

SUPPLEMENTRY INFORMATION

Quantification of Electric Fields inside the Protein Active Sites and Fullerenes

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1. Computational Methods

The method is a virtual reproduction of the experimental procedure to obtain VSTR. An external electric field was applied along the C≡N bond and then the change in bond lengths and vibrational frequencies were calculated. We performed geometry optimization, single-point energy, and vibrational frequency calculations of the various nitrile molecular probes at B3LYP/6-31G(d), B3LYP/6-31+G(d), HF/6-31G(d), and HF/6-31+G(d) level of theory by using the Gaussian 16 program.^[1] The frequency and coordinates analysis of molecules were performed with Chemcraft software. The protein crystal structures were downloaded from the Protein Data Bank (PDB) archive.^[2] The visualization and Cartesian coordinates of different residues were obtained by using *PyMOL*^[3] software.

In the first part of this study, full geometry optimization followed by vibration frequency calculation of the nitrile probes were performed in the presence of an external electric field. The C≡N bond of the nitrile probes was kept along Z-axis. The direction of the external electric field was set along the C→N bond vector, the arrow in C→N indicates the direction of the electric field from positive to negative, (see Figure 1E). The external electric field applied varied from 0.0 to +77.13 MV/cm with an increment of 12.85 MV/cm at every step. This range of electric field was selected based on estimated electric field strength experienced by the probes in proteins, water, and solvents as reported in the literature^[4]. We also ensured that the direction of the C≡N bond did not change during the optimization steps. Then the VSTR was calculated using this equation^[5],

$$|\Delta\vec{\mu}| = \left| \frac{\Delta\nu}{\Delta F_{ext}} \right| \quad (1)$$

Here $|\Delta\vec{\mu}|$ is the Stark tuning rate in $\text{cm}^{-1}/\text{MV}/\text{cm}$, $\Delta\nu$ is the change in C≡N stretching frequency in cm^{-1} , and ΔF_{ext} is the change in the applied external electric field in MV/cm . The slope of the $\Delta\nu$ vs ΔF_{ext} graph gave the Stark tuning rate.

2. Figures

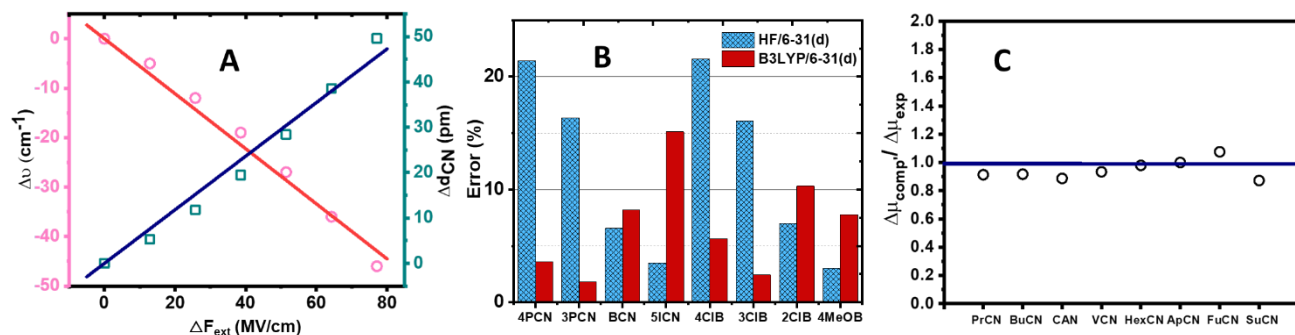


Figure S1: A) The dual y-axis plot for change in the external electric field (ΔF_{ext}) vs change in vibrational frequency ($\Delta\nu$) and bond length (Δd) of nitrile is shown by blue and red line fit respectively for BCN. B) Comparison of % error/deviation in computational VSTR with respect to experimental VSTR at HF/6-31G(d) and B3LYP/6-31G(d) level of theory for aromatic nitrile probes. C) The plot of $\Delta\mu_{\text{comp}} / \Delta\mu_{\text{exp}}$ for aliphatic nitrile probes.

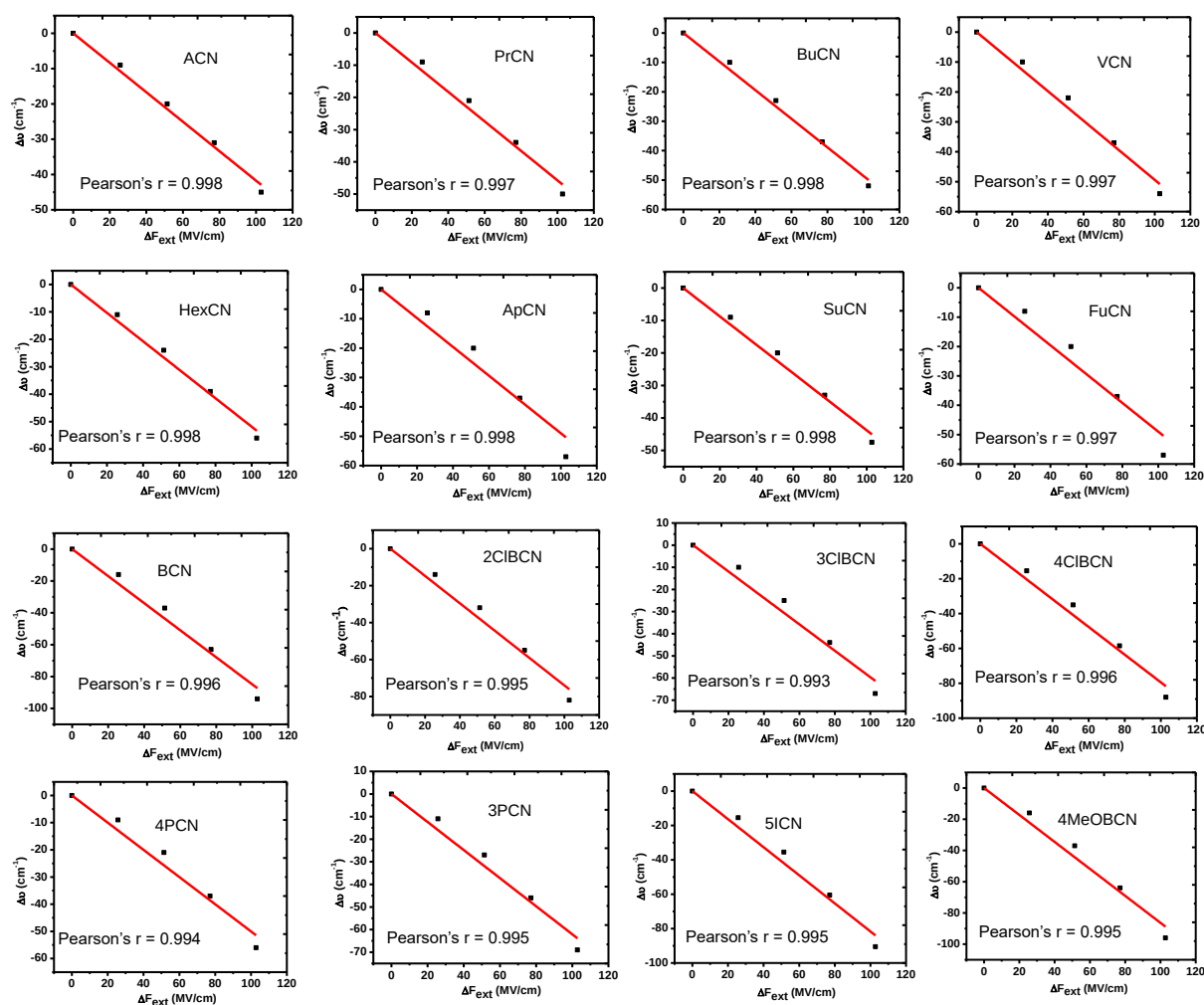


Fig S2: The linear plot for change in the external electric field (ΔF_{ext}) vs change in vibrational frequency ($\Delta\nu$) of the 16 probes shown in Fig 1 in main text.

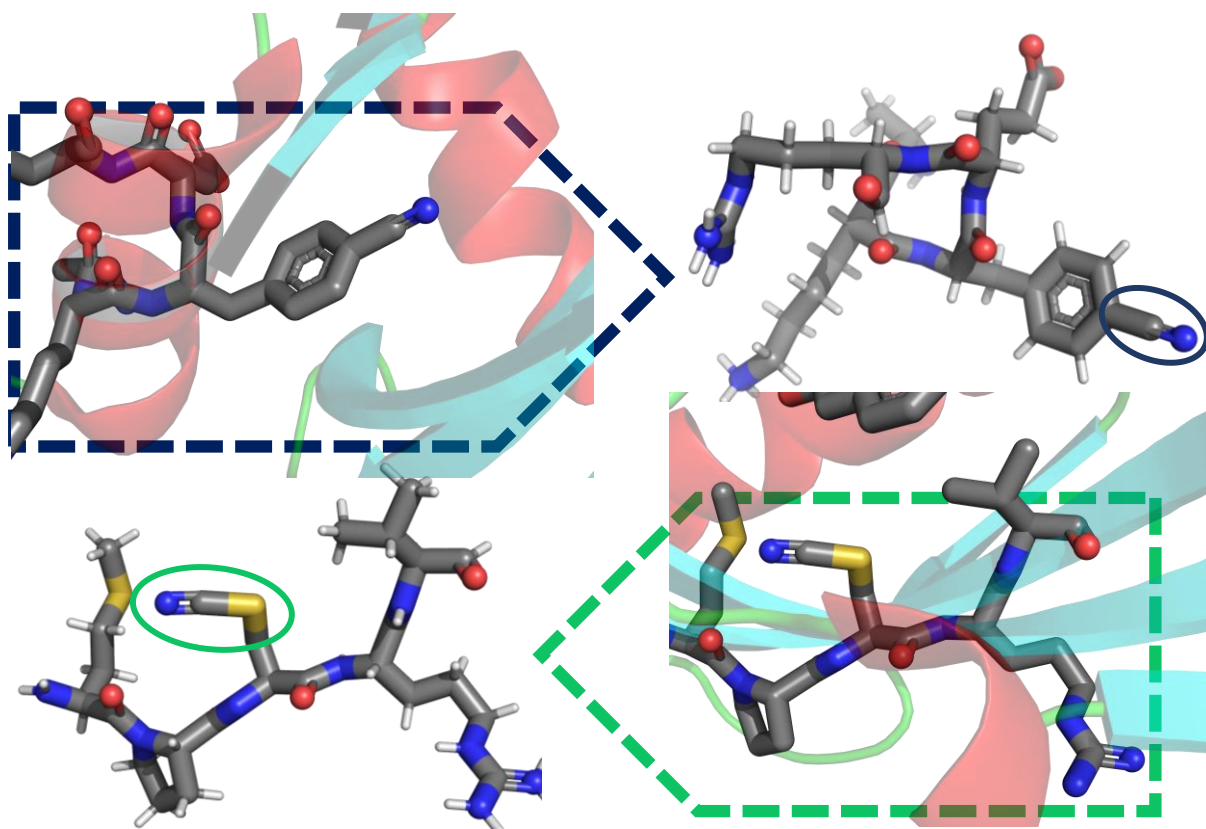


Figure S3:(Top) p-cyanophenylalanine probe near the active site of the semisynthetic enzyme ribonuclease S (PDB: 3OQY) and the residue near the probe were extracted. After adding H atoms to the residue, the freeze co-ordinate optimization was performed as shown in the right. (Bottom) Site-specific thiocyanate vibrational probe in bacterial ketosteroid isomerase (PDB: 3OWU). Grey, red, dark-yellow, and blue are carbon, oxygen, sulfur, and nitrogen respectively in the ball and stick diagram.

