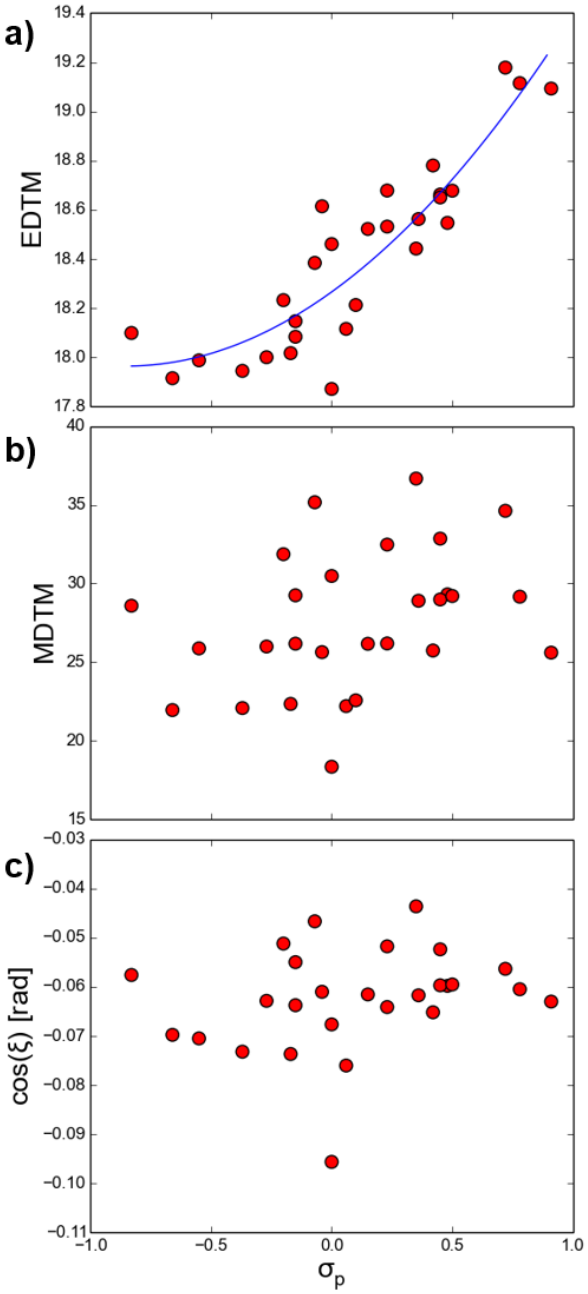


Figure S6. EDTM in ν(CH) (CN-IND) correlates well with σ_p. EDTM = 0.99 (± 0.07) σ_p^2 - 0.27 (± 0.04) σ_p + 0.65 (± 0.02) , r = 0.95, r^2 = 0.91, n = 27 (OMe excluded).

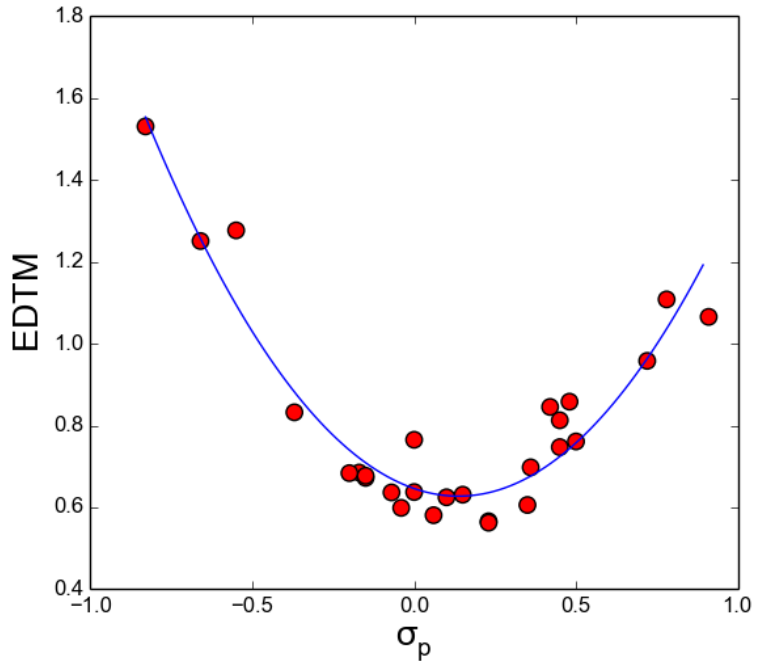
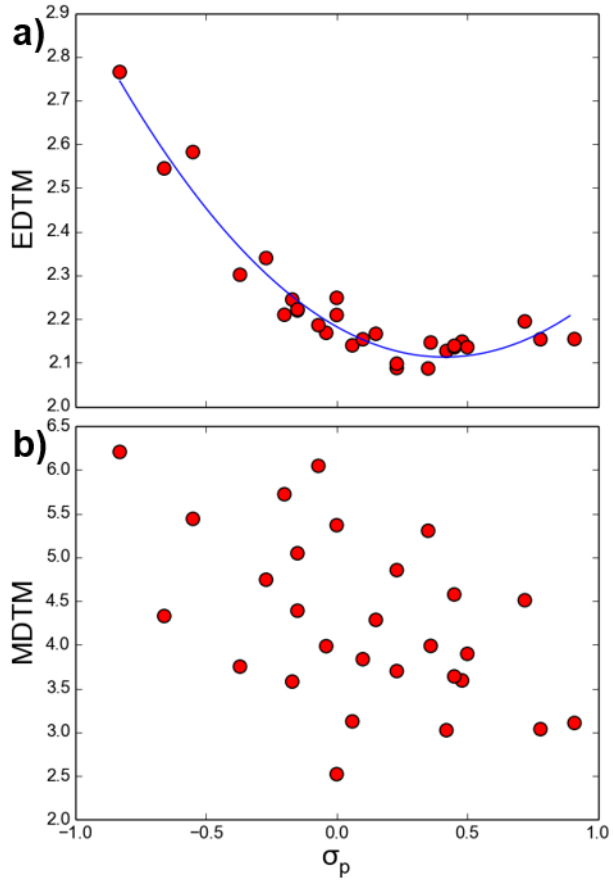


Figure S7. EDTM in ν(CH) (NC-IND) also correlates well with $\sigma_{p,}$ while no correlation is found for MDTM. a) EDTM = 0.41 (± 0.03) σ_p^2 - 0.34 (± 0.02) σ_p + 2.18 (± 0.01) , r = 0.97, r^2 = 0.94, n = 28.



Gaussian 09 input headings

Geometry optimization and harmonic frequencies

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VCD spectra and EDTM/MDTM details

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Full Gaussian 09 citation

Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, **2009**.

Coordinates and energies of CN-IND

BF_2-CN-IND
Total energy (hartree): -664.144789
Sum of electronic and thermal Free Energies (hartree): -664.044660

C	1.512170	2.034827	0.008671
C	2.727423	1.497857	-0.215338
C	2.600711	0.006953	-0.515552
C	1.103967	-0.237843	-0.358783
C	0.372552	-1.413251	-0.475202
C	-1.017150	-1.345832	-0.310731
C	-1.668612	-0.124982	-0.035458
C	-0.905963	1.056029	0.084359
C	0.478197	0.994107	-0.073871
H	1.313296	3.083549	0.221851
H	3.684983	2.012380	-0.210883
H	0.860836	-2.366225	-0.679253
H	-1.609158	-2.256930	-0.395864
H	-1.399145	2.003553	0.301552
H	2.899260	-0.187291	-1.561117
C	3.438322	-0.843296	0.340255
N	4.107575	-1.517597	1.006942
B	-3.202587	-0.079880	0.137645
F	-3.850650	1.065448	0.400514
F	-3.964891	-1.178099	0.032463

Br-CN-IND
Total energy (hartree): -3013.600737
Sum of electronic and thermal Free Energies (hartree): -3013.509236

C	-1.861455	2.034365	-0.076026
C	-3.077299	1.503960	0.161631
C	-2.951532	0.024904	0.515379
C	-1.454171	-0.222562	0.375259
C	-0.714176	-1.386086	0.535857
C	0.679018	-1.328910	0.376663
C	1.289132	-0.109986	0.063591
C	0.558663	1.069712	-0.107007
C	-0.828465	0.997322	0.049245
H	-1.662611	3.074988	-0.325850
H	-4.034904	2.017889	0.133725
H	-1.192887	-2.336580	0.772012
H	1.282736	-2.226602	0.493672
H	1.057453	2.004586	-0.355079
H	-3.260732	-0.130368	1.564264
C	-3.785599	-0.852562	-0.316656
N	-4.452040	-1.549605	-0.962554

Br	3.195729	-0.055360	-0.143214

CHO-1-CN-IND

Total energy (hartree): -553.386724

Sum of electronic and thermal Free Energies (hartree): -553.275490

C	0.974809	2.037859	0.022432
C	2.225391	1.595433	-0.212556
C	2.211478	0.101294	-0.522732
C	0.739196	-0.258494	-0.357068
C	0.101788	-1.486203	-0.473437
C	-1.288242	-1.525848	-0.295815
C	-2.013727	-0.357491	-0.010941
C	-1.359845	0.882986	0.110544
C	0.021173	0.922944	-0.059562
H	0.698430	3.067022	0.243770
H	3.141100	2.181374	-0.211218
H	0.660083	-2.397654	-0.686414
H	-1.818582	-2.475823	-0.377629
H	-1.944590	1.773860	0.336950
H	2.516732	-0.062061	-1.571664
C	3.117527	-0.689243	0.320668
N	3.840130	-1.317325	0.976692
C	-3.484973	-0.448637	0.164710
H	-3.907242	-1.475591	0.057023
O	-4.211788	0.495318	0.406859

CHO-2-CN-IND

Total energy (hartree): -553.386220

Sum of electronic and thermal Free Energies (hartree): -553.275032

C	-1.271430	2.028217	-0.091761
C	-2.442456	1.423264	0.188019
C	-2.210253	-0.043360	0.538887
C	-0.705688	-0.197480	0.348081
C	0.104304	-1.321037	0.489686
C	1.479840	-1.178771	0.286225
C	2.027837	0.072340	-0.053340
C	1.203636	1.200397	-0.200503
C	-0.170676	1.059373	-0.000775
H	-1.147940	3.078526	-0.349436
H	-3.431321	1.874688	0.192764
H	-0.318973	-2.292733	0.744372
H	2.151605	-2.030486	0.384714
H	1.639447	2.164389	-0.468533
H	-2.467997	-0.215412	1.599144
C	-3.013700	-0.977192	-0.260780
N	-3.655832	-1.716912	-0.883214

C	3.490806	0.215379	-0.263855
H	3.825008	1.244663	-0.536500
O	4.298460	-0.686504	-0.157915

Cl-CN-IND

Total energy (hartree): -899.664910

Sum of electronic and thermal Free Energies (hartree): -899.571723

C	-1.177463	2.034751	-0.077010
C	-2.392451	1.514249	0.185779
C	-2.271836	0.033311	0.533327
C	-0.780044	-0.226448	0.360681
C	-0.046713	-1.396711	0.502839
C	1.342518	-1.351225	0.313425
C	1.955959	-0.137043	-0.010755
C	1.232712	1.049414	-0.162839
C	-0.150858	0.988750	0.023549
H	-0.975320	3.074269	-0.328817
H	-3.345928	2.036507	0.179794
H	-0.528582	-2.343371	0.747519
H	1.945320	-2.251532	0.414254
H	1.738665	1.977992	-0.420180
H	-2.560686	-0.122078	1.587975
C	-3.130678	-0.834747	-0.283328
N	-3.816336	-1.524545	-0.916794
Cl	3.703177	-0.102693	-0.239823

$COCH_3$-1-CN-IND

Total energy (hartree): -592.711713

Sum of electronic and thermal Free Energies (hartree): -592.574952

C	1.442930	2.039870	-0.018255
C	2.672302	1.532274	-0.234379
C	2.584035	0.034715	-0.514893
C	1.093933	-0.245557	-0.357691
C	0.387304	-1.438697	-0.461373
C	-1.001442	-1.404607	-0.300854
C	-1.676533	-0.197036	-0.040624
C	-0.950287	1.003074	0.067967
C	0.436708	0.971348	-0.088865
H	1.217914	3.086117	0.181411
H	3.616069	2.071708	-0.235262
H	0.896571	-2.383078	-0.654039
H	-1.592200	-2.315966	-0.373121
H	-1.454121	1.946108	0.272833
H	2.891177	-0.165810	-1.556759
C	3.441714	-0.780284	0.355351
N	4.127912	-1.425425	1.033580

C	-3.172339	-0.238196	0.115961
O	-3.778648	-1.292245	0.002651
C	-3.915454	1.050225	0.416700
H	-3.754564	1.790122	-0.380830
H	-4.983577	0.828262	0.497807
H	-3.560692	1.495705	1.357426

$COCH_3$-2-CN-IND

Total energy (hartree): -592.712179

Sum of electronic and thermal Free Energies (hartree): -592.575392

C	1.548419	2.025480	0.024287
C	2.748979	1.459582	-0.207745
C	2.584727	-0.025378	-0.520527
C	1.083127	-0.233169	-0.360119
C	0.318770	-1.385008	-0.480339
C	-1.069458	-1.283121	-0.307940
C	-1.679383	-0.048130	-0.023263
C	-0.891476	1.111950	0.100731
C	0.487593	1.012049	-0.063166
H	1.376544	3.076970	0.246550
H	3.719177	1.949978	-0.202252
H	0.777450	-2.350521	-0.693247
H	-1.674229	-2.183426	-0.397127
H	-1.381192	2.058009	0.325767
H	2.876378	-0.217219	-1.568456
C	3.403388	-0.904225	0.324888
N	4.056670	-1.603216	0.982024
C	-3.166879	0.081154	0.160071
O	-3.666663	1.171453	0.392313
C	-4.035356	-1.158079	0.052878
H	-3.739063	-1.909162	0.799333
H	-5.077959	-0.870597	0.217430
H	-3.935195	-1.621766	-0.939206