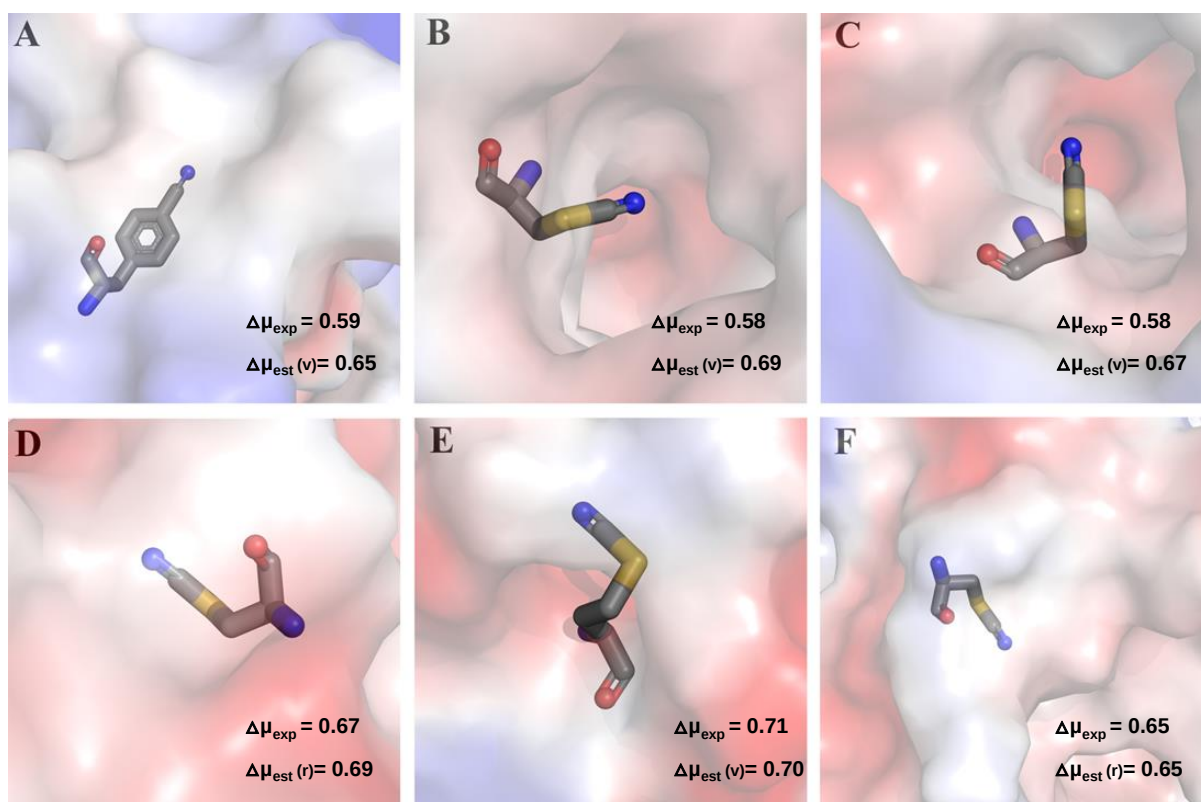


Figure S4: The local environment surrounding each of the six probes is shown in semi-transparent surface representation A) PDB: 3OQY B) PDB: 3OWU C) 3OX9 D) PDB: 3OXA E) 3OR0 F) 3OWS. As seen in figures B and C, the nitrile probe is solvent-exposed for 3OWU and 3OX9 because the probe is outside on the surface, whereas the rest of the probes are buried deep down in the hydrophobic core.

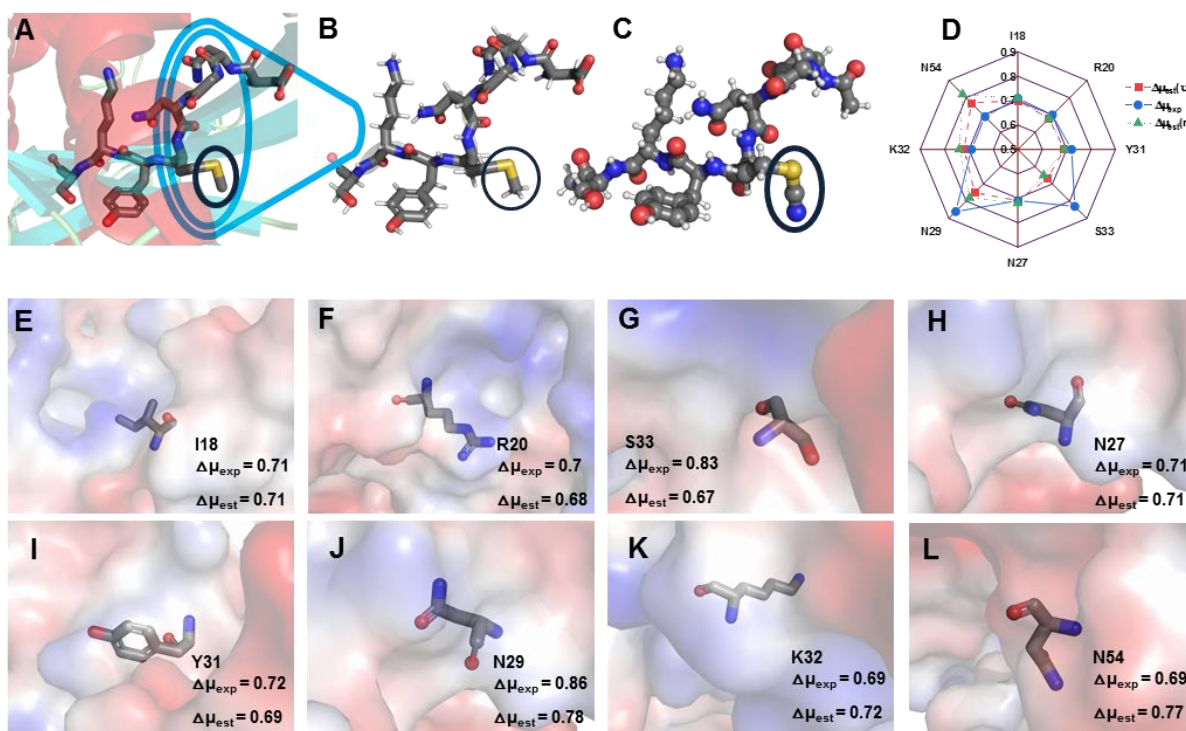


Figure S5:A-C) Incorporation of the thionitrile probe at the active site of interest by modifying the side chain of the respective amino acids; here the methionine side chain is modified to a thionitrile group. D) The spider web plot shows the comparison of estimated VSTR ($\Delta\mu_{est}$) with experimental VSTR ($\Delta\mu_{exp}$) using the expression for v_{comp} [$\Delta\mu_{est}(v)$] and r_{CN} [$\Delta\mu_{est}(r)$] for SCN probes in SCN-LabeledRas mutants (PDB: 1LFD). The X-axis contains the one letter form of the amino-acid and residue's location. The local environment surrounding the probes at different locations of the active Ras protein (PDB: 1LFD). E) I18: Isoluecene-18, F) R20: Arginine-20, G) S33: Serine-33, H) N27: Asparagine-27, I) Y31: Tyrosine-31, J) N29: Asparagine-29, K) K32: Lysine-32, L) N54: Asparagine-54. Grey, red, dark-yellow, and blue colors in the ball and stick diagram represent carbon, oxygen, sulfur, and nitrogen, respectively.

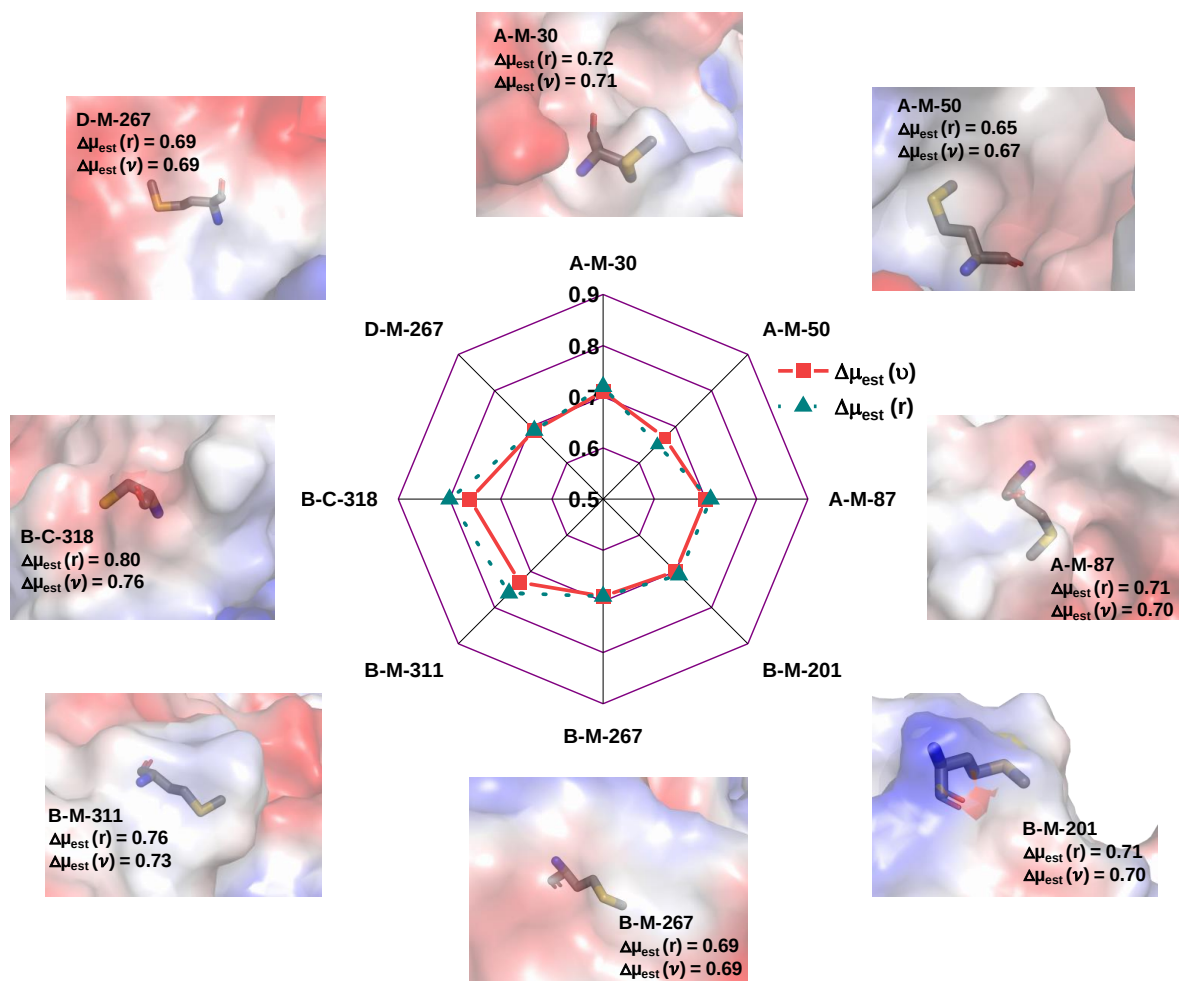


Figure S6: The pictures are the representation of the local environment surrounding the probes is shown in semi-transparent surface representation for residues at different locations in 1LFD. A-M-30: Chain-A-MET-30, A-M-50: Chain-A-MET-50, A-M-87: Chain-A-MET-87, B-M-201: Chain-B-MET-201, B-M-267: Chain-B-MET-267, B-M-311: Chain-B-MET-311, B-C-318: Chain-B-CYS-318, D-M-367: Chain-D-MET-267. The spider web plot shows the comparison of $[\Delta\mu_{\text{est}}(v)]$ and $[\Delta\mu_{\text{est}}(r)]$ for SCN probes in SCN-Labeled Ral β mutants (PDB: 1LFD). The horizontal-axis contains the one letter form of the amino-acid and residue's location.