$CONH_2$-1-CN-IND

Total energy (hartree): -608.779655

Sum of electronic and thermal Free Energies (hartree): -608.652785

C	1.472841	2.026654	-0.139152
C	2.692199	1.483754	-0.324291
C	2.575869	-0.026043	-0.514486
C	1.080055	-0.267671	-0.345190
C	0.347729	-1.447221	-0.398234
C	-1.042682	-1.375966	-0.251073
C	-1.687525	-0.145541	-0.040749
C	-0.939236	1.043478	0.009529
C	0.446906	0.975008	-0.144227

H	1.268010	3.087229	-0.003469
H	3.645914	2.004467	-0.356168
H	0.835529	-2.410723	-0.546475
H	-1.653817	-2.275267	-0.301064
H	-1.427693	2.010226	0.130189
H	2.883278	-0.295460	-1.540433
C	3.415018	-0.801014	0.408993
N	4.086134	-1.414625	1.130272
C	-3.186636	-0.169442	0.098144
O	-3.863270	-1.088696	-0.347230
N	-3.760305	0.909162	0.727105
H	-4.753443	0.844904	0.903838
H	-3.219644	1.506460	1.334208

$CONH_2$-2-CN-IND

Total energy (hartree): -608.779990

Sum of electronic and thermal Free Energies (hartree): -608.653423

C	1.501292	2.027786	-0.089421
C	2.711279	1.472206	-0.296751
C	2.572856	-0.030336	-0.527493
C	1.076199	-0.255855	-0.346464
C	0.331566	-1.426191	-0.390138
C	-1.057701	-1.339077	-0.218556
C	-1.687059	-0.100076	-0.006316
C	-0.920886	1.075874	0.056264
C	0.459825	0.991481	-0.115336
H	1.310801	3.086381	0.076975
H	3.672280	1.979744	-0.322889
H	0.806978	-2.396223	-0.535386
H	-1.638095	-2.261028	-0.216656
H	-1.424944	2.021693	0.247014
H	2.862573	-0.272313	-1.565568
C	3.413150	-0.847380	0.357600
N	4.084050	-1.499007	1.044982
C	-3.173419	0.042683	0.194775
O	-3.660473	1.049253	0.697472
N	-3.955531	-1.015527	-0.192178
H	-4.955320	-0.884338	-0.130102
H	-3.612731	-1.732901	-0.811775

$COOCH_3$-1-CN-IND

Total energy (hartree): -667.956046

Sum of electronic and thermal Free Energies (hartree): -667.815360

C	1.745122	2.058457	-0.048614
C	3.001406	1.604956	-0.226469
C	2.989287	0.100824	-0.484761

C	1.510105	-0.246262	-0.357972
C	0.863539	-1.472076	-0.457456
C	-0.530019	-1.500754	-0.328797
C	-1.258251	-0.319701	-0.105453
C	-0.598619	0.917334	-0.000807
C	0.790622	0.943886	-0.125244
H	1.466707	3.095770	0.128238
H	3.919205	2.187377	-0.213851
H	1.419597	-2.394889	-0.622108
H	-1.074760	-2.440404	-0.398242
H	-1.166809	1.827744	0.175999
H	3.330293	-0.100940	-1.515751
C	3.862463	-0.660623	0.417994
N	4.561422	-1.263518	1.121644
C	-2.742982	-0.434669	0.017270
O	-3.360754	-1.476919	-0.073346
O	-3.339763	0.759061	0.242425
C	-4.774276	0.717536	0.371537
H	-5.228558	0.330231	-0.548340
H	-5.062566	0.076816	1.213433
H	-5.079312	1.752334	0.549109

$COOCH_3$-2-CN-IND

Total energy (hartree): -667.956200

Sum of electronic and thermal Free Energies (hartree): -667.815601

C	2.047273	1.996164	0.043181
C	3.222080	1.376074	-0.182534
C	2.990113	-0.096968	-0.507871
C	1.478601	-0.234699	-0.363194
C	0.661631	-1.349133	-0.501725
C	-0.721292	-1.186959	-0.343536
C	-1.267268	0.075499	-0.053727
C	-0.434273	1.198283	0.090012
C	0.941352	1.034398	-0.062003
H	1.923153	3.052916	0.272162
H	4.214223	1.819974	-0.164412
H	1.077636	-2.332928	-0.718808
H	-1.382218	-2.044457	-0.443805
H	-0.879452	2.164948	0.319072
H	3.282318	-0.295208	-1.554442
C	3.758904	-1.018654	0.338715
N	4.373923	-1.750581	0.996928
C	-2.737464	0.280853	0.116977
O	-3.253299	1.353739	0.362225
O	-3.446042	-0.861463	-0.031430
C	-4.872401	-0.728751	0.123639

H	-5.113515	-0.359317	1.127540
H	-5.273604	-0.032694	-0.622723
H	-5.274800	-1.734016	-0.027033

COOH-1-CN-IND

Total energy (hartree): -628.654413

Sum of electronic and thermal Free Energies (hartree): -628.538830

C	1.455188	2.036300	0.004994
C	2.676653	1.514005	-0.220161
C	2.567716	0.021162	-0.517785
C	1.074542	-0.241290	-0.358560
C	0.354765	-1.424592	-0.472594
C	-1.033959	-1.376176	-0.307282
C	-1.683287	-0.159904	-0.033775
C	-0.950519	1.033911	0.086444
C	0.434228	0.982583	-0.074663
H	1.243896	3.082829	0.216928
H	3.627742	2.040452	-0.217886
H	0.851533	-2.373041	-0.676311
H	-1.635064	-2.280023	-0.386586
H	-1.459637	1.970614	0.302486
H	2.867689	-0.170880	-1.563346
C	3.417414	-0.816579	0.338525
N	4.097029	-1.480391	1.005237
C	-3.164781	-0.186181	0.125045
O	-3.857792	-1.178089	0.030031
O	-3.693627	1.038553	0.393637
H	-4.651756	0.909641	0.477580

COOH-2-CN-IND

Total energy (hartree): -628.654584

Sum of electronic and thermal Free Energies (hartree): -628.538987

C	1.505487	2.034123	0.021843
C	2.713287	1.483840	-0.210137
C	2.568136	-0.003549	-0.519862
C	1.069509	-0.231465	-0.358313
C	0.321866	-1.395609	-0.477798
C	-1.066797	-1.317041	-0.307645
C	-1.684625	-0.086559	-0.024648
C	-0.922090	1.087744	0.100669
C	0.459092	1.006146	-0.063496
H	1.319658	3.083593	0.242432
H	3.676864	1.987075	-0.206069
H	0.795447	-2.354199	-0.689274
H	-1.675118	-2.214354	-0.393176
H	-1.423661	2.027571	0.324848

H	2.860593	-0.193523	-1.567924
C	3.399608	-0.869506	0.326231
N	4.063871	-1.556999	0.984397
C	-3.159550	0.024673	0.156692
O	-3.752115	1.056509	0.398480
O	-3.807201	-1.163483	0.023612
H	-4.749881	-0.978148	0.160425

Et-1-CN-IND

Total energy (hartree): -518.683180

Sum of electronic and thermal Free Energies (hartree): -518.527153

C	-1.191809	2.029706	-0.115288
C	-2.390815	1.545552	0.265452
C	-2.276010	0.063243	0.612166
C	-0.812814	-0.235745	0.304492
C	-0.096952	-1.422384	0.382428
C	1.267236	-1.401593	0.056531
C	1.916515	-0.219238	-0.339510
C	1.174135	0.971342	-0.419541
C	-0.185800	0.958850	-0.101076
H	-0.988811	3.062329	-0.394530
H	-3.326650	2.093131	0.344259
H	-0.577874	-2.356397	0.674384
H	1.838037	-2.330169	0.104192
H	1.658646	1.896080	-0.737576
H	-2.472432	-0.080993	1.689348
C	-3.228702	-0.784393	-0.117299
N	-3.988640	-1.456862	-0.681217
C	3.399460	-0.222662	-0.645342
H	3.683767	-1.200911	-1.059356
H	3.612485	0.524454	-1.423941
C	4.265263	0.074181	0.591936
H	5.332942	0.064731	0.331756
H	4.024344	1.060178	1.012806
H	4.097784	-0.675573	1.377486

Et-2-CN-IND

Total energy (hartree): -518.682039

Sum of electronic and thermal Free Energies (hartree): -518.525732

C	1.453207	2.007711	0.102010
C	2.606569	1.368471	-0.176800
C	2.330136	-0.088560	-0.540068
C	0.819591	-0.192815	-0.358709
C	-0.038259	-1.270671	-0.506628
C	-1.414320	-1.070195	-0.299901
C	-1.934052	0.186499	0.047854

C	-1.045500	1.268956	0.196925
C	0.320800	1.077128	-0.001222
H	1.364250	3.059833	0.367804
H	3.609193	1.788792	-0.172327
H	0.335756	-2.260978	-0.767873
H	-2.084020	-1.920709	-0.412281
H	-1.430051	2.252970	0.471687
H	2.597222	-0.262921	-1.597364
C	3.099205	-1.048617	0.263217
N	3.714644	-1.810854	0.886098
C	-3.418521	0.425352	0.273304
H	-3.545955	0.855909	1.279030
H	-3.748349	1.211765	-0.424079
C	-4.337481	-0.788995	0.128750
H	-5.378805	-0.497271	0.318882
H	-4.291913	-1.215483	-0.883080
H	-4.078083	-1.581515	0.844527

Et-3-CN-IND

Total energy (hartree): -518.683178

Sum of electronic and thermal Free Energies (hartree): -518.527264

C	1.238871	2.024733	0.147271
C	2.463592	1.486290	-0.016925
C	2.345371	0.026023	-0.445701
C	0.837441	-0.200613	-0.435501
C	0.091753	-1.337801	-0.714137
C	-1.307174	-1.247985	-0.662487
C	-1.961424	-0.046190	-0.340035
C	-1.190212	1.095064	-0.061029
C	0.203391	1.013192	-0.104576
H	1.036503	3.057223	0.427423
H	3.422806	1.981744	0.110622
H	0.572683	-2.284138	-0.963263
H	-1.903707	-2.134884	-0.881473
H	-1.680649	2.038082	0.186257
H	2.736825	-0.090530	-1.471792
C	3.097878	-0.899712	0.411547
N	3.701728	-1.633777	1.078037
C	-3.472407	0.007685	-0.257149
H	-3.818562	1.005666	-0.564117
H	-3.901793	-0.709525	-0.971702
C	-4.005888	-0.301645	1.152897
H	-5.103626	-0.253562	1.173035
H	-3.701246	-1.306326	1.476880
H	-3.618483	0.418443	1.886826

F-CN-IND

Total energy (hartree): -539.295927

Sum of electronic and thermal Free Energies (hartree): -539.200550

C	-0.747922	2.035557	-0.077439
C	-1.961209	1.528785	0.218503
C	-1.848542	0.045277	0.557108
C	-0.365345	-0.231806	0.341645
C	0.355949	-1.412952	0.460332
C	1.739645	-1.385531	0.231530
C	2.344603	-0.176001	-0.105270
C	1.647180	1.022465	-0.236015
C	0.268499	0.977570	-0.009808
H	-0.540886	3.073560	-0.331590
H	-2.908011	2.062619	0.241437
H	-0.133246	-2.352794	0.716275
H	2.347160	-2.285679	0.308480
H	2.171038	1.937755	-0.506212
H	-2.111844	-0.110567	1.618313
C	-2.740657	-0.807681	-0.239772
N	-3.452175	-1.485890	-0.857119
F	3.687534	-0.166416	-0.321306

H-CN-IND

Total energy (hartree): -440.045876

Sum of electronic and thermal Free Energies (hartree): -439.940965

C	-0.278688	2.029888	-0.085174
C	-1.497144	1.566587	0.257273
C	-1.423711	0.076969	0.581348
C	0.039364	-0.252184	0.302358
C	0.718144	-1.460990	0.384864
C	2.091920	-1.473766	0.097013
C	2.758792	-0.295015	-0.261820
C	2.071456	0.922070	-0.347976
C	0.702092	0.936328	-0.066758
H	-0.045254	3.062124	-0.341047
H	-2.422394	2.133604	0.322820
H	0.201906	-2.382497	0.655439
H	2.644822	-2.411744	0.151013
H	2.594539	1.835507	-0.631917
H	-1.645544	-0.079890	1.651829
C	-2.378104	-0.738468	-0.181496
N	-3.139889	-1.385320	-0.772127
H	3.826424	-0.328380	-0.481051

iPr-1-CN-IND

Total energy (hartree): -557.999806

Sum of electronic and thermal Free Energies (hartree): -557.817476

C	1.718988	2.007553	0.260592
C	2.891598	1.424013	-0.058004
C	2.655492	-0.003940	-0.543670
C	1.147027	-0.160829	-0.387729
C	0.318555	-1.247653	-0.636661
C	-1.059744	-1.099764	-0.429321
C	-1.617196	0.112334	0.018729
C	-0.763259	1.198814	0.266619
C	0.613424	1.059222	0.067683
H	1.599147	3.031163	0.611683
H	3.882788	1.867631	-0.007756
H	0.722939	-2.201760	-0.975999
H	-1.710569	-1.953155	-0.619914
H	-1.176400	2.145748	0.617761
H	2.934794	-0.082740	-1.609270
C	3.442158	-1.008353	0.184614
N	4.071783	-1.804467	0.748074
C	-3.117891	0.248010	0.239014
H	-3.295007	1.276973	0.588249
C	-3.625111	-0.703908	1.337485
H	-4.694285	-0.535432	1.528134
H	-3.498830	-1.755308	1.042913
H	-3.080056	-0.550013	2.278223
C	-3.910548	0.064301	-1.067880
H	-3.798309	-0.955575	-1.462167
H	-4.981608	0.240587	-0.895619
H	-3.568046	0.764352	-1.841585

iPr-2-CN-IND

Total energy (hartree): -557.999849

Sum of electronic and thermal Free Energies (hartree): -557.817387

C	1.402608	2.021681	0.155879
C	2.659173	1.603535	-0.094670
C	2.654107	0.135920	-0.515174
C	1.179292	-0.234995	-0.401390
C	0.529725	-1.440298	-0.621614
C	-0.865032	-1.484438	-0.466956
C	-1.609921	-0.351359	-0.100271
C	-0.932410	0.861301	0.122438
C	0.454406	0.913729	-0.024903
H	1.121523	3.031417	0.450771
H	3.572213	2.190556	-0.034885
H	1.080173	-2.339796	-0.898719
H	-1.386026	-2.428111	-0.634406
H	-1.482466	1.756860	0.412747