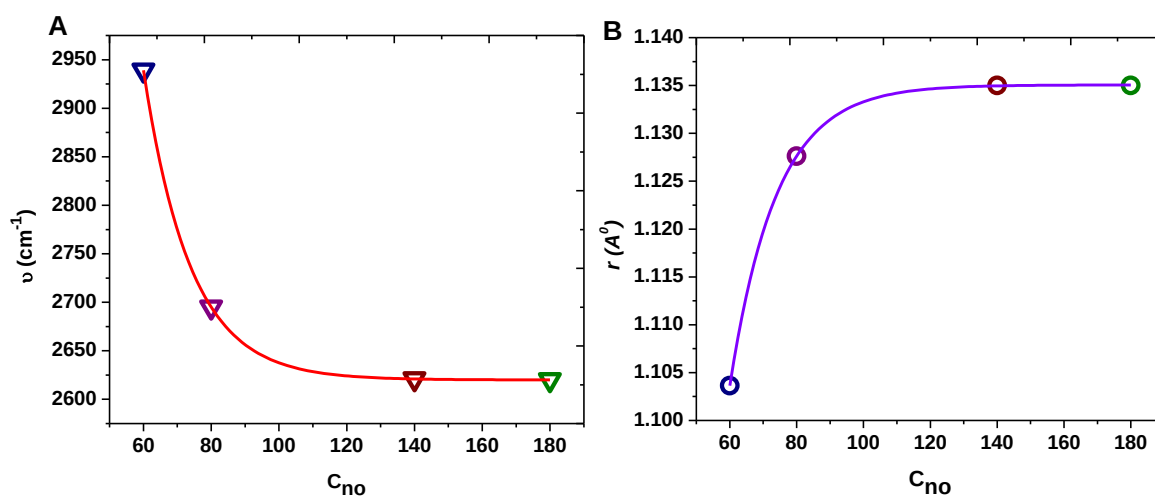


Figure S7: A) CN Frequency vs C_{no} plot, and B) CN bond length vs C_{no} plot for Fullerenes.

Tables

Table S1: VSTR for aromatic and aliphatic nitrile probes

		Alt-B3LYP/6-31G*		Alt-HF/6-31G*	
Molecule	Stark (expt)	Stark (comp)	%Error	Stark (comp)	%Error
4PCN	0.42	0.435	-4	0.51	-21
3PCN	0.55	0.56	-2	0.64	-16
BCN	0.61	0.56	8	0.65	-7
5ICN	0.86	0.73	15	0.83	3
4ClBCN	0.584	0.617	-6	0.71	-22
3ClBCN	0.534	0.521	2	0.62	-16
2ClBCN	0.514	0.461	10	0.55	-7
4MeOBCN	0.835	0.77	8	0.86	-3
PrCN	0.465	0.364	22	0.42	10
BuCN	0.475	0.39	18	0.44	7
CAN	0.433	0.305	30	0.39	10
VCN	0.448	0.41	8	0.42	6
HexCN	0.47	0.43	9	0.47	0
ApCN	0.446	0.4	10	0.452	-1
FuCN	0.4	0.28	30	0.427	-7
SuCN	0.47	0.32	32	0.41	13

Table S2: Estimated VSTR using bond length.

Molecule	Bond length (ang)	Stark (expt)	Stark (est)	% Error
3OQY	1.1363	0.59	0.65	10
3OQZ	1.1365	0.6	0.62	4
IDD743	1.1364	0.69	0.66	-4
3T42	1.1366	0.77	0.70	-9
3OXA	1.1373	0.67	0.69	3
3OWY	1.1373	0.70	0.70	0
3OWU	1.1365	0.58	0.57	-1
3OWS	1.1370	0.65	0.65	1
3OX9	1.1369	0.58	0.64	10
3Or0	1.1374	0.71	0.70	-1
I-18	1.1374	0.71	0.71	0
R-20	1.1372	0.7	0.68	-3
Y-31	1.1373	0.72	0.69	-4
M-30	1.1375		0.72	
S-33	1.1370	0.83	0.65	-22
N-27	1.1375	0.71	0.72	1
N-29	1.1379	0.86	0.78	-9
K-32	1.1376	0.69	0.74	7
N-54	1.1381	0.69	0.82	19

Table S3: Estimated VSTR using frequency.

Molecule	Freq (cm-1)	Scaled freq (cm-1)	Stark (expt)	Stark (est)	% Error
3OQY	2605.4	2239.1	0.59	0.65	11
3OQZ	2603.6	2237.5	0.6	0.68	14
IDD743	2606.8	2240.3	0.69	0.63	-8
3T42	2604.1	2238.0	0.77	0.68	-12
3OXA	2553.8	2194.7	0.67	0.70	5
3OWY	2555.2	2196.0	0.70	0.69	-1
3OWU	2555.5	2196.2	0.58	0.69	19
3OWS	2553.5	2194.5	0.65	0.71	9
3OX9	2558.1	2198.4	0.58	0.67	16
3Or0	2554.8	2195.6	0.71	0.70	-2
I-18	2554	2194.9	0.71	0.70	-1
R-20	2557	2197.5	0.7	0.68	-3
Y-31	2555	2195.8	0.72	0.69	-4
M-30	2553	2194.0		0.71	
S-33	2558	2198.3	0.83	0.67	-19
N-27	2553	2194.0	0.71	0.71	0
N-29	2548	2189.8	0.86	0.75	-13
K-32	2552	2193.2	0.69	0.72	4
N-54	2545	2187.2	0.69	0.77	12

Table S4: The predicted EF's (MV/cm) and VSRs (cm-1/MV/cm) data for C60, C80, C140, C180 Fullerenes and C60@C240 carbon nano-onion.

Fullerene	Frequency (cm⁻¹)	E.F.est (v)	E.F.est (r)	 Δμ_{est}(v) 	 Δμ_{est}(r)
C ₆₀	2939	-68.82 (~50)	-60.22 (~50)	4.59	5.25
C ₈₀	2695	-95.45	-78.35	0.75	0.92
C ₁₄₀	2621	-4.88	-4.82	0.41	0.41
C ₁₈₀	2620	-7.05	-7.20	0.43	0.42
C ₆₀ @C ₂₄₀	2944	-68.73	-59.80	4.67	5.37

The E.F in bracket is the reported by Tuchin *et. al.*^[6]

3. Cartesian coordinates of the optimized geometries

ACN, symmetry C1, imaginary frequency=0, HF = -131.927

C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.134761000
H	1.016539000	0.000000000	-1.835138000
C	-0.001244000	-0.000018000	-1.467750000
H	-0.510067000	-0.881792000	-1.834509000
H	-0.510342000	0.881538000	-1.834622000

PrCN, symmetry C1, imaginary frequency=0, HF = -170.966

C	-0.004415000	0.000012000	0.007806000
N	-0.021877000	-0.000011000	1.143728000
C	1.460036000	-0.000002000	-2.013152000
C	0.028760000	0.000072000	-1.466302000
H	-0.514194000	0.873142000	-1.809120000
H	-0.514315000	-0.872892000	-1.809199000
H	1.434728000	0.000048000	-3.096974000
H	2.001974000	-0.878448000	-1.683906000
H	2.002096000	0.878338000	-1.683826000

BuCN, symmetry C1, imaginary frequency=0, HF = -209.99789

C	-0.015584000	-0.009734000	0.009557000
N	-0.020474000	-0.023015000	1.144753000
C	1.434173000	0.007293000	-2.026154000
C	1.436875000	0.026092000	-3.553091000
C	0.005740000	0.007507000	-1.463016000
H	-0.543650000	-0.858783000	-1.815106000
H	-0.535196000	0.887147000	-1.794488000
H	1.967189000	0.870992000	-1.642719000
H	1.958578000	-0.870795000	-1.664114000

H	0.938987000	0.911346000	-3.937507000
H	2.452035000	0.025664000	-3.934547000
H	0.930096000	-0.844303000	-3.959211000

VCN, symmetry C1, imaginary frequency=0, HF = -249.027

C	-0.024950000	0.019667000	0.012470000
N	-0.031069000	0.035017000	1.147680000
C	1.427244000	-0.022003000	-2.020360000
C	1.440121000	-0.044344000	-3.549280000
C	2.855976000	-0.066744000	-4.123432000
C	-0.001923000	-0.000663000	-1.460076000
H	-0.555291000	-0.873048000	-1.789994000
H	-0.538663000	0.872738000	-1.813903000
H	1.947907000	-0.892657000	-1.633292000
H	1.964060000	0.849704000	-1.658544000
H	0.892697000	-0.915346000	-3.902616000
H	0.909776000	0.826528000	-3.928060000
H	3.400667000	-0.944761000	-3.789350000
H	3.418250000	0.809420000	-3.814588000
H	2.835928000	-0.082144000	-5.208117000

HexCN, symmetry C1, imaginary frequency=0, HF = -288.06746

C	-0.031836000	0.013194000	-0.004214000
N	-0.045265000	0.015190000	1.130979000
C	1.433555000	-0.005923000	-2.027967000
C	1.455245000	-0.008514000	-3.556712000
C	2.872971000	-0.025436000	-4.131201000
C	2.894044000	-0.028140000	-5.659114000
C	0.000680000	0.010567000	-1.476780000
H	-0.532653000	0.888893000	-1.823434000

H	-0.551666000	-0.856994000	-1.820754000
H	1.968832000	0.860143000	-1.650929000
H	1.949796000	-0.882323000	-1.648257000
H	0.927432000	0.868372000	-3.927560000
H	0.907733000	-0.874371000	-3.924898000
H	3.400471000	-0.901357000	-3.760678000
H	3.420149000	0.839515000	-3.763461000
H	2.403015000	0.853927000	-6.060041000
H	2.383536000	-0.900391000	-6.057181000
H	3.911570000	-0.040055000	-6.036166000

ApCN, symmetry C1, imaginary frequency=0, HF = -340.7640

C	-0.016463000	-0.000116000	0.011885000
N	-0.011109000	0.012823000	1.146773000
C	2.865529000	-0.013669000	-5.584283000
N	2.860132000	-0.025524000	-6.719189000
C	-0.004292000	-0.016707000	-1.460235000
C	1.423935000	0.001098000	-2.022093000
C	1.425143000	-0.015813000	-3.550297000
C	2.853377000	0.001657000	-4.112145000
H	3.413320000	-0.858875000	-3.763369000
H	3.384650000	0.887298000	-3.781887000
H	0.911113000	-0.900397000	-3.913330000
H	0.882190000	0.842995000	-3.932598000
H	1.967087000	-0.857563000	-1.639748000
H	1.937756000	0.885821000	-1.659118000
H	-0.535109000	-0.902886000	-1.789768000
H	-0.564681000	0.843244000	-1.809699000