H	2.984981	0.050580	-1.565348
C	3.548784	-0.706996	0.289401
N	4.264535	-1.374649	0.913621
C	-3.121272	-0.444758	0.060059
H	-3.402388	-1.480799	-0.183247
C	-3.863566	0.476605	-0.924744
H	-4.950085	0.336002	-0.837696
H	-3.646322	1.535037	-0.721949
H	-3.572752	0.265183	-1.962350
C	-3.560047	-0.177983	1.511435
H	-3.331193	0.853983	1.813511
H	-4.643847	-0.325550	1.618925
H	-3.050627	-0.854478	2.210363

Me-CN-IND

Total energy (hartree): -479.366380

Sum of electronic and thermal Free Energies (hartree): -479.237175

C	0.785436	2.029998	0.077798
C	2.002600	1.527264	-0.209558
C	1.894969	0.043069	-0.550538
C	0.409780	-0.235616	-0.347096
C	-0.315008	-1.411161	-0.472440
C	-1.701151	-1.368884	-0.251436
C	-2.360533	-0.176807	0.088903
C	-1.609055	1.005681	0.215230
C	-0.230560	0.971249	0.001483
H	0.576058	3.067930	0.331657
H	2.948670	2.062699	-0.224510
H	0.171076	-2.353377	-0.727047
H	-2.280773	-2.288107	-0.344351
H	-2.103876	1.941051	0.482432
H	2.167263	-0.113687	-1.609298
C	2.781578	-0.808704	0.253703
N	3.489928	-1.484724	0.877353
C	-3.853241	-0.156748	0.324660
H	-4.087357	0.145867	1.356037
H	-4.351365	0.559510	-0.345011
H	-4.298088	-1.144873	0.154361

MeS-1-CN-IND

Total energy (hartree): -877.570634

Sum of electronic and thermal Free Energies (hartree): -877.442501

C	-1.769367	2.001767	-0.073754
C	-2.926119	1.360136	0.183872
C	-2.657100	-0.101824	0.531980
C	-1.145787	-0.206493	0.365929

C	-0.290351	-1.287837	0.507602
C	1.088421	-1.095775	0.320589
C	1.599557	0.172031	-0.003990
C	0.725947	1.267693	-0.151967
C	-0.640229	1.067215	0.030452
H	-1.674970	3.056864	-0.324967
H	-3.927923	1.782432	0.173701
H	-0.668092	-2.281247	0.751097
H	1.752977	-1.949112	0.429504
H	1.117313	2.252078	-0.409938
H	-2.938382	-0.287772	1.583742
C	-3.419105	-1.050269	-0.292068
N	-4.027705	-1.805055	-0.930492
S	3.334631	0.513703	-0.255455
C	4.135136	-1.109986	-0.025791
H	3.984731	-1.491059	0.991601
H	3.783444	-1.837120	-0.767751
H	5.204731	-0.928883	-0.183398

MeS-2-CN-IND

Total energy (hartree): -877.570554

Sum of electronic and thermal Free Energies (hartree): -877.442357

C	1.358557	2.033363	-0.045696
C	2.625900	1.618790	-0.241884
C	2.654826	0.116143	-0.507990
C	1.188187	-0.271799	-0.367078
C	0.562030	-1.509516	-0.465177
C	-0.827049	-1.574852	-0.317870
C	-1.588373	-0.413070	-0.076773
C	-0.953039	0.835174	0.025424
C	0.437048	0.890810	-0.117477
H	1.053066	3.061640	0.140945
H	3.525925	2.228570	-0.236454
H	1.131932	-2.421803	-0.642930
H	-1.329590	-2.539700	-0.387659
H	-1.517310	1.745343	0.214493
H	2.998405	-0.068444	-1.541370
C	3.559858	-0.618917	0.386133
N	4.283546	-1.203054	1.080888
S	-3.351137	-0.651777	0.082984
C	-3.984877	1.026830	0.413926
H	-3.572811	1.433230	1.345677
H	-3.785685	1.703930	-0.425772
H	-5.068977	0.909300	0.525880

$MeSO_2$-1-CN-IND

Total energy (hartree): -1027.970794

Sum of electronic and thermal Free Energies (hartree): -1027.836697

C	-2.093765	2.037860	-0.096116
C	-3.303922	1.511471	0.175859
C	-3.171442	0.037171	0.545005
C	-1.678645	-0.216777	0.369750
C	-0.949248	-1.390530	0.511131
C	0.438892	-1.342787	0.313941
C	1.044314	-0.125495	-0.012072
C	0.322973	1.061523	-0.174353
C	-1.059180	1.001435	0.018807
H	-1.898705	3.074237	-0.364790
H	-4.261640	2.025615	0.164003
H	-1.436164	-2.335843	0.750093
H	1.045016	-2.244378	0.383612
H	0.831064	1.978518	-0.468441
H	-3.447712	-0.103268	1.605305
C	-4.029208	-0.853266	-0.247427
N	-4.715388	-1.560124	-0.860823
S	2.844592	-0.086092	-0.253076
O	3.289402	-1.459134	-0.633531
O	3.162980	1.093121	-1.112121
C	3.501935	0.258054	1.406914
H	4.590362	0.290512	1.287093
H	3.113397	1.225490	1.740304
H	3.203350	-0.556408	2.074368

$MeSO_2$-2-CN-IND

Total energy (hartree): -1027.971341

Sum of electronic and thermal Free Energies (hartree): -1027.837239

C	2.108663	2.031402	0.108176
C	3.323798	1.489252	-0.103863
C	3.190018	0.019366	-0.489802
C	1.685903	-0.212456	-0.400686
C	0.945727	-1.366537	-0.624269
C	-0.450715	-1.297375	-0.511085
C	-1.052688	-0.080314	-0.177760
C	-0.323033	1.091481	0.045490
C	1.067035	1.010347	-0.065633
H	1.914260	3.069661	0.369904
H	4.286745	1.989452	-0.038843
H	1.428088	-2.309000	-0.882856
H	-1.070799	-2.171063	-0.704148
H	-0.836689	2.024370	0.272089
H	3.525586	-0.121838	-1.532470
C	3.982651	-0.887281	0.351034

N	4.613945	-1.605944	1.008211
S	-2.862996	-0.013682	-0.038255
O	-3.280904	1.406835	-0.232923
O	-3.430623	-1.105321	-0.883525
C	-3.187317	-0.443644	1.697807
H	-4.276833	-0.408826	1.806821
H	-2.804778	-1.452251	1.883425
H	-2.703307	0.302463	2.335819

NH_2-CN-IND

Total energy (hartree): -495.415180

Sum of electronic and thermal Free Energies (hartree): -495.295515

C	-0.768509	2.027849	-0.071869
C	-1.984556	1.525283	0.220708
C	-1.876929	0.039900	0.556781
C	-0.394177	-0.237656	0.345557
C	0.340044	-1.410969	0.463149
C	1.720643	-1.374710	0.237010
C	2.373493	-0.172023	-0.104160
C	1.622570	1.014060	-0.225311
C	0.246740	0.967595	-0.003641
H	-0.560166	3.066277	-0.324974
H	-2.929916	2.061961	0.240853
H	-0.140183	-2.356075	0.718538
H	2.303748	-2.293186	0.317113
H	2.114615	1.948753	-0.498348
H	-2.151838	-0.118142	1.614896
C	-2.769721	-0.804897	-0.249191
N	-3.482525	-1.477656	-0.871545
N	3.742075	-0.171288	-0.385268
H	4.213135	0.719080	-0.296301
H	4.276161	-0.932650	0.011711

$NHNH_2$-1-CN-IND

Total energy (hartree): -550.739226

Sum of electronic and thermal Free Energies (hartree): -550.604154

C	-1.380875	2.013061	-0.061345
C	-2.542781	1.398531	0.237359
C	-2.295529	-0.072669	0.562591
C	-0.794865	-0.211310	0.337738
C	0.047355	-1.309676	0.446707
C	1.419812	-1.150827	0.213601
C	1.948217	0.108502	-0.129369
C	1.091861	1.224023	-0.236210
C	-0.271594	1.050804	-0.008790
H	-1.271995	3.067852	-0.309202

H	-3.533595	1.845160	0.267861
H	-0.342036	-2.295730	0.702625
H	2.094069	-1.999641	0.289128
H	1.493845	2.202903	-0.504027
H	-2.545467	-0.262224	1.621673
C	-3.114432	-0.990366	-0.242158
N	-3.769607	-1.719935	-0.863892
N	3.307954	0.279527	-0.432092
H	3.621484	1.241805	-0.353679
N	4.213110	-0.691291	0.048600
H	4.632567	-0.411632	0.935693
H	4.947910	-0.827033	-0.639133

$NHNH_2$-2-CN-IND

Total energy (hartree): -550.739820

Sum of electronic and thermal Free Energies (hartree): -550.604703

C	1.030545	2.024960	-0.034782
C	2.295809	1.600867	-0.224831
C	2.313611	0.099894	-0.504321
C	0.842176	-0.274366	-0.379964
C	0.200578	-1.502295	-0.489597
C	-1.189851	-1.552885	-0.348663
C	-1.942847	-0.383740	-0.107707
C	-1.291271	0.857329	0.011733
C	0.097248	0.893023	-0.124312
H	0.732835	3.054344	0.158681
H	3.201239	2.202535	-0.207153
H	0.760070	-2.421129	-0.667423
H	-1.703412	-2.512506	-0.430337
H	-1.871936	1.755220	0.206737
H	2.670465	-0.078628	-1.534268
C	3.202663	-0.649148	0.394932
N	3.912611	-1.246500	1.093037
N	-3.341098	-0.491203	-0.046973
H	-3.663033	-1.428349	0.173835
N	-4.045948	0.553516	0.590828
H	-4.225643	0.343429	1.573168
H	-4.931505	0.692562	0.113596

NMe_2-CN-IND

Total energy (hartree): -574.027127

Sum of electronic and thermal Free Energies (hartree): -573.855889

C	1.549370	2.020214	-0.018825
C	2.766759	1.492116	-0.255153
C	2.649338	-0.004948	-0.533378
C	1.157798	-0.253890	-0.354264

C	0.402992	-1.414816	-0.451093
C	-0.982491	-1.352268	-0.268081
C	-1.641529	-0.127682	0.020549
C	-0.857165	1.051933	0.106191
C	0.522264	0.969813	-0.072516
H	1.347739	3.070826	0.185033
H	3.719159	2.016394	-0.269602
H	0.870189	-2.377380	-0.661933
H	-1.552170	-2.273508	-0.348916
H	-1.313222	2.016120	0.313765
H	2.954154	-0.210334	-1.575084
C	3.506647	-0.825659	0.334013
N	4.191809	-1.479943	1.005340
N	-3.012160	-0.088138	0.227867
C	-3.815228	-1.270343	-0.034885
H	-4.861433	-1.049111	0.196741
H	-3.755990	-1.598854	-1.088299
H	-3.503884	-2.110160	0.603268
C	-3.682781	1.195655	0.340177
H	-3.568202	1.814966	-0.567909
H	-4.750785	1.027303	0.507641
H	-3.298951	1.769555	1.196440

NO-1-CN-IND

Total energy (hartree): -569.357742

Sum of electronic and thermal Free Energies (hartree): -569.259127

C	-1.252888	2.032755	-0.098048
C	-2.420688	1.423920	0.186131
C	-2.182286	-0.040630	0.540988
C	-0.678443	-0.191000	0.345155
C	0.132245	-1.316930	0.486920
C	1.505797	-1.178349	0.280391
C	2.035690	0.078726	-0.061069
C	1.224046	1.212402	-0.211189
C	-0.148980	1.067545	-0.007709
H	-1.132259	3.082490	-0.358570
H	-3.411274	1.871478	0.192810
H	-0.293280	-2.287055	0.744140
H	2.183238	-2.025271	0.376273
H	1.683182	2.163109	-0.481681
H	-2.433298	-0.209058	1.603595
C	-2.984964	-0.982442	-0.249900
N	-3.625547	-1.729353	-0.865184
N	3.444161	0.311480	-0.288133
O	4.162028	-0.663320	-0.159171

NO-2-CN-IND

Total energy (hartree): -569.358216

Sum of electronic and thermal Free Energies (hartree): -569.259507

C	0.944780	2.039046	0.024929
C	2.194664	1.598247	-0.215594
C	2.182692	0.104530	-0.526946
C	0.712219	-0.259283	-0.355947
C	0.081542	-1.490826	-0.472027
C	-1.307313	-1.537503	-0.290807
C	-2.021299	-0.365448	-0.003801
C	-1.386691	0.883408	0.120709
C	-0.008043	0.923243	-0.054329
H	0.667700	3.067467	0.248416
H	3.109460	2.185635	-0.217204
H	0.644262	-2.398740	-0.687653
H	-1.858940	-2.474279	-0.366614
H	-1.978651	1.768059	0.350120
H	2.483041	-0.057968	-1.577469
C	3.093712	-0.684926	0.312106
N	3.820687	-1.310819	0.965227
N	-3.444836	-0.551729	0.154105
O	-4.076926	0.460592	0.398165

NO_2-CN-IND

Total energy (hartree): -644.582826

Sum of electronic and thermal Free Energies (hartree): -644.479659

C	1.445486	2.038778	0.019872
C	2.658451	1.501194	-0.214356
C	2.530444	0.012514	-0.522980
C	1.035639	-0.233316	-0.358179
C	0.303734	-1.408509	-0.475400
C	-1.085218	-1.352400	-0.303542
C	-1.688761	-0.123508	-0.022838
C	-0.970324	1.068974	0.105425
C	0.412344	0.997868	-0.062800
H	1.247131	3.085808	0.240195
H	3.616145	2.015515	-0.212707
H	0.788805	-2.360931	-0.686836
H	-1.702524	-2.243227	-0.382834
H	-1.489399	1.997137	0.329738
H	2.821420	-0.173628	-1.572206
C	3.373227	-0.844286	0.321109
N	4.045503	-1.524533	0.978344
N	-3.157268	-0.081509	0.150252
O	-3.777981	-1.134929	0.037058
O	-3.670689	1.007149	0.396269

OCF_3-1-CN-IND

Total energy (hartree): -852.361967

Sum of electronic and thermal Free Energies (hartree): -852.256190

C	1.842636	2.001335	-0.048201
C	3.136387	1.660553	-0.210414
C	3.260479	0.164790	-0.484269
C	1.815834	-0.309290	-0.385811
C	1.270211	-1.580942	-0.507076
C	-0.117100	-1.728582	-0.399961
C	-0.924838	-0.608595	-0.177434
C	-0.396039	0.678271	-0.048479
C	0.992607	0.807719	-0.152142
H	1.471396	3.008075	0.134660
H	3.998883	2.321422	-0.176567
H	1.897403	-2.456660	-0.672397
H	-0.586981	-2.706767	-0.484468
H	-1.023948	1.546447	0.127644
H	3.638949	0.008684	-1.510021
C	4.181921	-0.525860	0.427872
N	4.918098	-1.075321	1.137337
O	-2.291283	-0.915908	-0.101764
C	-3.223744	0.028443	0.149797
F	-3.265668	0.998448	-0.797058
F	-3.043798	0.648457	1.341111
F	-4.415228	-0.579543	0.172682

OCF_3-2-CN-IND

Total energy (hartree): -852.361797

Sum of electronic and thermal Free Energies (hartree): -852.256087

C	-2.518744	2.002175	-0.149137
C	-3.633837	1.294908	0.119937
C	-3.275237	-0.133468	0.520491
C	-1.758533	-0.145674	0.371979
C	-0.840081	-1.166703	0.559941
C	0.527800	-0.903196	0.381643
C	0.932382	0.384579	0.018697
C	0.019471	1.424876	-0.179389
C	-1.334731	1.145633	-0.002215
H	-2.488966	3.051800	-0.435662
H	-4.660597	1.650641	0.086131
H	-1.158231	-2.172184	0.834675
H	1.248296	-1.702037	0.526637
H	0.379611	2.411305	-0.466256
H	-3.553226	-0.300344	1.576215
C	-3.964648	-1.157426	-0.276097

N	-4.515808	-1.971014	-0.893741
O	2.265972	0.771510	-0.179144
C	3.287333	-0.110012	-0.100078
F	3.180921	-1.126349	-0.988456
F	3.411282	-0.669475	1.128568
F	4.415458	0.559344	-0.365338

OCF_3-3-CN-IND

Total energy (hartree): -852.362205

Sum of electronic and thermal Free Energies (hartree): -852.256986

C	2.157875	2.029315	0.131379
C	3.378980	1.461710	0.080105
C	3.270097	0.006453	-0.365119
C	1.763732	-0.187717	-0.497710
C	1.030767	-1.313573	-0.848827
C	-0.365479	-1.207814	-0.928104
C	-0.978102	0.015362	-0.653290
C	-0.259053	1.159163	-0.305253
C	1.130456	1.041139	-0.221749
H	1.951383	3.064475	0.396631
H	4.332783	1.934966	0.299358
H	1.517276	-2.266922	-1.053907
H	-0.978933	-2.063518	-1.202996
H	-0.776045	2.096532	-0.110282
H	3.751657	-0.114028	-1.351730
C	3.918207	-0.940791	0.551603
N	4.440022	-1.692646	1.265375
O	-2.375707	0.117262	-0.823450
C	-3.158367	-0.071891	0.264915
F	-2.919141	0.829800	1.248416
F	-3.003610	-1.298239	0.817491
F	-4.433614	0.058526	-0.120885

OH-1-CN-IND

Total energy (hartree): -515.282992

Sum of electronic and thermal Free Energies (hartree): -515.175261

C	-0.765229	2.031000	-0.077591
C	-1.977982	1.521899	0.216731
C	-1.862696	0.038410	0.557264
C	-0.378411	-0.233095	0.345430
C	0.354024	-1.405657	0.464059
C	1.737002	-1.365555	0.234958
C	2.365555	-0.158242	-0.106693
C	1.630762	1.029136	-0.232133
C	0.255437	0.976543	-0.007220
H	-0.561322	3.069546	-0.332729

H	-2.926147	2.053549	0.237040
H	-0.125054	-2.350857	0.720308
H	2.328400	-2.279155	0.319483
H	2.141693	1.952020	-0.502812
H	-2.132892	-0.117497	1.616767
C	-2.750468	-0.815839	-0.243768
N	-3.458194	-1.496458	-0.863148
O	3.714711	-0.077001	-0.336282
H	4.117018	-0.947996	-0.231979

OH-2-CN-IND

Total energy (hartree): -515.282679

Sum of electronic and thermal Free Energies (hartree): -515.174964

C	-0.749656	2.030842	-0.071642
C	-1.966613	1.530959	0.221833
C	-1.861922	0.045655	0.556766
C	-0.379818	-0.236762	0.344543
C	0.345637	-1.416723	0.462380
C	1.726439	-1.390757	0.236237
C	2.365114	-0.188112	-0.102794
C	1.640149	1.005705	-0.227365
C	0.261357	0.967182	-0.004073
H	-0.538109	3.068731	-0.323762
H	-2.910469	2.070074	0.243784
H	-0.142682	-2.357651	0.716967
H	2.325600	-2.296616	0.315427
H	2.143158	1.936776	-0.495209
H	-2.133211	-0.112293	1.615706
C	-2.756885	-0.797356	-0.248105
N	-3.471443	-1.467234	-0.871297
O	3.719860	-0.246274	-0.305066
H	4.054117	0.628019	-0.539988

OMe-1-CN-IND

Total energy (hartree): -554.583688

Sum of electronic and thermal Free Energies (hartree): -554.449898

C	0.997543	2.023942	-0.006047
C	2.262720	1.616763	-0.230772
C	2.289968	0.118952	-0.522621
C	0.826624	-0.274437	-0.364669
C	0.199495	-1.512454	-0.474725
C	-1.184572	-1.584272	-0.306173
C	-1.937533	-0.426467	-0.030907
C	-1.311045	0.824629	0.084434
C	0.077862	0.880442	-0.082344
H	0.692654	3.048041	0.203620

H	3.161117	2.228956	-0.229740
H	0.768608	-2.419715	-0.678695
H	-1.709301	-2.535660	-0.380527
H	-1.874215	1.728974	0.300573
H	2.619610	-0.047044	-1.563644
C	3.210796	-0.627325	0.345920
N	3.946867	-1.220453	1.019866
O	-3.281644	-0.626217	0.110623
C	-4.104199	0.498345	0.402897
H	-3.819919	0.962532	1.359862
H	-4.055211	1.248887	-0.401184
H	-5.124214	0.109234	0.475728

OMe-2-CN-IND

Total energy (hartree): -554.583814

Sum of electronic and thermal Free Energies (hartree): -554.450025

C	-1.392665	2.013270	-0.101886
C	-2.551151	1.386014	0.182176
C	-2.290846	-0.074101	0.544854
C	-0.783041	-0.194869	0.358092
C	0.065070	-1.280104	0.503103
C	1.444485	-1.107520	0.294183
C	1.953077	0.154367	-0.056286
C	1.092963	1.257483	-0.208136
C	-0.270241	1.070266	-0.002896
H	-1.292857	3.064120	-0.368394
H	-3.548938	1.817928	0.181536
H	-0.318047	-2.266294	0.766561
H	2.104577	-1.963674	0.405232
H	1.511859	2.224010	-0.484889
H	-2.561206	-0.244551	1.602017
C	-3.074269	-1.023481	-0.258073
N	-3.699747	-1.778985	-0.879231
O	3.276564	0.413476	-0.275884
C	4.207144	-0.657057	-0.150243
H	4.207022	-1.068457	0.870841
H	3.992171	-1.459606	-0.872301
H	5.187983	-0.223994	-0.368241

SH-CN-IND

Total energy (hartree): -838.255821

Sum of electronic and thermal Free Energies (hartree): -838.154997

C	-1.189280	2.031714	-0.069675
C	-2.405514	1.512644	0.190485
C	-2.287243	0.030064	0.533023
C	-0.795541	-0.229533	0.362378

C	-0.057144	-1.397103	0.502128
C	1.330225	-1.345877	0.313212
C	1.967114	-0.134822	-0.010153
C	1.219451	1.045027	-0.155482
C	-0.163340	0.984369	0.028918
H	-0.986705	3.072131	-0.318277
H	-3.358226	2.036363	0.184710
H	-0.535821	-2.346213	0.744233
H	1.920077	-2.256707	0.415748
H	1.705020	1.986970	-0.409347
H	-2.581662	-0.129361	1.585561
C	-3.145739	-0.831690	-0.291125
N	-3.831555	-1.516326	-0.930192
S	3.744582	-0.179186	-0.223617
H	3.906963	1.129315	-0.535667

SiH_3-CN-IND

Total energy (hartree): -730.753260

Sum of electronic and thermal Free Energies (hartree): -730.638444

C	1.231396	2.032764	0.078779
C	2.447892	1.512211	-0.176872
C	2.327248	0.031331	-0.526422
C	0.833335	-0.226997	-0.362513
C	0.101073	-1.395480	-0.510851
C	-1.290291	-1.337581	-0.327494
C	-1.947908	-0.134636	-0.002469
C	-1.181525	1.039915	0.147356
C	0.202522	0.989155	-0.028585
H	1.029988	3.072742	0.330133
H	3.402042	2.033061	-0.164595
H	0.585480	-2.341685	-0.753840
H	-1.869326	-2.255050	-0.440348
H	-1.660492	1.987324	0.402438
H	2.619946	-0.125346	-1.579792
C	3.180034	-0.839183	0.293671
N	3.862018	-1.529539	0.930632
Si	-3.825843	-0.101166	0.234951
H	-4.174091	0.335856	1.621580
H	-4.370538	-1.470555	-0.004459
H	-4.457989	0.857765	-0.722446

$SiMe_3$-CN-IND

Total energy (hartree): -848.745922

Sum of electronic and thermal Free Energies (hartree): -848.551657

C	2.194160	2.023382	0.068507
C	3.415761	1.500548	-0.156935

C	3.299563	0.020680	-0.513388
C	1.800777	-0.232933	-0.389992
C	1.065986	-1.396746	-0.561475
C	-0.329755	-1.331475	-0.414424
C	-0.997619	-0.130180	-0.102740
C	-0.223360	1.036738	0.070480
C	1.164929	0.983429	-0.068731
H	1.989835	3.063411	0.317568
H	4.370779	2.018485	-0.118213
H	1.551979	-2.344622	-0.795054
H	-0.903971	-2.248738	-0.546691
H	-0.700972	1.987317	0.317175
H	3.620995	-0.135023	-1.558444
C	4.127563	-0.853291	0.328277
N	4.790648	-1.546214	0.982338
Si	-2.891612	-0.055147	0.097213
C	-3.642777	-1.761298	-0.230487
H	-3.269605	-2.517715	0.474776
H	-4.735800	-1.718545	-0.117335
H	-3.431939	-2.115459	-1.249774
C	-3.592468	1.202201	-1.137108
H	-4.683320	1.294564	-1.028787
H	-3.159910	2.201867	-0.985289
H	-3.382241	0.904460	-2.174313
C	-3.305319	0.498785	1.862300
H	-2.880768	1.488368	2.085973
H	-4.393464	0.565386	2.009858
H	-2.908208	-0.207236	2.605497

tBu-1-CN-IND

Total energy (hartree): -597.314011

Sum of electronic and thermal Free Energies (hartree): -597.104273

C	1.829392	2.020287	0.070662
C	3.051961	1.505716	-0.168589
C	2.942347	0.025210	-0.526134
C	1.446780	-0.236682	-0.388339
C	0.708685	-1.397129	-0.551958
C	-0.686099	-1.338220	-0.388942
C	-1.352806	-0.143111	-0.067998
C	-0.578784	1.023279	0.097449
C	0.805667	0.973712	-0.057818
H	1.621399	3.058657	0.323811
H	4.003724	2.030148	-0.138559
H	1.188667	-2.346097	-0.792565
H	-1.249665	-2.258764	-0.517140
H	-1.054010	1.970003	0.351756