FuCN, symmetry C1, imaginary frequency=0, HF = -261.4959

C	0.002550000	-0.000037000	0.013780000
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N	-0.009757000	-0.000275000	1.149046000
C	1.125244000	0.000038000	-3.559273000
N	1.137542000	0.000181000	-4.694537000
C	0.000187000	0.000231000	-1.426180000
C	1.127540000	-0.000136000	-2.119316000
H	-0.961532000	0.000706000	-1.903351000
H	2.089238000	-0.000607000	-1.642104000

SuCN, symmetry C1, imaginary frequency=0, HF = -262.6902

C	-0.000118000	0.000498000	0.000194000
N	-0.000143000	0.001164000	1.134641000
C	0.021508000	-0.000362000	-1.470786000
H	-0.511709000	-0.873943000	-1.823780000
H	-0.509295000	0.874305000	-1.824726000
C	1.467749000	-0.002629000	-1.995742000
H	2.001001000	0.870858000	-1.642566000
H	1.998509000	-0.877389000	-1.641963000
C	1.489394000	-0.003162000	-3.466710000
N	1.489483000	-0.003622000	-4.601156000

4PCN, symmetry C1, imaginary frequency=0, HF = -340.5245

C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.162642000
C	1.209168000	0.000000000	-2.148319000
C	0.001963000	0.000030000	-1.435436000
C	-1.202768000	0.000112000	-2.152390000
C	-1.138157000	0.000179000	-3.544842000
C	1.149263000	0.000094000	-3.540976000
H	-2.156810000	0.000125000	-1.636407000
H	2.161567000	-0.000070000	-1.629323000
H	2.067493000	0.000099000	-4.124836000
H	-2.054409000	0.000244000	-4.131804000

N	0.006704000	0.000178000	-4.238910000
3PCN, symmetry C1, imaginary frequency=0, HF = -340.5259			
C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.163161000
C	1.197910000	0.000000000	-2.160388000
C	-0.001746000	0.000261000	-1.432210000
C	-1.215986000	0.000959000	-2.142366000
C	-0.132094000	0.001388000	-4.154437000
C	1.126872000	0.000603000	-3.548647000
H	-2.159768000	0.001129000	-1.601623000
H	-0.220084000	0.001909000	-5.239153000
H	2.027832000	0.000495000	-4.153870000
H	2.151135000	-0.000573000	-1.641328000
N	-1.285551000	0.001524000	-3.473418000
BCN, symmetry C1, imaginary frequency=0, HF = -324.4922			
C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.163367000
H	2.150727000	0.000000000	-1.588050000
C	-0.004774000	0.000000000	-4.225570000
C	-1.214844000	0.000000000	-3.527392000
C	1.206939000	0.000000000	-3.530232000
H	-2.156644000	0.000000000	-4.068332000
H	2.147500000	0.000000000	-4.073316000
C	-1.219807000	0.000000000	-2.134874000
C	1.215022000	0.000000000	-2.137747000
H	-2.154494000	0.000000000	-1.583416000
C	-0.001571000	0.000000000	-1.434713000
H	-0.006081000	0.000000000	-5.311963000
5ICN, symmetry C1, imaginary frequency=0, HF = -456.0631			
C	0.000000000	0.000000000	0.000000000

N	0.000000000	0.000000000	1.164068000
C	1.236144000	0.000000000	-2.129524000
C	-0.001398000	-0.000075000	-1.433216000
C	-1.218484000	-0.000251000	-2.122882000
C	-1.203678000	-0.000339000	-3.522735000
C	0.051854000	-0.000215000	-4.199073000
C	1.272875000	-0.000046000	-3.514029000
C	-2.224224000	-0.000500000	-4.534577000
C	-1.586699000	-0.000459000	-5.745146000
H	-1.993812000	-0.000500000	-6.746567000
H	0.477313000	-0.000238000	-6.280682000
H	2.220971000	0.000020000	-4.044496000
H	2.159565000	0.000145000	-1.560258000
H	-2.153773000	-0.000312000	-1.571964000
H	-3.293712000	-0.000610000	-4.377718000
N	-0.215699000	-0.000280000	-5.548222000

4ClBCN, symmetry C1, imaginary frequency=0, HF = -784.0866

C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.163289000
C	1.215244000	0.000000000	-2.138610000
C	0.000143000	0.000000000	-1.433564000
C	-1.214939000	0.000000000	-2.138631000
C	-1.216679000	0.000000000	-3.529912000
C	0.000107000	0.000000000	-4.214248000
C	1.216895000	0.000000000	-3.529818000
H	2.153619000	0.000000000	-1.593983000
H	2.151073000	0.000000000	-4.080474000
H	-2.150926000	0.000000000	-4.080400000
H	-2.153239000	0.000000000	-1.593899000
Cl	0.000480000	0.000000000	-5.966331000

3ClBCN, symmetry C1, imaginary frequency=0, HF = -784.0857

C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.162999000
C	1.214734000	0.000000000	-2.130314000
C	-0.005307000	-0.000164000	-1.434871000
C	-1.223394000	-0.000573000	-2.133575000
C	-1.213940000	-0.000851000	-3.525908000
C	-0.008525000	-0.000740000	-4.229731000
C	1.194362000	-0.000329000	-3.521618000
H	-2.158224000	-0.000678000	-1.583546000
H	-2.152079000	-0.001168000	-4.072531000
H	0.002648000	-0.000972000	-5.314315000
H	2.154535000	0.000326000	-1.590598000
Cl	2.712790000	-0.000189000	-4.399741000

2ClBCN, symmetry C1, imaginary frequency=0, HF = -784.0834

C	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	1.162891000
H	2.204968000	0.000000000	-1.457059000
H	2.368762000	-0.003525000	-3.938176000
H	-1.932917000	-0.008273000	-4.200309000
C	1.309429000	-0.001819000	-2.069738000
C	-1.109906000	-0.004426000	-2.219736000
C	0.056041000	-0.002103000	-1.431013000
H	0.288233000	-0.007705000	-5.309714000
Cl	-2.684451000	-0.004745000	-1.463223000
C	0.228827000	-0.006143000	-4.225296000
C	1.395514000	-0.003822000	-3.457553000
C	-1.023039000	-0.006475000	-3.610187000

4MeOBCN, symmetry C1, imaginary frequency=0, HF = -439.0168

C	0.000000000	0.000000000	0.000000000
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N	0.000000000	0.000000000	1.164016000
C	1.211250000	0.000000000	-2.140496000
C	0.001230000	0.000154000	-1.431487000
C	-1.213325000	0.000663000	-2.145904000
C	-1.210072000	0.001031000	-3.530257000
C	0.005750000	0.000933000	-4.235611000
C	1.219600000	0.000434000	-3.533128000
H	2.150781000	-0.000395000	-1.597108000
H	2.167805000	0.000365000	-4.057380000
H	-2.136564000	0.001429000	-4.094944000
H	-2.153361000	0.000766000	-1.603575000
O	-0.102264000	0.001366000	-5.588569000
C	1.087504000	0.001230000	-6.367577000
H	1.691778000	-0.894568000	-6.176264000
H	1.692304000	0.896569000	-6.175777000
H	0.759736000	0.001611000	-7.408011000

3OQZ, symmetry C1, imaginary frequency=0, HF = -1704.56705

C	67.952999000000	7.996000000000	28.781000000000
O	67.605000000000	8.904000000000	28.010000000000
C	69.366000000000	7.961000000000	29.374000000000
N	67.144001000000	7.008998000000	29.152001000000
C	65.770999000000	6.948000000000	28.684999000000
C	65.018002000000	8.232997000000	29.005001000000
O	64.292002000000	8.760002000000	28.160999000000
C	65.038000000000	5.750000000000	29.289000000000
C	63.719999000000	5.444001000000	28.591000000000
C	62.980000000000	4.253999000000	29.210001000000
C	61.708000000000	3.957000000000	28.421998000000
N	66.339969000000	11.028020000000	26.642989000000
C	65.845010000000	10.801984000000	25.293999000000

N	60.793000000000	2.982001000000	29.097001000000
C	64.912991000000	11.166052000000	29.810002000000
N	65.201995000000	8.744003000000	30.215996000000
C	64.500007000000	9.942000000000	30.614008000000
C	64.606000000000	10.064999000000	32.146001000000
C	64.237002000000	11.497001000000	32.545000000000
C	63.654000000000	14.147000000000	33.171000000000
C	65.221000000000	12.454000000000	32.557001000000
C	62.945000000000	11.875000000000	32.852998000000
C	64.939000000000	13.761000000000	32.868001000000
C	62.650000000000	13.195000000000	33.171999000000
O	64.124998000000	11.997997000000	29.556994000000
N	66.192049000000	11.250915000000	29.462980000000
C	66.686947000000	12.348043000000	28.638019000000
C	66.198026000000	12.220987000000	27.210011000000
O	65.702002000000	13.183001000000	26.626999000000
C	68.211001000000	12.401001000000	28.656005000000
C	68.762999000000	13.186004000000	29.825000000000
C	70.267000000000	13.130998000000	29.906000000000
O	70.936000000000	13.365996000000	28.866999000000
O	70.781000000000	12.851004000000	31.012001000000
H	66.735152000000	10.419750000000	29.463232000000
H	66.261484000000	13.266814000000	29.010041000000
H	68.610645000000	11.392135000000	28.640160000000
H	68.558316000000	12.868929000000	27.744179000000
H	68.338437000000	12.846619000000	30.764380000000
H	68.499149000000	14.233837000000	29.724482000000
H	66.620225000000	10.239767000000	27.171576000000
H	64.766679000000	10.893473000000	25.251885000000
H	66.128771000000	9.802301000000	24.992245000000

H	66.278595000000	11.518314000000	24.609964000000
H	69.623253000000	6.994501000000	29.789007000000
H	69.431324000000	8.707750000000	30.158110000000
H	70.071793000000	8.227168000000	28.599596000000
H	67.507850000000	6.257874000000	29.692726000000
H	65.766822000000	6.876448000000	27.606443000000
H	64.873544000000	5.914189000000	30.351591000000
H	65.685170000000	4.877958000000	29.208563000000
H	63.076713000000	6.316967000000	28.613138000000
H	63.919865000000	5.242842000000	27.541327000000
H	62.712189000000	4.470976000000	30.240023000000
H	63.623542000000	3.375897000000	29.227242000000
H	61.142989000000	4.876528000000	28.315171000000
H	61.978169000000	3.636533000000	27.415309000000
H	61.196633000000	2.064094000000	29.080489000000
H	59.935194000000	2.927568000000	28.582480000000
H	65.787879000000	8.274428000000	30.866501000000
H	63.456164000000	9.823245000000	30.359600000000
H	63.947920000000	9.338231000000	32.605762000000
H	65.620401000000	9.857798000000	32.473575000000
H	63.436929000000	15.171534000000	33.408565000000
H	66.234170000000	12.183581000000	32.323933000000
H	62.154974000000	11.144561000000	32.848448000000
H	61.641068000000	13.477990000000	33.408103000000
C	66.012081000000	14.731228000000	32.872297000000
N	66.867619000000	15.479337000000	32.877429000000
H	71.731325000000	12.888831000000	30.931791000000
3OQY, symmetry C1, imaginary frequency=0, HF = -1832.8462			
C	20.045005000000	10.577001000000	4.421992000000
C	19.077978000000	11.696048000000	4.019010000000