H	3.257476	-0.127115	-1.573538
C	3.783584	-0.843030	0.308627
N	4.456915	-1.531706	0.956750
C	-2.880205	-0.069214	0.113361
C	-3.201410	0.402175	1.550811
H	-2.786152	1.397023	1.755563
H	-4.289275	0.455741	1.699151
H	-2.788556	-0.294922	2.292445
C	-3.563318	-1.430415	-0.110038
H	-4.647540	-1.322805	0.027221
H	-3.394226	-1.810875	-1.126422
H	-3.213332	-2.186809	0.605283
C	-3.468525	0.938081	-0.901926
H	-3.251944	0.626767	-1.932855
H	-4.559695	1.000596	-0.785477
H	-3.058890	1.946431	-0.760940

tBu-2-CN-IND

Total energy (hartree): -597.314011

Sum of electronic and thermal Free Energies (hartree): -597.104270

C	1.829392	2.020286	0.070659
C	3.051961	1.505716	-0.168590
C	2.942347	0.025208	-0.526132
C	1.446780	-0.236683	-0.388337
C	0.708684	-1.397130	-0.551958
C	-0.686101	-1.338220	-0.388944
C	-1.352808	-0.143110	-0.068000
C	-0.578784	1.023278	0.097451
C	0.805667	0.973711	-0.057816
H	1.621399	3.058657	0.323804
H	4.003725	2.030147	-0.138563
H	1.188665	-2.346099	-0.792563
H	-1.249667	-2.258763	-0.517142
H	-1.054010	1.970002	0.351756
H	3.257477	-0.127115	-1.573536
C	3.783589	-0.843033	0.308623
N	4.456924	-1.531697	0.956752
C	-2.880208	-0.069213	0.113361
C	-3.468528	0.938082	-0.901926
H	-3.251949	0.626770	-1.932857
H	-4.559698	1.000597	-0.785478
H	-3.058896	1.946432	-0.760940
C	-3.201411	0.402175	1.550813
H	-4.289277	0.455740	1.699153
H	-2.788556	-0.294921	2.292446
H	-2.786155	1.397023	1.755565

C	-3.563319	-1.430416	-0.110037
H	-3.213333	-2.186808	0.605285
H	-4.647540	-1.322805	0.027220
H	-3.394227	-1.810878	-1.126421

tBu-3-CN-IND

Total energy (hartree): -597.314011

Sum of electronic and thermal Free Energies (hartree): -597.104281

C	1.829392	2.020289	0.070654
C	3.051961	1.505715	-0.168588
C	2.942344	0.025209	-0.526129
C	1.446778	-0.236679	-0.388333
C	0.708685	-1.397126	-0.551962
C	-0.686101	-1.338219	-0.388945
C	-1.352806	-0.143111	-0.067997
C	-0.578785	1.023281	0.097449
C	0.805666	0.973714	-0.057815
H	1.621401	3.058662	0.323794
H	4.003725	2.030147	-0.138562
H	1.188666	-2.346093	-0.792577
H	-1.249667	-2.258761	-0.517151
H	-1.054016	1.970003	0.351752
H	3.257479	-0.127122	-1.573532
C	3.783577	-0.843034	0.308634
N	4.456927	-1.531704	0.956743
C	-2.880206	-0.069214	0.113360
C	-3.563314	-1.430420	-0.110031
H	-3.213324	-2.186807	0.605295
H	-4.647535	-1.322811	0.027227
H	-3.394221	-1.810887	-1.126413
C	-3.468529	0.938076	-0.901929
H	-4.559699	1.000591	-0.785473
H	-3.058894	1.946426	-0.760949
H	-3.251956	0.626756	-1.932858
C	-3.201408	0.402179	1.550813
H	-2.786137	1.397022	1.755562
H	-4.289273	0.455760	1.699147
H	-2.788565	-0.294924	2.292445

Vin-1-CN-IND

Total energy (hartree): -517.453920

Sum of electronic and thermal Free Energies (hartree): -517.319332

C	0.981515	2.030092	0.008543
C	2.238542	1.601502	-0.219279
C	2.242211	0.104723	-0.519550
C	0.772632	-0.267426	-0.359531

C	0.133264	-1.493108	-0.471177
C	-1.257271	-1.536125	-0.298368
C	-2.011800	-0.379011	-0.019518
C	-1.341712	0.857563	0.094743
C	0.040063	0.904363	-0.071157
H	0.695181	3.058343	0.223204
H	3.147325	2.198176	-0.216944
H	0.689518	-2.407558	-0.678037
H	-1.773493	-2.493233	-0.379884
H	-1.895783	1.769196	0.314924
H	2.561366	-0.062481	-1.563635
C	3.152788	-0.664937	0.338884
N	3.880691	-1.275834	1.005575
C	-3.471187	-0.512578	0.145054
H	-3.850484	-1.532646	0.039305
C	-4.355020	0.463797	0.403620
H	-4.066391	1.508163	0.524106
H	-5.416233	0.239744	0.504352

Vin-2-CN-IND

Total energy (hartree): -517.453776

Sum of electronic and thermal Free Energies (hartree): -517.319198

C	-1.306305	2.018455	-0.090138
C	-2.477351	1.410501	0.184790
C	-2.241541	-0.056115	0.536334
C	-0.735729	-0.201857	0.352351
C	0.090940	-1.311322	0.494285
C	1.465878	-1.154463	0.292881
C	2.026451	0.095391	-0.047283
C	1.171470	1.205994	-0.190521
C	-0.202196	1.053391	0.005282
H	-1.186072	3.069462	-0.347373
H	-3.467592	1.859066	0.185117
H	-0.316528	-2.290123	0.748136
H	2.112702	-2.023656	0.401065
H	1.588759	2.178062	-0.456917
H	-2.509932	-0.230071	1.593576
C	-3.038144	-0.989768	-0.271109
N	-3.674702	-1.731393	-0.897460
C	3.473193	0.285909	-0.262948
H	3.763698	1.307658	-0.522943
C	4.441735	-0.638995	-0.176265
H	4.245846	-1.681167	0.076238
H	5.481632	-0.372206	-0.360629

Coordinates and energies of NC-IND

BF_2-NC-IND
Total energy (hartree): -664.110249
Sum of electronic and thermal Free Energies (hartree): -664.010806

C	1.535726	2.019322	0.010421
C	2.748330	1.467011	-0.183404
C	2.609177	-0.019937	-0.484740
C	1.111445	-0.255513	-0.328991
C	0.377430	-1.429048	-0.427995
C	-1.014333	-1.351609	-0.274878
C	-1.661315	-0.122148	-0.033971
C	-0.893049	1.058655	0.066977
C	0.491083	0.984893	-0.074077
H	1.341699	3.072261	0.207275
H	3.713152	1.967850	-0.168262
H	0.863884	-2.387740	-0.608092
H	-1.610305	-2.261548	-0.343655
H	-1.383912	2.013057	0.257948
H	2.905454	-0.212912	-1.529848
N	3.422204	-0.857938	0.341079
C	4.102198	-1.550179	1.005967
B	-3.196517	-0.065753	0.123943
F	-3.841274	1.088466	0.354340
F	-3.963500	-1.162391	0.037385

Br-NC-IND
Total energy (hartree): -3013.566235
Sum of electronic and thermal Free Energies (hartree): -3013.475412

C	-1.882104	2.019015	-0.066575
C	-3.095381	1.472541	0.139962
C	-2.958506	-0.005237	0.485649
C	-1.460892	-0.244140	0.344267
C	-0.718888	-1.407437	0.482639
C	0.676303	-1.340603	0.333746
C	1.282440	-0.111473	0.059571
C	0.547179	1.070392	-0.086017
C	-0.839664	0.986012	0.053448
H	-1.687039	3.065326	-0.295180
H	-4.059812	1.973393	0.105010
H	-1.196302	-2.364991	0.691305
H	1.283317	-2.238479	0.430420
H	1.044263	2.013698	-0.303918
H	-3.265538	-0.166524	1.532831
N	-3.770173	-0.862994	-0.322413
C	-4.448450	-1.573061	-0.969857

Br	3.190289	-0.041072	-0.130417

CHO-1-NC-IND
Total energy (hartree): -553.352239
Sum of electronic and thermal Free Energies (hartree): -553.241701

C	1.001361	2.024743	0.020379
C	2.250373	1.565191	-0.183009
C	2.222547	0.073562	-0.492059
C	0.748064	-0.275394	-0.327818
C	0.106961	-1.501015	-0.425331
C	-1.286070	-1.529167	-0.259226
C	-2.006997	-0.350840	-0.010259
C	-1.346470	0.889624	0.090537
C	0.035618	0.916087	-0.062096
H	0.730321	3.059117	0.223866
H	3.174972	2.137140	-0.171181
H	0.663248	-2.419190	-0.613001
H	-1.821339	-2.477752	-0.323653
H	-1.928688	1.788657	0.289637
H	2.526086	-0.090782	-1.539945
N	3.101632	-0.705441	0.323894
C	3.835638	-1.349831	0.979414
C	-3.480389	-0.429269	0.151545
H	-3.907675	-1.455993	0.063310
O	-4.204021	0.524344	0.363907

CHO-2-NC-IND
Total energy (hartree): -553.351638
Sum of electronic and thermal Free Energies (hartree): -553.241180

C	-1.299495	2.010913	-0.083831
C	-2.466938	1.385756	0.159542
C	-2.220018	-0.076987	0.506514
C	-0.713855	-0.217250	0.320527
C	0.100378	-1.338076	0.442277
C	1.477759	-1.181353	0.253892
C	2.019535	0.081863	-0.044862
C	1.187870	1.208829	-0.170333
C	-0.186265	1.051359	0.008129
H	-1.182547	3.066944	-0.320819
H	-3.463589	1.820046	0.152449
H	-0.319744	-2.318230	0.668021
H	2.154645	-2.030891	0.334698
H	1.619908	2.182646	-0.407380
H	-2.477789	-0.251565	1.565036
N	-2.994086	-0.995235	-0.269471
C	-3.642150	-1.753194	-0.893444

C	3.483375	0.241196	-0.236965
H	3.812689	1.280348	-0.476148
O	4.296733	-0.657625	-0.149780

Cl-NC-IND

Total energy (hartree): -899.630409

Sum of electronic and thermal Free Energies (hartree): -899.537904

C	-1.204071	2.019494	-0.068207
C	-2.416295	1.480018	0.161749
C	-2.281509	0.000867	0.502301
C	-0.788544	-0.246651	0.331050
C	-0.050860	-1.414630	0.453342
C	1.340848	-1.356089	0.276759
C	1.948630	-0.130389	-0.008218
C	1.218286	1.056215	-0.137592
C	-0.165605	0.980170	0.029433
H	-1.007496	3.065021	-0.299131
H	-3.378153	1.986777	0.146855
H	-0.530041	-2.369365	0.670361
H	1.948677	-2.254870	0.359189
H	1.721258	1.994337	-0.364549
H	-2.569521	-0.160504	1.554849
N	-3.114039	-0.850420	-0.291455
C	-3.808910	-1.555410	-0.926715
Cl	3.697749	-0.077060	-0.218282

$COCH_3$-1-NC-IND

Total energy (hartree): -592.677139

Sum of electronic and thermal Free Energies (hartree): -592.541058

C	1.465985	2.025519	-0.012908
C	2.693082	1.503635	-0.199665
C	2.593181	0.009686	-0.483998
C	1.101670	-0.261988	-0.327599
C	0.392656	-1.453127	-0.415721
C	-0.998384	-1.410007	-0.266099
C	-1.669551	-0.194834	-0.038236
C	-0.937877	1.005244	0.052550
C	0.449223	0.962549	-0.087279
H	1.245306	3.075415	0.172513
H	3.644282	2.030100	-0.188845
H	0.900302	-2.402560	-0.586511
H	-1.592774	-2.320067	-0.323946
H	-1.439529	1.954375	0.233281
H	2.896932	-0.187241	-1.526265
N	3.426770	-0.795002	0.354213
C	4.124604	-1.458838	1.029627

C	-3.166920	-0.225470	0.105722
O	-3.777463	-1.279109	0.012887
C	-3.906522	1.073581	0.367095
H	-3.733436	1.792933	-0.446531
H	-4.976565	0.858997	0.442510
H	-3.559098	1.540238	1.300266

$COCH_3$-2-NC-IND

Total energy (hartree): -592.677669

Sum of electronic and thermal Free Energies (hartree): -592.541539

C	1.572831	2.008277	0.025449
C	2.770054	1.426213	-0.176638
C	2.593122	-0.054603	-0.490310
C	1.090409	-0.252046	-0.331682
C	0.322873	-1.401458	-0.435482
C	-1.067245	-1.288706	-0.274836
C	-1.671889	-0.044902	-0.023955
C	-0.877838	1.114695	0.081536
C	0.500843	1.002013	-0.064778
H	1.406431	3.063888	0.232334
H	3.747487	1.902144	-0.159860
H	0.779096	-2.372956	-0.625168
H	-1.676532	-2.187423	-0.348240
H	-1.364652	2.067963	0.281111
H	2.883768	-0.246636	-1.537135
N	3.386301	-0.919089	0.328160
C	4.048275	-1.635263	0.985913
C	-3.160011	0.096909	0.143453
O	-3.655440	1.195228	0.345569
C	-4.034866	-1.139639	0.058613
H	-3.749486	-1.874081	0.825578
H	-5.077116	-0.842281	0.207069
H	-3.928939	-1.627754	-0.921054