O	19.323007000000	12.865002000000	4.317988000000
N	17.995925000000	11.330843000000	3.328998000000
C	16.900109000000	12.248189000000	3.021037000000
C	15.721988000000	11.893936000000	3.913973000000
O	15.354005000000	10.726999000000	4.014006000000
C	16.417006000000	12.098003000000	1.566015000000
C	15.145983000000	12.915972000000	1.329997000000
C	17.508996000000	12.486000000000	0.583995000000
C	12.916000000000	13.547070000000	5.368008000000
N	15.111986000000	12.894049000000	4.538985000000
O	13.074002000000	14.752998000000	5.305976000000
C	14.101994000000	12.636907000000	5.545010000000
C	14.709996000000	12.962023000000	6.906997000000
S	15.628001000000	11.600000000000	7.549999000000
N	11.722948000000	12.968849000000	5.282052000000
C	10.502087000000	13.766190000000	5.317971000000
C	9.857974000000	13.569951000000	6.678974000000
O	9.702013000000	12.440001000000	7.138006000000
C	9.538022000000	13.363000000000	4.199975000000
C	8.260980000000	14.200969000000	4.141035000000
C	7.322979000000	13.735031000000	3.027029000000
N	6.472053000000	12.614984000000	3.431946000000
C	6.645963000000	11.353990000000	3.046015000000
N	7.644001000000	11.034000000000	2.232001000000
N	5.816005000000	10.410999000000	3.472006000000
N	9.506985000000	14.669990000000	7.334998000000
C	8.851010000000	14.606006000000	8.634005000000
H	9.745527000000	15.559077000000	6.961545000000
H	9.528096000000	14.237036000000	9.393574000000
H	8.522072000000	15.600392000000	8.901524000000

H	7.996857000000	13.946210000000	8.584949000000
H	19.822079000000	9.627987000000	3.949483000000
H	19.998363000000	10.459053000000	5.498287000000
H	21.047627000000	10.887885000000	4.161742000000
H	17.765553000000	10.362997000000	3.279591000000
H	17.260273000000	13.248128000000	3.208116000000
H	16.172459000000	11.049214000000	1.422500000000
H	15.294915000000	13.963537000000	1.580152000000
H	14.302949000000	12.547718000000	1.901001000000
H	14.867579000000	12.871839000000	0.282202000000
H	17.182662000000	12.312456000000	-0.436701000000
H	18.413616000000	11.912471000000	0.745532000000
H	17.762659000000	13.538925000000	0.674834000000
H	11.621542000000	12.002206000000	5.505158000000
H	10.807350000000	14.791302000000	5.181921000000
H	10.074095000000	13.451622000000	3.259201000000
H	9.284626000000	12.316597000000	4.341362000000
H	8.528284000000	15.241251000000	3.964336000000
H	7.726686000000	14.168387000000	5.084227000000
H	6.673901000000	14.557503000000	2.743910000000
H	7.863294000000	13.461846000000	2.133226000000
H	5.767841000000	12.786357000000	4.109138000000
H	8.529890000000	11.467592000000	2.353241000000
H	7.698129000000	10.049079000000	2.086218000000
H	5.053438000000	10.822499000000	3.976871000000
H	15.448875000000	13.827602000000	4.457056000000
H	13.822467000000	11.599118000000	5.460715000000
H	15.333079000000	13.838969000000	6.817753000000
H	13.925821000000	13.198221000000	7.616060000000
N	16.510578000000	12.755407000000	9.994168000000

C 16.155249000000 12.305182000000 9.012291000000

3OXA, symmetry C1, imaginary frequency=0, HF = -1794.4675

C 10.608000000000 -0.951000000000 10.222000000000

C 9.947000000000 -1.961000000000 9.287000000000

O 10.412000000000 -2.191000000000 8.169000000000

N 8.844000000000 -2.544000000000 9.750000000000

C 8.146000000000 -3.606000000000 9.027000000000

C 6.634000000000 -3.476000000000 9.195000000000

O 6.150000000000 -3.255000000000 10.313000000000

C 8.564000000000 -4.985000000000 9.592000000000

O 9.696000000000 -5.472000000000 8.870000000000

C 7.423000000000 -5.980000000000 9.486000000000

C 3.945000000000 -4.807000000000 7.296000000000

N 5.890000000000 -3.600000000000 8.100000000000

O 4.376000000000 -4.964000000000 6.161000000000

C 4.435000000000 -3.666000000000 8.163000000000

C 3.773000000000 -2.373000000000 7.684000000000

S 2.021000000000 -2.455000000000 7.996000000000

N 3.033000000000 -5.610000000000 7.840000000000

C 2.415000000000 -6.706000000000 7.097000000000

C 0.914000000000 -6.642000000000 7.252000000000

O 0.406000000000 -6.662000000000 8.371000000000

C 2.934000000000 -8.057000000000 7.590000000000

C 4.426000000000 -8.230000000000 7.358000000000

C 5.117000000000 -8.945000000000 8.492000000000

O 4.987000000000 -8.565000000000 9.657000000000

N 5.872000000000 -9.983000000000 8.157000000000

N 0.199000000000 -6.547000000000 6.130000000000

C -1.260000000000 -6.442000000000 6.176000000000

H	0.658910000000	-6.282222000000	5.289295000000
H	-1.572606000000	-5.466672000000	6.527971000000
H	-1.650463000000	-7.196605000000	6.841216000000
H	-1.645539000000	-6.604019000000	5.179079000000
H	10.715776000000	-0.014416000000	9.690244000000
H	11.600897000000	-1.308906000000	10.466589000000
H	10.051819000000	-0.786767000000	11.136439000000
H	8.494806000000	-2.325531000000	10.656318000000
H	8.432338000000	-3.543489000000	7.988989000000
H	8.823078000000	-4.853055000000	10.636785000000
H	10.314348000000	-4.764633000000	8.731790000000
H	6.601283000000	-5.720317000000	10.133995000000
H	7.773947000000	-6.960083000000	9.787551000000
H	7.075825000000	-6.070713000000	8.463052000000
H	6.309969000000	-3.816766000000	7.222032000000
H	4.179437000000	-3.826289000000	9.198177000000
H	3.971101000000	-2.184649000000	6.639093000000
H	4.147108000000	-1.540192000000	8.264112000000
H	2.715606000000	-5.467127000000	8.773931000000
H	2.694230000000	-6.559263000000	6.064866000000
H	2.381443000000	-8.849890000000	7.094117000000
H	2.713403000000	-8.130037000000	8.646592000000
H	4.608564000000	-8.727004000000	6.410270000000
H	4.913029000000	-7.266546000000	7.289097000000
H	6.394075000000	-10.442152000000	8.869852000000
H	6.018266000000	-10.257501000000	7.214642000000
N	0.991290000000	-3.331714000000	5.495398000000
C	1.425758000000	-2.980575000000	6.486029000000
3OQY, symmetry C1, imaginary frequency=0, HF = -1704.5698			
C	-0.036318000000	0.002510000000	-0.074345000000

N	-0.090445000000	0.012453000000	1.060657000000
C	0.020536000000	-0.002105000000	-1.517691000000
C	0.116160000000	-3.732990000000	-10.112080000000
C	1.443130000000	-3.137200000000	-9.669150000000
O	2.209810000000	-3.775230000000	-8.949940000000
N	1.715439000000	-1.913699000000	-10.101391000000
C	2.917791000000	-1.226069000000	-9.676980000000
C	2.922451000000	-1.003811000000	-8.163488000000
O	3.958139000000	-1.155894000000	-7.514369000000
C	3.070150000000	0.101800000000	-10.418021000000
C	4.310351000000	0.869230000000	-10.029069000000
C	4.475119000000	2.102001000000	-10.901042000000
C	5.648751000000	2.947320000000	-10.448628000000
N	6.049459000000	3.923560000000	-11.489051000000
C	2.057267000000	-1.795505000000	-5.418308000000
N	1.768086000000	-0.649487000000	-7.593903000000
O	2.733400000000	-1.796860000000	-4.443060000000
C	1.681581000000	-0.506274000000	-6.146149000000
C	0.243560000000	-0.051937000000	-5.822760000000
C	0.097289000000	-0.010724000000	-4.299580000000
C	-0.348071000000	-1.133340000000	-3.607920000000
C	0.512671000000	1.106659000000	-3.585539000000
C	-0.385291000000	-1.124688000000	-2.225610000000
C	0.472771000000	1.117188000000	-2.198190000000
N	1.537188000000	-2.903417000000	-5.937336000000
C	1.798725000000	-4.210043000000	-5.358128000000
C	3.282808000000	-4.555261000000	-5.448317000000
O	3.869647000000	-5.063150000000	-4.486614000000
C	0.932666000000	-5.279998000000	-6.034308000000
C	-0.572842000000	-5.090019000000	-5.798619000000

C	-1.380329000000	-6.352180000000	-6.058052000000
O	-0.799269000000	-7.458770000000	-5.979572000000
O	-2.601390000000	-6.248360000000	-6.340508000000
N	3.898138000000	-4.252747000000	-6.589863000000
C	5.322202000000	-4.529264000000	-6.745605000000
H	-0.327599000000	-3.207514000000	-10.948815000000
H	-0.578635000000	-3.704495000000	-9.279322000000
H	0.273158000000	-4.769358000000	-10.376842000000
H	1.113733000000	-1.482480000000	-10.765572000000
H	3.774592000000	-1.854385000000	-9.871285000000
H	2.187851000000	0.716801000000	-10.245427000000
H	3.094311000000	-0.114063000000	-11.484052000000
H	4.264592000000	1.158258000000	-8.984334000000
H	5.185330000000	0.233376000000	-10.127169000000
H	3.565726000000	2.700971000000	-10.895265000000
H	4.636801000000	1.792493000000	-11.931605000000
H	5.416208000000	3.489974000000	-9.539686000000
H	6.510937000000	2.324472000000	-10.237757000000
H	5.280255000000	4.522925000000	-11.720197000000
H	6.310705000000	3.441858000000	-12.327429000000
H	0.953571000000	-0.532705000000	-8.150376000000
H	2.389680000000	0.237208000000	-5.812164000000
H	0.071778000000	0.927193000000	-6.255747000000
H	-0.473827000000	-0.745655000000	-6.248295000000
H	-0.663890000000	-2.009525000000	-4.142019000000
H	0.870105000000	1.976322000000	-4.107778000000
H	-0.728990000000	-1.990985000000	-1.691409000000
H	0.792663000000	1.985575000000	-1.653345000000
H	1.233904000000	-2.884778000000	-6.881774000000
H	1.580573000000	-4.167579000000	-4.301450000000

H	1.150080000000	-5.317150000000	-7.095868000000
H	1.237532000000	-6.231927000000	-5.618965000000
H	-1.014671000000	-4.314997000000	-6.407341000000
H	-0.760209000000	-4.826473000000	-4.760716000000
H	3.410220000000	-3.838214000000	-7.346367000000
H	5.886599000000	-4.042280000000	-5.962855000000
H	5.637115000000	-4.143764000000	-7.705531000000
H	5.517622000000	-5.593633000000	-6.702559000000
H	-1.432320000000	-8.154180000000	-6.142020000000