$CONH_2$-1-NC-IND

Total energy (hartree): -608.745066

Sum of electronic and thermal Free Energies (hartree): -608.618933

C	1.495439	2.012115	-0.138715
C	2.712491	1.456516	-0.291351
C	2.584567	-0.050122	-0.480732
C	1.087763	-0.283096	-0.313711
C	0.353342	-1.460195	-0.349009
C	-1.039143	-1.380551	-0.214073
C	-1.680353	-0.143674	-0.039606
C	-0.926839	1.044517	-0.009424
C	0.459326	0.965834	-0.144597

H	1.294881	3.075771	-0.021012
H	3.673334	1.964840	-0.311907
H	0.839703	-2.427909	-0.472248
H	-1.653452	-2.278466	-0.247638
H	-1.412702	2.015684	0.083295
H	2.890304	-0.319725	-1.505730
N	3.400010	-0.814117	0.412706
C	4.082298	-1.444708	1.134008
C	-3.180801	-0.158155	0.085694
O	-3.857193	-1.086647	-0.340518
N	-3.756149	0.939416	0.679453
H	-4.751089	0.883396	0.848657
H	-3.218998	1.551591	1.274713

$CONH_2$-2-NC-IND

Total energy (hartree): -608.745462

Sum of electronic and thermal Free Energies (hartree): -608.619555

C	1.525426	2.011621	-0.090439
C	2.732671	1.441483	-0.265845
C	2.581256	-0.057447	-0.495426
C	1.083652	-0.272921	-0.316637
C	0.336052	-1.440043	-0.342119
C	-1.055215	-1.342811	-0.182244
C	-1.679687	-0.096774	-0.005823
C	-0.907738	1.078048	0.036734
C	0.472985	0.981828	-0.117044
H	1.340052	3.073905	0.058033
H	3.701159	1.935347	-0.281095
H	0.809280	-2.414538	-0.462383
H	-1.640375	-2.261555	-0.162396
H	-1.409417	2.030208	0.200476
H	2.869790	-0.300594	-1.532140
N	3.396319	-0.861773	0.362108
C	4.077020	-1.530364	1.049784
C	-3.166979	0.057788	0.178517
O	-3.653257	1.077702	0.654459
N	-3.951172	-1.004481	-0.192895
H	-4.950770	-0.866736	-0.143198
H	-3.606351	-1.736325	-0.794208

$COOCH_3$-1-NC-IND

Total energy (hartree): -667.921492

Sum of electronic and thermal Free Energies (hartree): -667.781509

C	1.763916	2.046373	-0.040861
C	3.018529	1.581585	-0.192404
C	2.996608	0.080983	-0.456165

C	1.517014	-0.260893	-0.327521
C	0.869874	-1.485824	-0.411026
C	-0.525771	-1.508572	-0.290049
C	-1.251518	-0.321894	-0.096115
C	-0.588362	0.916323	-0.009290
C	0.800848	0.935007	-0.119754
H	1.488417	3.086697	0.123127
H	3.942983	2.153323	-0.169421
H	1.425615	-2.412156	-0.555608
H	-1.072843	-2.447875	-0.344475
H	-1.155684	1.831355	0.145232
H	3.332750	-0.116067	-1.488235
N	3.849939	-0.671546	0.410940
C	4.564388	-1.292103	1.109443
C	-2.737525	-0.429621	0.017218
O	-3.358315	-1.471478	-0.055801
O	-3.331967	0.770706	0.211868
C	-4.767570	0.736784	0.330271
H	-5.215870	0.330439	-0.584317
H	-5.064838	0.116086	1.183980
H	-5.070435	1.776310	0.482115

$COOCH_3$-2-NC-IND

Total energy (hartree): -667.921660

Sum of electronic and thermal Free Energies (hartree): -667.781703

C	2.067768	1.978867	0.043468
C	3.239108	1.344190	-0.152150
C	2.996768	-0.124599	-0.478047
C	1.484868	-0.254122	-0.334520
C	0.666448	-1.367578	-0.455162
C	-0.717956	-1.196550	-0.308061
C	-1.259854	0.074013	-0.052709
C	-0.422258	1.197689	0.071059
C	0.952423	1.023047	-0.063829
H	1.947909	3.039539	0.256578
H	4.237061	1.774703	-0.123212
H	1.081011	-2.356907	-0.648528
H	-1.381966	-2.053431	-0.392095
H	-0.865440	2.171091	0.274096
H	3.287735	-0.322541	-1.523657
N	3.742381	-1.029842	0.341038
C	4.366186	-1.778844	0.999469
C	-2.730181	0.290042	0.102403
O	-3.242735	1.371491	0.315029
O	-3.443236	-0.852577	-0.020321

C	-4.869987	-0.708881	0.120339
H	-5.116657	-0.310186	1.111618
H	-5.262342	-0.032246	-0.648268
H	-5.276200	-1.716091	-0.005022

COOH-1-NC-IND

Total energy (hartree): -628.619855

Sum of electronic and thermal Free Energies (hartree): -628.504963

C	1.478804	2.021289	0.006974
C	2.697902	1.483715	-0.187374
C	2.576644	-0.005401	-0.486577
C	1.082216	-0.258650	-0.329000
C	0.359851	-1.440030	-0.426153
C	-1.031084	-1.381736	-0.272197
C	-1.676107	-0.157094	-0.032563
C	-0.937723	1.036740	0.068740
C	0.447138	0.973599	-0.074836
H	1.272219	3.072000	0.202827
H	3.656460	1.996563	-0.173769
H	0.854873	-2.394122	-0.606305
H	-1.636055	-2.284252	-0.335971
H	-1.444571	1.980269	0.259086
H	2.874503	-0.195751	-1.531675
N	3.401265	-0.831618	0.339709
C	4.091578	-1.513694	1.004434
C	-3.159060	-0.172298	0.113567
O	-3.856486	-1.162715	0.036732
O	-3.683981	1.061312	0.347296
H	-4.643484	0.939212	0.425518

COOH-2-NC-IND

Total energy (hartree): -628.620052

Sum of electronic and thermal Free Energies (hartree): -628.505132

C	1.529572	2.017931	0.022221
C	2.734557	1.451681	-0.178652
C	2.576741	-0.031744	-0.488960
C	1.076985	-0.249786	-0.329405
C	0.326483	-1.411835	-0.431772
C	-1.064203	-1.322725	-0.273052
C	-1.677215	-0.083423	-0.024722
C	-0.908780	1.090665	0.081579
C	0.472276	0.996626	-0.064994
H	1.348860	3.071745	0.226316
H	3.705465	1.940707	-0.163370
H	0.797972	-2.376419	-0.619195

H	-1.676667	-2.218630	-0.342504
H	-1.407803	2.037733	0.279559
H	2.867854	-0.221275	-1.536082
N	3.382673	-0.884575	0.328921
C	4.056495	-1.589938	0.986191
C	-3.152967	0.040027	0.140712
O	-3.741785	1.080757	0.351865
O	-3.806337	-1.147423	0.031052
H	-4.749086	-0.953373	0.154617

Et-1-NC-IND
Total energy (hartree): -518.648631
Sum of electronic and thermal Free Energies (hartree): -518.493242

C	-1.215572	2.015625	-0.110743
C	-2.415128	1.513647	0.240706
C	-2.286684	0.034181	0.583864
C	-0.822683	-0.254174	0.277125
C	-0.104556	-1.438610	0.338209
C	1.263336	-1.406003	0.023277
C	1.911170	-0.213108	-0.338406
C	1.164005	0.977553	-0.398944
C	-0.198170	0.950994	-0.097755
H	-1.016218	3.053615	-0.372609
H	-3.360175	2.046583	0.311270
H	-0.585434	-2.379783	0.606212
H	1.837206	-2.333407	0.053994
H	1.648421	1.911127	-0.690424
H	-2.482922	-0.113134	1.659252
N	-3.212368	-0.800289	-0.121992
C	-3.982230	-1.489914	-0.682827
C	3.396908	-0.201999	-0.629788
H	3.694061	-1.176088	-1.044426
H	3.610749	0.549950	-1.403624
C	4.247858	0.098306	0.616959
H	5.318017	0.100313	0.367003
H	3.993405	1.080163	1.039493
H	4.079946	-0.656310	1.397742

Et-2-NC-IND
Total energy (hartree): -518.647531
Sum of electronic and thermal Free Energies (hartree): -518.491868

C	1.479563	1.988975	0.093293
C	2.628424	1.330283	-0.152224
C	2.337849	-0.123078	-0.508720
C	0.827390	-0.214349	-0.331730
C	-0.034660	-1.289187	-0.462256

C	-1.412039	-1.074796	-0.270253
C	-1.925249	0.193510	0.039018
C	-1.029555	1.274690	0.168282
C	0.335822	1.067013	-0.009231
H	1.396994	3.046602	0.339006
H	3.637995	1.733804	-0.137771
H	0.335888	-2.287590	-0.696197
H	-2.086753	-1.923490	-0.365127
H	-1.410381	2.268139	0.412805
H	2.606914	-0.305233	-1.562686
N	3.081051	-1.064060	0.274946
C	3.701072	-1.842352	0.901428
C	-3.409553	0.449761	0.244499
H	-3.542200	0.910127	1.236296
H	-3.727144	1.218464	-0.477933
C	-4.336720	-0.761208	0.126680
H	-5.377324	-0.456344	0.299383
H	-4.285883	-1.216795	-0.872119
H	-4.089520	-1.534841	0.867002

Et-3-NC-IND

Total energy (hartree): -518.648636

Sum of electronic and thermal Free Energies (hartree): -518.493269

C	1.256672	2.011218	0.115830
C	2.478008	1.457187	-0.009174
C	2.352912	-0.007015	-0.413262
C	0.845739	-0.229123	-0.403393
C	0.100204	-1.372024	-0.649683
C	-1.300042	-1.275320	-0.613930
C	-1.951353	-0.060056	-0.344838
C	-1.177225	1.088905	-0.099711
C	0.214888	0.998096	-0.122411
H	1.056517	3.052691	0.362836
H	3.441598	1.943494	0.121642
H	0.580783	-2.328019	-0.859506
H	-1.898587	-2.167417	-0.804474
H	-1.666509	2.042515	0.106061
H	2.746646	-0.142275	-1.434693
N	3.086034	-0.900163	0.433021
C	3.700773	-1.638296	1.111277
C	-3.462767	0.004793	-0.280229
H	-3.801179	0.986322	-0.643883
H	-3.888569	-0.748105	-0.959248
C	-4.011426	-0.225745	1.139163
H	-5.109068	-0.172082	1.145806
H	-3.714387	-1.212835	1.519294

H	-3.627790	0.531134	1.837185

F-NC-IND
Total energy (hartree): -539.261436
Sum of electronic and thermal Free Energies (hartree): -539.166739

C	-0.782226	2.020565	-0.069420
C	-1.992463	1.490619	0.191516
C	-1.860890	0.009455	0.524339
C	-0.375117	-0.250033	0.313856
C	0.354435	-1.425931	0.415680
C	1.741519	-1.380474	0.203132
C	2.338016	-0.157590	-0.094477
C	1.629749	1.038236	-0.205302
C	0.249753	0.972916	-0.001763
H	-0.583406	3.065074	-0.303117
H	-2.950109	2.005397	0.203085
H	-0.129853	-2.375428	0.643840
H	2.356885	-2.276467	0.264563
H	2.148595	1.964885	-0.444860
H	-2.125271	-0.152632	1.582895
N	-2.721591	-0.831192	-0.251233
C	-3.438894	-1.527898	-0.870409
F	3.683446	-0.127964	-0.292298

H-NC-IND
Total energy (hartree): -440.011320
Sum of electronic and thermal Free Energies (hartree): -439.907080

C	-0.328572	2.017896	-0.078283
C	-1.543807	1.522835	0.225136
C	-1.441241	0.036918	0.547132
C	0.028666	-0.264218	0.279281
C	0.723567	-1.462898	0.348795
C	2.102845	-1.448025	0.081964
C	2.755883	-0.251358	-0.237292
C	2.049731	0.957603	-0.308199
C	0.676482	0.942087	-0.053941
H	-0.109520	3.058016	-0.314679
H	-2.485238	2.064471	0.275380
H	0.216728	-2.397396	0.591036
H	2.669874	-2.378219	0.122814
H	2.563301	1.885498	-0.561074
H	-1.667197	-0.124496	1.614669
N	-2.353796	-0.777591	-0.196700
C	-3.113383	-1.451276	-0.790101
H	3.827600	-0.262112	-0.438203

iPr-1-NC-IND

Total energy (hartree): -557.965223

Sum of electronic and thermal Free Energies (hartree): -557.783547

C	1.742298	1.993442	0.228101
C	2.911313	1.385949	-0.052564
C	2.662565	-0.045272	-0.513955
C	1.154383	-0.189705	-0.357155
C	0.322870	-1.279068	-0.574685
C	-1.057103	-1.115401	-0.382826
C	-1.609632	0.116039	0.012446
C	-0.749736	1.206704	0.227530
C	0.626473	1.049204	0.049264
H	1.627504	3.028344	0.546646
H	3.909126	1.814556	-0.000415
H	0.724980	-2.246866	-0.875734
H	-1.712306	-1.971227	-0.545479
H	-1.160285	2.168971	0.537847
H	2.941895	-0.142887	-1.576570
N	3.426381	-1.020506	0.204853
C	4.064150	-1.825357	0.777763
C	-3.111262	0.270757	0.213331
H	-3.284726	1.315545	0.514050
C	-3.633619	-0.627292	1.349487
H	-4.702893	-0.442897	1.524355
H	-3.512783	-1.691653	1.103131
H	-3.094295	-0.435309	2.286530
C	-3.894253	0.032458	-1.090612
H	-3.784392	-1.004759	-1.437537
H	-4.965691	0.221858	-0.935422
H	-3.541492	0.695131	-1.892130

iPr-2-NC-IND

Total energy (hartree): -557.965313

Sum of electronic and thermal Free Energies (hartree): -557.783786

C	1.424172	2.010313	0.132539
C	2.679152	1.573027	-0.086205
C	2.662380	0.102695	-0.487422
C	1.187372	-0.259321	-0.367576
C	0.535818	-1.467308	-0.555655
C	-0.861404	-1.500540	-0.409765
C	-1.603194	-0.352623	-0.089356
C	-0.921024	0.864938	0.099405
C	0.466295	0.904072	-0.033706
H	1.146773	3.029025	0.399172
H	3.599903	2.148054	-0.025898
H	1.085373	-2.377036	-0.799020