3T42, symmetry C1, imaginary frequency=0, HF = -1722.6169

Cl	-8.640003000000	-3.712998000000	7.684000000000
C	-1.799000000000	3.484000000000	12.873999000000
N	-1.109001000000	4.598000000000	13.390002000000
O	-1.486000000000	5.724000000000	13.102000000000
O	-0.099000000000	4.452000000000	14.069000000000
C	-2.881998000000	3.717000000000	12.027998000000
C	-3.589008000000	2.656995000000	11.476008000000
C	-4.765002000000	2.954007000000	10.566997000000
N	-5.310992000000	1.775991000000	9.908998000000
C	-6.328002000000	1.103006000000	10.402002000000
C	-6.870015000000	-0.087992000000	9.682998000000
C	-7.529993000000	-1.037004000000	10.446002000000
C	-8.061994000000	-2.152003000000	9.827000000000
C	-7.937999000000	-2.293000000000	8.453001000000
C	-7.299000000000	-1.352000000000	7.676999000000
C	-6.764054000000	-0.237980000000	8.298980000000
O	-6.132931000000	0.723948000000	7.589032000000
C	-5.704023000000	0.419004000000	6.278990000000
C	-4.328995000000	-0.167988000000	6.499003000000

O	-3.797006000000	-0.666013000000	5.523003000000
O	-3.777987000000	-0.123973000000	7.629993000000
O	-6.830001000000	1.428001000000	11.474000000000
C	-3.204000000000	1.359999000000	11.777000000000
C	-2.124998000000	1.117002000000	12.613996000000
C	-1.413998000000	2.180999000000	13.152999000000
H	-3.157121000000	4.730927000000	11.816402000000
H	-4.456124000000	3.652219000000	9.798028000000
H	-5.555878000000	3.414672000000	11.139450000000
H	-4.930298000000	1.512163000000	9.032396000000
H	-7.622662000000	-0.882401000000	11.501963000000
H	-8.572343000000	-2.905015000000	10.395704000000
H	-7.263736000000	-1.515893000000	6.623700000000
H	-6.321524000000	-0.244991000000	5.710970000000
H	-5.606393000000	1.355407000000	5.750194000000
H	-3.742998000000	0.531659000000	11.363196000000
H	-1.825128000000	0.114862000000	12.849899000000
H	-2.922389000000	-0.542220000000	7.560811000000
C	-0.303402000000	1.808148000000	14.003841000000
N	0.528527000000	1.370726000000	14.639928000000
3OWS, symmetry C1, imaginary frequency=0, HF = -2247.0996			
N	-19.930011000000	17.035003000000	16.392984000000
C	-20.997008000000	16.263968000000	17.019024000000
C	-21.650018000000	15.352999000000	15.996988000000
O	-22.051984000000	14.237993000000	16.303997000000
C	-22.046979000000	17.195048000000	17.627031000000
C	-23.070017000000	16.481948000000	18.467964000000
C	-22.449954000000	15.850018000000	19.691985000000
N	-22.569024000000	14.523003000000	19.808015000000
O	-21.863011000000	16.542001000000	20.526005000000

N	-21.738982000000	15.842055000000	14.772973000000
C	-22.460025000000	15.160943000000	13.711052000000
C	-21.736992000000	15.448002000000	12.393006000000
O	-21.239000000000	16.562000000000	12.187000000000
C	-23.905999000000	15.696006000000	13.627985000000
C	-24.584999000000	15.240018000000	12.344993000000
O	-24.656995000000	15.226991000000	14.756000000000
N	-21.674001000000	14.447002000000	11.513998000000
C	-21.069005000000	14.606014000000	10.202992000000
C	-21.810994000000	13.745993000000	9.210002000000
O	-22.057998000000	12.570999000000	9.454999000000
C	-19.614002000000	14.142989000000	10.241003000000
S	-18.844001000000	14.461005000000	8.681001000000
N	-22.160999000000	14.333010000000	8.073992000000
C	-22.872994000000	13.604996000000	7.036040000000
C	-22.185005000000	13.824000000000	5.706990000000
O	-22.037010000000	14.962000000000	5.260996000000
C	-24.317006000000	14.086013000000	6.981973000000
C	-24.995011000000	13.985968000000	8.328001000000
C	-25.947984000000	15.103014000000	8.563997000000
N	-27.219000000000	14.768000000000	8.751998000000
O	-25.551999000000	16.268999000000	8.583006000000
H	-22.832249000000	12.565154000000	7.318739000000
H	-24.861317000000	13.519115000000	6.232125000000
H	-24.305032000000	15.117952000000	6.655039000000
H	-24.276726000000	14.060398000000	9.127923000000
H	-25.475069000000	13.018406000000	8.441292000000
H	-21.959466000000	15.294143000000	7.903087000000
H	-27.882794000000	15.488183000000	8.931799000000
H	-27.532571000000	13.826547000000	8.748069000000

N	-21.763990000000	12.726526000000	5.067813000000
C	-21.024989000000	12.788006000000	3.821013000000
C	-21.963000000000	12.499002000000	2.662001000000
O	-22.440999000000	11.373000000000	2.508998000000
C	-19.875006000000	11.778993000000	3.821995000000
H	-20.646540000000	13.794723000000	3.733827000000
H	-22.212700000000	13.301640000000	1.970803000000
H	-19.204154000000	11.974817000000	4.647053000000
H	-20.256986000000	10.769136000000	3.907700000000
H	-19.317203000000	11.845508000000	2.893894000000
H	-21.875217000000	11.834336000000	5.494710000000
C	-18.965039000000	12.939719000000	7.919347000000
N	-19.023112000000	11.939921000000	7.380924000000
H	-19.146349000000	16.451482000000	16.171433000000
H	-19.602535000000	17.750161000000	17.012761000000
H	-20.623023000000	15.602660000000	17.795424000000
H	-22.536772000000	17.751737000000	16.834857000000
H	-21.534625000000	17.916339000000	18.254372000000
H	-23.622882000000	15.754246000000	17.887063000000
H	-23.789308000000	17.207076000000	18.833349000000
H	-22.079094000000	14.083744000000	20.555851000000
H	-22.800647000000	13.966081000000	19.015917000000
H	-22.472968000000	14.101319000000	13.922495000000
H	-23.872469000000	16.776803000000	13.668403000000
H	-25.638458000000	15.488020000000	12.399045000000
H	-24.178319000000	15.733535000000	11.471227000000
H	-24.510706000000	14.163400000000	12.223309000000
H	-24.118544000000	14.675329000000	15.309661000000
H	-21.311998000000	16.720594000000	14.564725000000
H	-21.114704000000	15.652160000000	9.944619000000

H	-19.545514000000	13.097677000000	10.502125000000
H	-19.074598000000	14.723317000000	10.977398000000
H	-22.060593000000	13.553260000000	11.725229000000
IDD743, symmetry C1, imaginary frequency=0, HF = -1362.5689			
F	-5.183629000000	7.658938000000	7.812475000000
C	-12.655001000000	1.001002000000	4.272001000000
N	-13.582998000000	-0.102001000000	4.050997000000
O	-13.604000000000	-1.051000000000	4.874000000000
O	-14.305000000000	-0.063000000000	3.085000000000
C	-11.668007000000	0.807002000000	5.246010000000
C	-10.758001000000	1.834018000000	5.478007000000
C	-9.677974000000	1.540963000000	6.495988000000
N	-8.717015000000	2.609011000000	6.706006000000
C	-8.778011000000	3.385013000000	7.783984000000
C	-7.770979000000	4.429981000000	7.890046000000
C	-8.142004000000	5.647002000000	8.402989000000
C	-7.305008000000	6.766007000000	8.373984000000
C	-6.041994000000	6.657000000000	7.770990000000
C	-5.557006000000	5.384001000000	7.396993000000
C	-6.437870000000	4.314009000000	7.405175000000
O	-6.066246000000	3.025046000000	7.174664000000
C	-4.955749000000	2.818051000000	6.298140000000
C	-5.314142000000	3.077911000000	4.833019000000
O	-4.341998000000	3.169052000000	4.074009000000
O	-6.540998000000	3.091933000000	4.523987000000
O	-9.746002000000	3.308003000000	8.583997000000
C	-10.849000000000	3.015997000000	4.762996000000
C	-11.847999000000	3.234000000000	3.785000000000
C	-12.758001000000	2.197001000000	3.516000000000
H	-11.631179000000	-0.116915000000	5.786916000000

H	-9.130420000000	0.661709000000	6.173146000000
H	-10.130500000000	1.318107000000	7.449108000000
H	-7.962056000000	2.695665000000	6.061835000000
H	-9.124282000000	5.741941000000	8.824687000000
H	-4.533518000000	5.307760000000	7.095130000000
H	-4.714847000000	1.766925000000	6.384403000000
H	-4.084083000000	3.376756000000	6.600824000000
H	-10.138954000000	3.797184000000	4.958036000000
H	-11.900714000000	4.161113000000	3.248018000000
H	-13.527685000000	2.293947000000	2.776903000000
H	-4.618262000000	3.261661000000	3.162984000000
C	-7.744660000000	8.031872000000	8.898125000000
N	-8.097369000000	9.028337000000	9.313807000000
3OR0, symmetry C1, imaginary frequency=0, HF = -1924.0557			
C	-0.481841000000	-0.276871000000	-0.759309000000
N	-0.877185000000	-0.286483000000	0.307090000000
S	0.106263000000	-0.268194000000	-2.361732000000
C	6.474562000000	-6.001858000000	1.397107000000
C	5.267766000000	-6.252175000000	0.491745000000
O	5.208290000000	-7.279110000000	-0.175851000000
N	4.301509000000	-5.342823000000	0.469593000000
C	3.008166000000	-5.671092000000	-0.141543000000
C	2.464173000000	-4.582062000000	-1.044588000000
O	1.446010000000	-4.774530000000	-1.719020000000
C	1.967151000000	-5.984958000000	0.932530000000
C	2.403047000000	-7.026500000000	1.910241000000
N	2.417441000000	-8.369050000000	1.607190000000
C	2.836851000000	-6.923360000000	3.188000000000
C	2.848520000000	-9.049670000000	2.654280000000
N	3.110770000000	-8.195980000000	3.626000000000

C	3.453874000000	-2.234245000000	-3.266514000000
N	3.140111000000	-3.439892000000	-1.040873000000
O	4.596807000000	-1.919406000000	-3.336445000000
C	2.785351000000	-2.329697000000	-1.900135000000
C	2.642761000000	-0.964530000000	-1.243438000000
C	1.871791000000	0.095420000000	-2.028191000000
N	2.706649000000	-2.494787000000	-4.330434000000
C	3.217287000000	-2.267860000000	-5.675995000000
C	2.222549000000	-1.441717000000	-6.482382000000
O	1.469513000000	-1.973110000000	-7.302595000000
C	3.499943000000	-3.582463000000	-6.387912000000
C	4.262267000000	-3.387933000000	-7.680634000000
O	5.004676000000	-2.381320000000	-7.783857000000
O	4.120566000000	-4.229780000000	-8.595741000000
N	2.217633000000	-0.138386000000	-6.242571000000
C	1.240289000000	0.730745000000	-6.880327000000
H	6.343756000000	-6.589312000000	2.299189000000
H	6.594169000000	-4.959054000000	1.668972000000
H	7.358841000000	-6.351763000000	0.884792000000
H	4.278054000000	-4.707163000000	1.238414000000
H	3.180288000000	-6.532781000000	-0.764516000000
H	1.749067000000	-5.077613000000	1.489790000000
H	1.043449000000	-6.265814000000	0.440189000000
H	2.198974000000	-8.747102000000	0.712764000000
H	2.949136000000	-6.064574000000	3.815456000000
H	2.966255000000	-10.110749000000	2.692040000000
H	4.062300000000	-3.465356000000	-0.665704000000
H	1.757247000000	-2.586800000000	-2.127439000000
H	3.622614000000	-0.537877000000	-1.039862000000
H	2.163131000000	-1.108831000000	-0.281614000000