H	-1.385677	-2.447068	-0.548657
H	-1.469754	1.772130	0.354030
H	2.991227	0.002704	-1.535486
N	3.535955	-0.716038	0.298705
C	4.264820	-1.391590	0.927253
C	-3.116390	-0.432095	0.059188
H	-3.401081	-1.474791	-0.148903
C	-3.843379	0.456743	-0.966139
H	-4.931481	0.324882	-0.885601
H	-3.622492	1.520698	-0.799529
H	-3.542872	0.206297	-1.992235
C	-3.568179	-0.110237	1.495440
H	-3.337303	0.930968	1.762260
H	-4.653727	-0.248783	1.597298
H	-3.069207	-0.763249	2.223623

Me-NC-IND

Total energy (hartree): -479.331856

Sum of electronic and thermal Free Energies (hartree): -479.203348

C	0.817928	2.015286	0.069468
C	2.032164	1.490390	-0.184012
C	1.906702	0.008597	-0.518585
C	0.419467	-0.253999	-0.319326
C	-0.312452	-1.425113	-0.427361
C	-1.701647	-1.366025	-0.221700
C	-2.353603	-0.160601	0.079645
C	-1.592258	1.019385	0.186328
C	-0.212666	0.966034	-0.006143
H	0.616270	3.059616	0.302983
H	2.988434	2.007865	-0.188704
H	0.169228	-2.376563	-0.654504
H	-2.288418	-2.282304	-0.297473
H	-2.082492	1.965391	0.423015
H	2.180694	-0.155211	-1.574363
N	2.763658	-0.830044	0.264871
C	3.477641	-1.523551	0.890963
C	-3.848671	-0.119860	0.295960
H	-4.092362	0.214398	1.315304
H	-4.331326	0.581961	-0.399897
H	-4.301257	-1.108096	0.148118

MeS-NC-IND

Total energy (hartree): -877.536196

Sum of electronic and thermal Free Energies (hartree): -877.408711

C	-1.792433	1.982682	-0.066535
C	-2.944837	1.323893	0.160396

C	-2.663227	-0.134851	0.501712
C	-1.152561	-0.228710	0.338014
C	-0.293808	-1.307697	0.462437
C	1.086143	-1.104087	0.287587
C	1.591471	0.173866	-0.000422
C	0.711765	1.269294	-0.127880
C	-0.653222	1.055028	0.035664
H	-1.703432	3.042699	-0.298748
H	-3.952992	1.730827	0.141252
H	-0.668801	-2.308111	0.680216
H	1.754948	-1.956262	0.378501
H	1.100052	2.262081	-0.356851
H	-2.945563	-0.328839	1.550160
N	-3.402204	-1.062579	-0.301974
C	-4.017663	-1.831891	-0.944049
S	3.325404	0.533499	-0.231223
C	4.135825	-1.088897	-0.029532
H	3.978285	-1.493051	0.977826
H	3.796233	-1.802115	-0.790386
H	5.205517	-0.896944	-0.172939

$MeSO_2$-NC-IND

Total energy (hartree): -1027.936300

Sum of electronic and thermal Free Energies (hartree): -1027.802896

C	-2.114739	2.022102	-0.087085
C	-3.322945	1.478562	0.153535
C	-3.178677	0.006105	0.516073
C	-1.685129	-0.238613	0.338542
C	-0.953936	-1.412027	0.455577
C	0.436414	-1.353478	0.267752
C	1.038294	-0.125554	-0.018610
C	0.312243	1.063640	-0.154291
C	-1.070092	0.990665	0.023247
H	-1.923622	3.064590	-0.334581
H	-4.287886	1.979066	0.134654
H	-1.439707	-2.364536	0.666553
H	1.046374	-2.253885	0.316260
H	0.818679	1.990509	-0.418912
H	-3.451064	-0.137642	1.575643
N	-4.011735	-0.865882	-0.251104
C	-4.710607	-1.587004	-0.864015
S	2.840157	-0.071889	-0.244118
O	3.295230	-1.434095	-0.650610
O	3.159538	1.127236	-1.074806
C	3.482284	0.239292	1.428310
H	4.571484	0.279793	1.318185

H	3.086131	1.197275	1.779606
H	3.182428	-0.591050	2.075331

NH_2-NC-IND

Total energy (hartree): -495.380737

Sum of electronic and thermal Free Energies (hartree): -495.261729

C	-0.801698	2.012655	-0.063652
C	-2.014283	1.487672	0.197080
C	-1.888082	0.004109	0.525221
C	-0.404028	-0.256652	0.317480
C	0.338701	-1.424407	0.420118
C	1.722333	-1.370800	0.209441
C	2.366800	-0.154676	-0.094326
C	1.605082	1.028168	-0.197302
C	0.228290	0.961815	0.002742
H	-0.601388	3.057367	-0.297040
H	-2.970263	2.005754	0.207731
H	-0.136360	-2.378781	0.649451
H	2.313376	-2.285410	0.273973
H	2.092048	1.973739	-0.440595
H	-2.165315	-0.163882	1.579582
N	-2.752587	-0.826211	-0.261741
C	-3.471052	-1.515736	-0.886928
N	3.738394	-0.131710	-0.357710
H	4.198409	0.761222	-0.241320
H	4.276475	-0.897466	0.025130

$NHNH_2$-NC-IND

Total energy (hartree): -550.704784

Sum of electronic and thermal Free Energies (hartree): -550.570357

C	-1.408497	1.994653	-0.052196
C	-2.566289	1.360519	0.214960
C	-2.303553	-0.107576	0.531739
C	-0.803286	-0.232098	0.310636
C	0.044459	-1.325932	0.403881
C	1.418638	-1.152648	0.184678
C	1.940132	0.117982	-0.121704
C	1.075689	1.231020	-0.209263
C	-0.287180	1.041119	-0.001865
H	-1.306180	3.054629	-0.280394
H	-3.565210	1.789608	0.236331
H	-0.341030	-2.319843	0.634074
H	2.098384	-1.998310	0.244327
H	1.473610	2.219091	-0.448050
H	-2.555903	-0.307627	1.586689
N	-3.096624	-1.006673	-0.255229

C	-3.756484	-1.752008	-0.880878
N	3.300635	0.308451	-0.406971
H	3.605948	1.270647	-0.300242
N	4.209918	-0.668677	0.052146
H	4.619601	-0.412172	0.950739
H	4.951500	-0.777919	-0.633027

NMe_2-NC-IND

Total energy (hartree): -573.992710

Sum of electronic and thermal Free Energies (hartree): -573.822075

C	1.572719	2.004067	-0.016463
C	2.787024	1.461055	-0.227185
C	2.656366	-0.033116	-0.503244
C	1.165622	-0.272533	-0.324758
C	0.406548	-1.430041	-0.410596
C	-0.980897	-1.357563	-0.238412
C	-1.634845	-0.124595	0.020915
C	-0.843854	1.053488	0.091604
C	0.535340	0.959047	-0.069893
H	1.375916	3.058407	0.172938
H	3.747309	1.971218	-0.232436
H	0.871181	-2.398030	-0.601483
H	-1.555067	-2.277065	-0.306043
H	-1.296810	2.024001	0.275435
H	2.962057	-0.244055	-1.541870
N	3.492525	-0.839055	0.339148
C	4.186988	-1.509157	1.010627
N	-3.006619	-0.072165	0.215188
C	-3.814432	-1.255275	-0.028157
H	-4.861018	-1.023722	0.191313
H	-3.749275	-1.606147	-1.073943
H	-3.511669	-2.083006	0.629653
C	-3.670915	1.217221	0.298593
H	-3.545903	1.819003	-0.619767
H	-4.741115	1.057580	0.460407
H	-3.290936	1.804775	1.147257

NO-1-NC-IND

Total energy (hartree): -569.323175

Sum of electronic and thermal Free Energies (hartree): -569.225270

C	-1.281752	2.015051	-0.089691
C	-2.445865	1.385286	0.157033
C	-2.192273	-0.075180	0.508313
C	-0.686533	-0.210936	0.317592
C	0.128695	-1.333952	0.438914
C	1.504136	-1.180179	0.248105

C	2.027453	0.089308	-0.051735
C	1.208004	1.221759	-0.179646
C	-0.164884	1.059775	0.001989
H	-1.167992	3.070700	-0.329018
H	-3.444394	1.815207	0.151512
H	-0.293446	-2.312883	0.666526
H	2.187112	-2.024466	0.326578
H	1.663123	2.182841	-0.418575
H	-2.442840	-0.245240	1.569486
N	-2.964733	-1.001487	-0.258617
C	-3.611376	-1.766799	-0.875266
N	3.436421	0.338974	-0.257115
O	4.160374	-0.634170	-0.151254

NO-2-NC-IND

Total energy (hartree): -569.323789

Sum of electronic and thermal Free Energies (hartree): -569.225765

C	0.971837	2.025940	0.022988
C	2.220323	1.567680	-0.185460
C	2.194275	0.076580	-0.496262
C	0.721236	-0.275970	-0.327090
C	0.086787	-1.505432	-0.423465
C	-1.305192	-1.540378	-0.253952
C	-2.014625	-0.358216	-0.003181
C	-1.373220	0.890734	0.100161
C	0.006599	0.916763	-0.057219
H	0.700259	3.059625	0.228828
H	3.144218	2.140836	-0.176001
H	0.647497	-2.420239	-0.613466
H	-1.861832	-2.475403	-0.312956
H	-1.962590	1.783739	0.302217
H	2.492857	-0.086403	-1.545833
N	3.076913	-0.701912	0.315430
C	3.815170	-1.344483	0.968283
N	-3.440615	-0.532220	0.143029
O	-4.069204	0.489683	0.354897

NO_2-NC-IND

Total energy (hartree): -644.548322

Sum of electronic and thermal Free Energies (hartree): -644.445853

C	1.469899	2.022781	0.020760
C	2.680302	1.469103	-0.182014
C	2.539490	-0.015833	-0.491533
C	1.043203	-0.251557	-0.328513
C	0.308305	-1.424644	-0.427951
C	-1.082865	-1.357691	-0.268123

C	-1.681639	-0.119931	-0.022531
C	-0.957176	1.072505	0.085930
C	0.425621	0.988632	-0.064128
H	1.276589	3.074274	0.224260
H	3.645586	1.969115	-0.168838
H	0.791339	-2.383198	-0.614822
H	-1.704485	-2.246788	-0.331800
H	-1.473637	2.008158	0.283727
H	2.827995	-0.200406	-1.540406
N	3.356007	-0.859939	0.322995
C	4.039749	-1.557890	0.978487
N	-3.151408	-0.065810	0.135436
O	-3.777136	-1.118376	0.043616
O	-3.660978	1.031655	0.348452

OCF_3-1-NC-IND

Total energy (hartree): -852.327447

Sum of electronic and thermal Free Energies (hartree): -852.222424

C	1.859121	1.990610	-0.046230
C	3.151787	1.638910	-0.182984
C	3.267001	0.144211	-0.455269
C	1.822416	-0.325487	-0.351618
C	1.276452	-1.597094	-0.453333
C	-0.113061	-1.739800	-0.352580
C	-0.918920	-0.613695	-0.161906
C	-0.387238	0.675654	-0.055137
C	1.001548	0.797768	-0.146073
H	1.489711	3.001010	0.120098
H	4.021281	2.290394	-0.142531
H	1.903852	-2.476561	-0.596420
H	-0.584929	-2.718400	-0.419205
H	-1.014745	1.548879	0.095862
H	3.639656	-0.012969	-1.481523
N	4.170811	-0.532837	0.423600
C	4.926065	-1.093815	1.129531
O	-2.287193	-0.914298	-0.092738
C	-3.218061	0.037480	0.135477
F	-3.249089	0.991709	-0.827732
F	-3.045117	0.676643	1.317677
F	-4.411973	-0.565748	0.159072

OCF_3-2-NC-IND

Total energy (hartree): -852.327326

Sum of electronic and thermal Free Energies (hartree): -852.222247

C	-2.536947	1.983981	-0.132437
C	-3.647588	1.260397	0.104960

C	-3.279234	-0.166850	0.492131
C	-1.763889	-0.171181	0.341885
C	-0.844222	-1.193424	0.504811
C	0.524272	-0.920261	0.336563
C	0.924536	0.379075	0.015869
C	0.007466	1.422673	-0.154087
C	-1.344969	1.131441	0.006005
H	-2.511060	3.040096	-0.394932
H	-4.678796	1.602871	0.066285
H	-1.160794	-2.207154	0.749403
H	1.247414	-1.720629	0.457976
H	0.365324	2.418803	-0.408601
H	-3.554592	-0.343932	1.545445
N	-3.950475	-1.163484	-0.285432
C	-4.513601	-1.989031	-0.905881
O	2.256648	0.777867	-0.167222
C	3.283969	-0.097012	-0.090693
F	3.198232	-1.096859	-0.999957
F	3.395430	-0.678982	1.128389
F	4.410103	0.586125	-0.327824