H	1.920853000000	1.036962000000	-1.501323000000
H	2.286731000000	0.252680000000	-3.015529000000
H	1.800682000000	-2.894709000000	-4.215423000000
H	4.140900000000	-1.725772000000	-5.569631000000
H	4.125250000000	-4.196142000000	-5.745296000000
H	2.584627000000	-4.127380000000	-6.574624000000
H	2.963614000000	0.264341000000	-5.723947000000
H	1.425362000000	0.816448000000	-7.943561000000
H	1.302041000000	1.710800000000	-6.427164000000
H	0.247107000000	0.331978000000	-6.734863000000
H	4.660586000000	-3.975276000000	-9.340038000000

3OWU, symmetry C1, imaginary frequency=0, HF = -1831.6682

C	-0.839099000000	-1.123825000000	-0.956839000000
N	-1.594200000000	-1.962894000000	-0.818140000000
S	0.267923000000	0.155479000000	-1.165341000000
C	1.696019000000	-0.827159000000	-1.773150000000
C	3.985630000000	-1.064060000000	4.040630000000
C	3.854650000000	0.024910000000	3.006160000000
O	2.897750000000	0.798240000000	3.038480000000
N	4.820720000000	0.090230000000	2.079490000000
C	4.760069000000	0.979660000000	0.918830000000
C	4.207321000000	0.203906000000	-0.267186000000
O	4.585521000000	-0.950940000000	-0.449911000000
C	6.234780000000	1.305340000000	0.654160000000
C	7.058530000000	0.327830000000	1.526370000000
C	6.080160000000	-0.667210000000	2.105460000000
C	2.474950000000	1.037600000000	-3.341808000000
N	3.346771000000	0.806959000000	-1.078633000000
O	2.445059000000	2.244270000000	-3.156100000000
C	2.840589000000	0.085961000000	-2.224412000000

N	2.227552000000	0.475124000000	-4.520680000000
C	1.816599000000	1.258090000000	-5.676414000000
C	0.515344000000	0.727959000000	-6.253564000000
O	0.392210000000	-0.458940000000	-6.561519000000
C	2.899365000000	1.261202000000	-6.745866000000
C	2.357211000000	1.472318000000	-8.138402000000
C	3.406933000000	2.080451000000	-9.030394000000
N	3.869528000000	3.346053000000	-8.471097000000
C	4.499353000000	4.288228000000	-9.165002000000
N	4.741293000000	4.114199000000	-10.458919000000
N	4.883898000000	5.408261000000	-8.565241000000
N	-0.451617000000	1.628278000000	-6.386852000000
C	-1.784796000000	1.293800000000	-6.861473000000
H	4.773364000000	-0.831858000000	4.750411000000
H	4.209376000000	-2.023532000000	3.589977000000
H	3.050224000000	-1.123666000000	4.576581000000
H	4.157034000000	1.842215000000	1.155778000000
H	6.481701000000	1.204840000000	-0.395461000000
H	6.444579000000	2.330948000000	0.931085000000
H	7.538918000000	0.878775000000	2.326911000000
H	7.840913000000	-0.157868000000	0.956018000000
H	5.996106000000	-1.559572000000	1.502962000000
H	6.338203000000	-0.943507000000	3.115631000000
H	3.111267000000	1.770782000000	-0.984516000000
H	3.626009000000	-0.571572000000	-2.574056000000
H	2.058486000000	-1.456608000000	-0.977129000000
H	1.348083000000	-1.453850000000	-2.582856000000
H	2.223568000000	-0.515756000000	-4.628051000000
H	1.668183000000	2.262517000000	-5.313899000000
H	3.406356000000	0.301271000000	-6.720132000000

H	3.644137000000	1.984132000000	-6.447639000000
H	2.008440000000	0.534159000000	-8.549064000000
H	1.513107000000	2.153740000000	-8.129992000000
H	2.990456000000	2.273921000000	-10.010563000000
H	4.236207000000	1.383121000000	-9.157734000000
H	3.874569000000	3.471582000000	-7.491036000000
H	4.976680000000	3.204710000000	-10.787643000000
H	5.297231000000	4.846120000000	-10.844067000000
H	4.519863000000	5.443171000000	-7.631181000000
H	-0.315990000000	2.532071000000	-5.996621000000
H	-1.708709000000	0.620493000000	-7.701613000000
H	-2.278467000000	2.203202000000	-7.174627000000
H	-2.371344000000	0.816418000000	-6.085599000000

3OX9, symmetry C1, imaginary frequency=0, HF = -2631.8926

N	9.291999000000	11.687994000000	21.319997000000
C	8.925004000000	11.006026000000	22.568008000000
C	9.604994000000	9.645997000000	22.683997000000
O	9.831996000000	8.974998000000	21.677000000000
C	7.410005000000	10.730973000000	22.578005000000
C	6.943000000000	9.843004000000	21.396996000000
S	5.154998000000	9.561011000000	21.520996000000
C	4.736001000000	8.827995000000	19.965002000000
N	9.878006000000	9.206003000000	23.923001000000
C	10.527998000000	7.926008000000	24.169995000000
C	9.504004000000	6.922998000000	24.645005000000
O	8.742998000000	7.259001000000	25.538998000000
C	11.470003000000	8.246990000000	25.342008000000
C	10.759000000000	9.381004000000	26.112991000000
C	9.668994000000	9.951998000000	25.177003000000
C	9.275997000000	3.383999000000	24.600996000000

N	9.495999000000	5.710000000000	24.090999000000
O	10.383998000000	3.237998000000	24.121995000000
C	8.576001000000	4.712001000000	24.557002000000
C	7.315000000000	4.711000000000	23.664000000000
S	7.609000000000	4.062000000000	22.044000000000
H	10.195000000000	5.473000000000	23.276000000000
H	8.259000000000	4.966000000000	25.579000000000
H	6.983000000000	5.759000000000	23.623000000000
H	6.570000000000	4.111000000000	24.208000000000
N	8.619015000000	2.403006000000	25.210006000000
C	9.123029000000	1.049979000000	25.225979000000
C	8.067980000000	0.112009000000	24.636018000000
O	6.920000000000	0.099001000000	25.069999000000
C	9.474992000000	0.634999000000	26.641969000000
C	9.464971000000	-0.870884000000	26.866081000000
C	10.265050000000	-1.233220000000	28.109950000000
N	11.663979000000	-0.816895000000	27.983944000000
C	12.710988000000	-1.603003000000	28.232039000000
N	12.515000000000	-2.850991000000	28.637028000000
N	13.953000000000	-1.144001000000	28.075996000000
N	8.470001000000	-0.680998000000	23.648998000000
C	7.543013000000	-1.550994000000	22.961994000000
C	7.819980000000	-2.984013000000	23.395011000000
O	8.941004000000	-3.457988000000	23.292994000000
C	7.698007000000	-1.447004000000	21.435998000000
C	6.750000000000	-2.417999000000	20.734000000000
C	7.461996000000	-0.018000000000	20.970002000000
H	9.439016000000	-0.764514000000	23.436182000000
H	6.549839000000	-1.258264000000	23.263130000000
H	7.000599000000	-3.585091000000	23.786838000000

H	8.718020000000	-1.734344000000	21.195054000000
H	5.714454000000	-2.213206000000	20.994941000000
H	6.962797000000	-3.452101000000	20.983422000000
H	6.840038000000	-2.324577000000	19.656820000000
H	8.167500000000	0.671848000000	21.415998000000
H	6.458952000000	0.315143000000	21.224708000000
H	7.568597000000	0.053758000000	19.891582000000
H	8.616585000000	12.403479000000	21.060098000000
H	9.350289000000	11.005087000000	20.567278000000
H	10.209742000000	12.128813000000	21.384009000000
H	9.185639000000	11.680164000000	23.363119000000
H	6.872249000000	11.674472000000	22.565832000000
H	7.168771000000	10.246474000000	23.516823000000
H	7.136676000000	10.343004000000	20.451381000000
H	7.460045000000	8.899712000000	21.376164000000
H	3.678806000000	8.600897000000	20.012894000000
H	5.282410000000	7.911818000000	19.791101000000
H	4.900009000000	9.509864000000	19.139009000000
H	11.043139000000	7.606147000000	23.278890000000
H	11.664082000000	7.382072000000	25.961114000000
H	12.418017000000	8.589604000000	24.944473000000
H	11.464272000000	10.151748000000	26.398152000000
H	10.302403000000	9.002630000000	27.015283000000
H	8.678451000000	9.774783000000	25.563174000000
H	9.818054000000	11.011059000000	25.027650000000
C	7.535277000000	5.487207000000	21.112237000000
N	7.484533000000	6.413611000000	20.454278000000
H	7.737116000000	2.553554000000	25.647896000000
H	10.006394000000	1.038627000000	24.609074000000
H	8.744609000000	1.074898000000	27.317747000000

H	10.433555000000	1.061897000000	26.900216000000
H	8.438426000000	-1.214337000000	26.965980000000
H	9.905373000000	-1.398975000000	26.023404000000
H	10.198345000000	-2.305772000000	28.261462000000
H	9.792684000000	-0.773073000000	28.985822000000
H	11.715832000000	-0.496132000000	27.008407000000
H	12.881824000000	-3.609882000000	28.042638000000
H	12.876435000000	-3.088303000000	29.561546000000
H	14.516817000000	-1.641989000000	27.387037000000
H	14.550507000000	-1.103698000000	28.905941000000

1LFD-I18, symmetry C1, imaginary frequency=0, HF = -2633.3317

N	81.878247000000	76.741134000000	43.336664000000
C	81.838250000000	78.198146000000	43.284672000000
C	80.844236000000	78.721120000000	42.260686000000
O	80.528253000000	78.049135000000	41.275663000000
C	83.230254000000	78.783127000000	43.021668000000
S	84.010250000000	78.284136000000	41.480666000000
N	80.322269000000	79.910152000000	42.536644000000
C	79.357214000000	80.571097000000	41.672655000000
C	80.105254000000	81.407155000000	40.643682000000
O	80.836249000000	82.322133000000	41.006669000000
C	78.438270000000	81.503146000000	42.498677000000
C	77.613244000000	80.679137000000	43.491666000000
N	79.947241000000	81.073129000000	39.366664000000
C	80.613267000000	81.827142000000	38.309675000000
C	79.609254000000	82.528130000000	37.401669000000
O	78.473247000000	82.070137000000	37.236671000000
C	81.549243000000	80.940128000000	37.432662000000
C	80.736251000000	79.922129000000	36.626672000000
C	82.582250000000	80.236138000000	38.312670000000