OCF_3-3-NC-IND

Total energy (hartree): -852.327706

Sum of electronic and thermal Free Energies (hartree): -852.223074

C	2.174830	2.015279	0.103412
C	3.389720	1.434658	0.088762
C	3.274235	-0.024375	-0.334344
C	1.768335	-0.217116	-0.463919
C	1.033942	-1.350311	-0.780910
C	-0.362490	-1.240683	-0.872429
C	-0.969019	-0.005209	-0.648184
C	-0.245309	1.147777	-0.336454
C	1.141218	1.023724	-0.235586
H	1.971996	3.058923	0.336841
H	4.346719	1.900463	0.310592
H	1.517971	-2.312222	-0.948452
H	-0.979155	-2.102639	-1.119104
H	-0.758871	2.094385	-0.180732
H	3.753839	-0.159707	-1.318518
N	3.907870	-0.937855	0.565933
C	4.444636	-1.693393	1.290359
O	-2.364669	0.100629	-0.831813
C	-3.156667	-0.055423	0.254946
F	-2.914383	0.865665	1.219518
F	-3.018970	-1.270533	0.836302
F	-4.427849	0.079444	-0.142661

OH-1-NC-IND

Total energy (hartree): -515.248546

Sum of electronic and thermal Free Energies (hartree): -515.141485

C	-0.799321	2.015507	-0.069128
C	-2.008555	1.483299	0.192089
C	-1.874214	0.001963	0.525337
C	-0.388094	-0.251978	0.317790
C	0.352955	-1.418944	0.420680
C	1.739022	-1.360786	0.207351
C	2.358812	-0.139853	-0.096089
C	1.613033	1.044344	-0.202550
C	0.236646	0.971230	0.000179
H	-0.603871	3.060495	-0.304246
H	-2.967481	1.995855	0.202157
H	-0.120836	-2.373652	0.650197
H	2.338541	-2.270423	0.275938
H	2.118668	1.978454	-0.443181
H	-2.146559	-0.162958	1.581367
N	-2.732208	-0.838361	-0.256387
C	-3.445280	-1.536195	-0.878767
O	3.709551	-0.038010	-0.306426
H	4.120565	-0.906676	-0.217457

OH-2-NC-IND

Total energy (hartree): -515.248181

Sum of electronic and thermal Free Energies (hartree): -515.141138

C	-0.783096	2.016190	-0.063709
C	-1.996986	1.493748	0.196067
C	-1.873814	0.010354	0.524213
C	-0.389751	-0.255134	0.316389
C	0.343977	-1.429781	0.418460
C	1.728035	-1.386395	0.208183
C	2.358597	-0.170406	-0.092512
C	1.622958	1.020516	-0.198053
C	0.242909	0.962060	0.002966
H	-0.579401	3.060450	-0.295627
H	-2.951582	2.014222	0.207433
H	-0.139452	-2.380105	0.646089
H	2.334884	-2.288336	0.272052
H	2.120953	1.962542	-0.435432
H	-2.146726	-0.155393	1.580021
N	-2.739096	-0.819667	-0.259970
C	-3.459360	-1.507549	-0.885193
O	3.716286	-0.208957	-0.278486
H	4.043894	0.674327	-0.487720

OMe-1-NC-IND

Total energy (hartree): -554.549141

Sum of electronic and thermal Free Energies (hartree): -554.416020

C	1.021480	2.012329	-0.006886
C	2.285264	1.589834	-0.202474
C	2.299737	0.093285	-0.491289
C	0.835830	-0.291023	-0.333085
C	0.205135	-1.526996	-0.426869
C	-1.181811	-1.589191	-0.269429
C	-1.930993	-0.422448	-0.027936
C	-1.298616	0.828988	0.067948
C	0.091259	0.872659	-0.081366
H	0.720542	3.041170	0.185095
H	3.192419	2.189137	-0.192558
H	0.772696	-2.440215	-0.607157
H	-1.710743	-2.539343	-0.328004
H	-1.859842	1.740562	0.257333
H	2.627668	-0.076061	-1.530790
N	3.198607	-0.640958	0.348838
C	3.947502	-1.249598	1.020712
O	-3.277774	-0.610851	0.102746
C	-4.097160	0.524144	0.361761
H	-3.821141	1.007160	1.311802
H	-4.035361	1.257138	-0.457482
H	-5.120059	0.142078	0.431401

OMe-2-NC-IND

Total energy (hartree): -554.549400

Sum of electronic and thermal Free Energies (hartree): -554.416281

C	-1.419901	1.994179	-0.091418
C	-2.573606	1.346991	0.160875
C	-2.298365	-0.110226	0.514445
C	-0.790951	-0.217093	0.331482
C	0.062322	-1.298564	0.459923
C	1.443085	-1.111630	0.264657
C	1.944289	0.161988	-0.048482
C	1.076403	1.263651	-0.179946
C	-0.285834	1.059761	0.005042
H	-1.326856	3.050666	-0.337779
H	-3.578833	1.761535	0.151362
H	-0.316777	-2.292969	0.697079
H	2.108705	-1.965511	0.358646
H	1.491117	2.239963	-0.427274
H	-2.571175	-0.291958	1.567470
N	-3.056214	-1.038773	-0.271733

C	-3.686767	-1.808498	-0.898298
O	3.266988	0.438092	-0.250005
C	4.206185	-0.626951	-0.142824
H	4.200461	-1.063984	0.867532
H	4.004863	-1.412905	-0.886761
H	5.184935	-0.179809	-0.340847

SH-1-NC-IND

Total energy (hartree): -838.221422

Sum of electronic and thermal Free Energies (hartree): -838.121079

C	-1.215392	2.015639	-0.063530
C	-2.428850	1.477981	0.164513
C	-2.296784	-0.002467	0.502219
C	-0.804349	-0.250282	0.333399
C	-0.061753	-1.414950	0.454177
C	1.329085	-1.352158	0.278558
C	1.959909	-0.130759	-0.007120
C	1.204317	1.049538	-0.131758
C	-0.177846	0.975028	0.033882
H	-1.017975	3.061484	-0.293035
H	-3.389989	1.986166	0.148958
H	-0.537710	-2.371874	0.669844
H	1.919437	-2.263694	0.365573
H	1.691280	1.998194	-0.358366
H	-2.591332	-0.167062	1.552435
N	-3.129506	-0.849222	-0.298003
C	-3.823082	-1.551554	-0.937340
S	3.731150	0.006904	-0.231242
H	4.022893	-1.305213	-0.061508

SH-2-NC-IND

Total energy (hartree): -838.221324

Sum of electronic and thermal Free Energies (hartree): -838.121171

C	-1.215340	2.016465	-0.061306
C	-2.428754	1.478945	0.167159
C	-2.296566	-0.001991	0.502267
C	-0.804126	-0.249775	0.332845
C	-0.061371	-1.414942	0.453763
C	1.328365	-1.351101	0.277284
C	1.959764	-0.128690	-0.007725
C	1.205077	1.051061	-0.131221
C	-0.177913	0.975395	0.034062
H	-1.018150	3.062685	-0.289522
H	-3.389756	1.987409	0.152835
H	-0.537361	-2.371853	0.668989
H	1.923099	-2.260671	0.361174

H	1.687700	2.002174	-0.354964
H	-2.590831	-0.168540	1.552247
N	-3.129751	-0.846591	-0.299635
C	-3.824416	-1.546038	-0.940972
S	3.739442	-0.153980	-0.204118
H	3.894167	1.162628	-0.484366

SiH_3-NC-IND

Total energy (hartree): -730.718730

Sum of electronic and thermal Free Energies (hartree): -730.604573

C	1.257134	2.017903	0.070057
C	2.470927	1.478877	-0.153138
C	2.336603	0.000116	-0.496028
C	0.841733	-0.246823	-0.332917
C	0.105846	-1.413706	-0.460221
C	-1.287804	-1.343505	-0.288933
C	-1.940327	-0.128955	-0.003397
C	-1.167417	1.045869	0.123518
C	0.216823	0.980663	-0.034172
H	1.061124	3.063833	0.300608
H	3.433076	1.984832	-0.132572
H	0.587880	-2.367816	-0.675394
H	-1.871435	-2.260324	-0.381758
H	-1.643610	2.002455	0.347891
H	2.628421	-0.162099	-1.547373
N	3.163836	-0.853885	0.300670
C	3.854480	-1.559918	0.939143
Si	-3.820192	-0.076998	0.213371
H	-4.179904	0.400311	1.583768
H	-4.371890	-1.448787	0.005855
H	-4.435809	0.859633	-0.776378

$SiMe_3$-NC-IND

Total energy (hartree): -848.711400

Sum of electronic and thermal Free Energies (hartree): -848.518066

C	2.213753	2.008412	0.060662
C	3.432670	1.470247	-0.136061
C	3.305554	-0.008000	-0.484335
C	1.807327	-0.254502	-0.356387
C	1.071128	-1.419114	-0.502429
C	-0.326159	-1.345364	-0.362199
C	-0.990661	-0.133926	-0.089149
C	-0.212104	1.035871	0.056199
C	1.175634	0.971840	-0.069733
H	2.013181	3.054081	0.288841
H	4.394113	1.976027	-0.092471

H	1.555964	-2.373977	-0.708237
H	-0.903005	-2.264150	-0.470049
H	-0.687383	1.995004	0.272745
H	3.623420	-0.169582	-1.528126
N	4.114660	-0.862717	0.331089
C	4.791001	-1.569011	0.984188
Si	-2.886423	-0.045958	0.087658
C	-3.634438	-1.773551	-0.107156
H	-3.259741	-2.472207	0.654529
H	-4.727503	-1.723043	0.002350
H	-3.423447	-2.204962	-1.096163
C	-3.578873	1.106127	-1.249945
H	-4.671660	1.198668	-1.163159
H	-3.154205	2.117441	-1.170156
H	-3.352949	0.730677	-2.258213
C	-3.316707	0.649317	1.798050
H	-2.892479	1.653190	1.944706
H	-4.406215	0.729586	1.927655
H	-2.929543	0.005614	2.600695

tBu-NC-IND

Total energy (hartree): -597.279492

Sum of electronic and thermal Free Energies (hartree): -597.070541

C	1.850558	2.004803	0.061659
C	3.070544	1.473709	-0.147394
C	2.949267	-0.005477	-0.495979
C	1.453764	-0.258571	-0.357057
C	0.713404	-1.418723	-0.498759
C	-0.683394	-1.349748	-0.346321
C	-1.346190	-0.143926	-0.063759
C	-0.567048	1.024167	0.077568
C	0.817235	0.962433	-0.061361
H	1.646671	3.049028	0.293724
H	4.029350	1.985038	-0.111142
H	1.191858	-2.374982	-0.711971
H	-1.250462	-2.270924	-0.453195
H	-1.040215	1.979496	0.301914
H	3.263886	-0.165480	-1.540866
N	3.768801	-0.854301	0.316112
C	4.452547	-1.555810	0.966476
C	-2.874378	-0.057192	0.103154
C	-3.204315	0.450416	1.526270
H	-2.785047	1.447556	1.710991
H	-4.293009	0.513591	1.664396
H	-2.801569	-0.231079	2.287705
C	-3.563242	-1.419660	-0.092751

H	-4.647976	-1.303050	0.032556
H	-3.387609	-1.825814	-1.098031
H	-3.223383	-2.160104	0.643805
C	-3.449081	0.928380	-0.940863
H	-3.227433	0.590062	-1.962155
H	-4.540600	1.000579	-0.833614
H	-3.034090	1.937396	-0.822200

Vin-1-NC-IND
Total energy (hartree): -517.419440
Sum of electronic and thermal Free Energies (hartree): -517.285522

C	1.006916	2.017548	0.006956
C	2.262280	1.572802	-0.191694
C	2.252542	0.078031	-0.489478
C	0.781705	-0.284146	-0.329978
C	0.138723	-1.507646	-0.424758
C	-1.254674	-1.540149	-0.262918
C	-2.004958	-0.373691	-0.018001
C	-1.328462	0.862816	0.077153
C	0.054196	0.897022	-0.071813
H	0.725467	3.050702	0.204470
H	3.179797	2.156115	-0.180297
H	0.693083	-2.428259	-0.607945
H	-1.775497	-2.496046	-0.328005
H	-1.880182	1.781914	0.270757
H	2.571076	-0.092576	-1.531661
N	3.138394	-0.679270	0.342609
C	3.877307	-1.305870	1.009219
C	-3.466573	-0.494802	0.133710
H	-3.851166	-1.514474	0.044623
C	-4.346943	0.492086	0.362907
H	-4.053117	1.536908	0.465359
H	-5.410567	0.276603	0.456611

Vin-2-NC-IND
Total energy (hartree): -517.419201
Sum of electronic and thermal Free Energies (hartree): -517.285362

C	-1.333445	2.000931	-0.081884
C	-2.500522	1.373461	0.158964
C	-2.250236	-0.089701	0.504801
C	-0.743834	-0.222362	0.324792
C	0.087217	-1.328805	0.448745
C	1.463796	-1.158032	0.262021
C	2.018012	0.103562	-0.039251
C	1.155677	1.212858	-0.162153
C	-0.217470	1.044306	0.013042

H	-1.219521	3.057509	-0.318815
H	-3.498299	1.805258	0.148862
H	-0.316931	-2.315691	0.675101
H	2.115785	-2.025405	0.352563
H	1.569211	2.194315	-0.398490
H	-2.519585	-0.269321	1.559388
N	-3.020309	-1.006015	-0.280954
C	-3.662310	-1.764264	-0.910123
C	3.465090	0.310738	-0.236477
H	3.750116	1.341420	-0.465411
C	4.440033	-0.608941	-0.166917
H	4.249962	-1.659221	0.054540
H	5.479387	-0.329265	-0.334417