C	81.514248000000	79.255136000000	35.495665000000
N	80.035249000000	83.652140000000	36.835666000000
C	79.203219000000	84.431142000000	35.928650000000
C	79.595247000000	84.125135000000	34.483664000000
O	80.754247000000	84.287133000000	34.101665000000
C	79.372349000000	85.925126000000	36.212706000000
C	78.915205000000	86.349127000000	37.596662000000
C	79.227220000000	87.813028000000	37.852692000000
N	78.730305000000	88.262281000000	39.150531000000
C	78.746146000000	89.525114000000	39.568741000000
N	79.240245000000	90.481131000000	38.791667000000
N	78.246314000000	89.831129000000	40.761694000000
N	78.637249000000	83.649138000000	33.695668000000
C	78.894251000000	83.324135000000	32.294668000000
C	78.120254000000	84.254140000000	31.369661000000
O	76.899251000000	84.406129000000	31.495672000000
C	78.510255000000	81.865135000000	31.959667000000
C	78.790250000000	81.572134000000	30.490668000000
C	79.281246000000	80.902136000000	32.838670000000
H	78.654030000000	84.759849000000	30.568182000000
H	77.444806000000	81.755707000000	32.142889000000
H	79.838075000000	81.736741000000	30.252382000000
H	78.563982000000	80.536206000000	30.262507000000
H	78.191951000000	82.181149000000	29.820324000000
H	80.351693000000	81.016255000000	32.694292000000
H	77.705794000000	83.555297000000	34.034793000000
H	79.066242000000	81.052713000000	33.888833000000
H	79.022906000000	79.875979000000	32.595603000000
H	79.952637000000	83.463964000000	32.143192000000
S	76.515573000000	81.680939000000	44.559890000000

C	75.415185000000	82.254765000000	43.388177000000
N	74.674225000000	82.644267000000	42.618164000000
H	77.780592000000	82.032807000000	41.818871000000
H	80.974007000000	76.386278000000	43.581779000000
H	82.082743000000	76.385967000000	42.422102000000
H	81.533955000000	78.551540000000	44.266022000000
H	83.888663000000	78.425030000000	43.801476000000
H	83.209772000000	79.864390000000	43.084131000000
H	83.234935000000	78.952207000000	40.645745000000
H	79.039489000000	82.243865000000	43.010671000000
H	78.247973000000	80.163435000000	44.199524000000
H	80.761823000000	80.477980000000	43.227308000000
H	77.009426000000	79.937245000000	42.987603000000
H	78.779536000000	79.794979000000	41.193722000000
H	79.268404000000	80.394933000000	39.103952000000
H	82.059002000000	81.611384000000	36.745190000000
H	79.862394000000	80.390889000000	36.197341000000
H	80.364210000000	79.154290000000	37.301368000000
H	83.097391000000	80.938271000000	38.961382000000
H	82.095578000000	79.490775000000	38.928956000000
H	83.332162000000	79.736075000000	37.710605000000
H	82.349057000000	78.665339000000	35.859179000000
H	80.868238000000	78.588194000000	34.934126000000
H	81.907114000000	79.994009000000	34.803234000000
H	81.212336000000	82.567417000000	38.814886000000
H	80.991894000000	83.916513000000	36.917120000000
H	78.903400000000	87.618415000000	39.888047000000
H	78.640018000000	90.833746000000	38.052814000000
H	80.114534000000	90.255461000000	38.376032000000
H	77.259812000000	90.065325000000	40.782855000000

H	78.738763000000	90.598780000000	41.160411000000
H	78.811648000000	86.476552000000	35.461105000000
H	80.416245000000	86.182670000000	36.056498000000
H	79.400319000000	85.739984000000	38.354189000000
H	77.846565000000	86.190832000000	37.706741000000
H	78.185431000000	84.126661000000	36.117504000000
H	78.769921000000	88.416900000000	37.077042000000
H	80.311397000000	87.960919000000	37.760015000000
H	79.804570000000	89.453529000000	40.067395000000

1LFD-R18, symmetry C1, imaginary frequency=0, HF = -2429.3558

N	81.894000000000	76.724000000000	43.349000000000
C	81.853999000000	78.180999000000	43.297000000000
C	80.860008000000	78.704002000000	42.273008000000
O	80.544001000000	78.032001000000	41.287999000000
C	83.245999000000	78.766000000000	43.033999000000
S	84.026000000000	78.267000000000	41.493000000000
N	80.337991000000	79.892986000000	42.548984000000
C	79.373001000000	80.554013000000	41.685011000000
C	80.120995000000	81.389994000000	40.655999000000
O	80.851999000000	82.305001000000	41.019000000000
C	78.454002000000	81.486004000000	42.511000000000
C	77.629001000000	80.661999000000	43.504000000000
C	77.555999000000	82.299998000000	41.597000000000
C	76.942999000000	81.488000000000	44.579000000000
N	79.963009000000	81.056008000000	39.379004000000
C	80.628996000000	81.809994000000	38.321995000000
C	79.625006000000	82.511000000000	37.414002000000
O	78.489000000000	82.053000000000	37.249000000000
C	81.564999000000	80.922999000000	37.445000000000

C	80.752000000000	79.905000000000	36.638999000000
C	82.598000000000	80.219000000000	38.325000000000
C	81.530000000000	79.238000000000	35.508000000000
N	80.050988000000	83.634996000000	36.848000000000
C	79.219005000000	84.414007000000	35.940998000000
C	79.610996000000	84.108000000000	34.496004000000
O	80.770001000000	84.269994000000	34.114002000000
C	79.388002000000	85.908000000000	36.224999000000
N	78.653005000000	83.632001000000	33.707995000000
C	78.910063000000	83.307026000000	32.306960000000
C	78.135930000000	84.236937000000	31.382082000000
O	76.915001000000	84.389042000000	31.507955000000
C	78.526016000000	81.848005000000	31.971992000000
C	78.806005000000	81.554998000000	30.503001000000
C	79.296984000000	80.884995000000	32.851009000000
H	78.670142000000	84.740008000000	30.579637000000
H	77.460476000000	81.739016000000	32.154958000000
H	79.853840000000	81.718769000000	30.264548000000
H	78.579132000000	80.519130000000	30.275957000000
H	78.207748000000	82.163681000000	29.832463000000
H	80.367461000000	80.999010000000	32.707173000000
H	77.720840000000	83.535685000000	34.045488000000
H	79.081459000000	81.033333000000	33.901515000000
H	79.039040000000	79.859141000000	32.607174000000
H	79.968306000000	83.446431000000	32.154827000000
S	78.946010000000	86.254096000000	37.969383000000
C	78.839646000000	87.953689000000	37.864309000000
N	78.762807000000	89.087203000000	37.814976000000
H	80.990094000000	76.372185000000	43.600214000000
H	82.087866000000	76.370440000000	42.431477000000

H	81.550452000000	78.534280000000	44.278541000000
H	83.905620000000	78.408874000000	43.813315000000
H	83.223269000000	79.847122000000	43.094639000000
H	83.238409000000	78.919756000000	40.657630000000
H	79.101363000000	82.168280000000	43.055832000000
H	78.269109000000	79.934096000000	43.991393000000
H	80.732776000000	80.439013000000	43.281728000000
H	76.885759000000	80.088021000000	42.953797000000
H	76.889540000000	82.932155000000	42.170654000000
H	78.122035000000	82.953660000000	40.944361000000
H	78.791952000000	79.778853000000	41.206958000000
H	76.939888000000	81.655679000000	40.974768000000
H	76.426511000000	80.843578000000	45.283486000000
H	77.663393000000	82.075798000000	45.141568000000
H	76.207029000000	82.172278000000	44.171921000000
H	79.296312000000	80.364700000000	39.120867000000
H	82.076655000000	81.592684000000	36.756515000000
H	79.877689000000	80.372628000000	36.208747000000
H	80.380040000000	79.137483000000	37.313666000000
H	83.112794000000	80.920879000000	38.973869000000
H	82.110958000000	79.474348000000	38.941445000000
H	83.347474000000	79.719276000000	37.722203000000
H	82.364548000000	78.648372000000	35.871870000000
H	80.884166000000	78.570766000000	34.946573000000
H	81.923533000000	79.976528000000	34.815372000000
H	81.226936000000	82.550946000000	38.828408000000
H	81.013610000000	83.884619000000	36.912459000000
H	78.731406000000	86.480170000000	35.584490000000
H	80.406573000000	86.217110000000	36.041316000000
H	78.200372000000	84.114772000000	36.131845000000

1LFD-S33, symmetry C1, imaginary frequency=0, HF = -3705.7516

C	72.263000000000	90.677000000000	22.171000000000
O	71.517000000000	90.994001000000	21.239000000000
C	73.770000000000	90.915999000000	22.085000000000
N	71.828000000000	90.093000000000	23.286000000000
C	70.418000000000	89.777999000000	23.492999000000
C	69.816000000000	90.355000000000	24.771000000000
O	68.763000000000	89.905000000000	25.222000000000
C	70.201000000000	88.257000000000	23.449000000000
C	70.989000000000	87.506000000000	24.521000000000
N	71.676000000000	88.237000000000	25.396000000000
O	70.969000000000	86.276000000000	24.559000000000
N	70.495000000000	91.336000000000	25.359000000000
C	69.996000000000	91.956000000000	26.575000000000
C	70.533000000000	91.394000000000	27.880000000000
O	70.421000000000	92.033000000000	28.922000000000
N	71.105000000000	90.197000000000	27.834000000000
C	71.654000000000	89.578000000000	29.031000000000
C	73.125000000000	89.927000000000	29.215000000000
O	73.911000000000	89.826000000000	28.273000000000
C	71.498000000000	88.057000000000	28.967000000000
C	72.146000000000	87.356000000000	30.149000000000
N	71.466000000000	87.367000000000	31.290000000000
O	73.252000000000	86.828000000000	30.041000000000
N	73.491000000000	90.321000000000	30.433000000000
C	74.878000000000	90.659000000000	30.746000000000
C	75.632000000000	89.388000000000	31.118000000000
O	76.752000000000	89.159000000000	30.659000000000
C	74.945000000000	91.678000000000	31.884000000000
C	74.355000000000	93.025000000000	31.512000000000

S	75.053000000000	93.639000000000	29.956000000000
C	76.677000000000	94.181000000000	30.492000000000
N	75.002000000000	88.568000000000	31.952000000000
C	75.571000000000	87.296000000000	32.388000000000
C	74.501000000000	86.477000000000	33.092000000000
O	73.420000000000	86.980000000000	33.414000000000
C	76.774000000000	87.496000000000	33.333000000000
C	76.449000000000	88.147000000000	34.670000000000
C	75.816999000000	87.429000000000	35.688000000000
C	76.756001000000	89.491000000000	34.909000000000
C	75.493001000000	88.030000000000	36.904000000000
C	76.435999000000	90.103000000000	36.122000000000
C	75.803000000000	89.366000000000	37.113000000000
N	74.803000000000	85.202000000000	33.295000000000
C	73.920000000000	84.291000000000	33.998000000000
C	74.837000000000	83.424000000000	34.849000000000
O	75.804000000000	82.853000000000	34.349000000000
C	73.113000000000	83.433000000000	33.025000000000
C	72.082000000000	84.203000000000	32.215000000000
C	71.184000000000	83.254000000000	31.442000000000
C	70.138000000000	84.006000000000	30.638000000000
N	69.151000000000	83.092000000000	29.982000000000
N	74.565000000000	83.388000000000	36.147000000000
C	75.372000000000	82.619000000000	37.083000000000
C	75.045000000000	81.130000000000	37.125000000000
O	73.880000000000	80.736000000000	37.101000000000
C	75.226000000000	83.198000000000	38.493000000000
N	76.090000000000	80.312000000000	37.185000000000
C	75.949000000000	78.862000000000	37.284000000000
O	75.478239000000	89.954896000000	38.310022000000

S	76.014712000000	84.841604000000	38.596291000000
C	75.945047000000	85.041795000000	40.289024000000
N	75.907397000000	85.185607000000	41.416286000000
H	74.163557000000	90.339184000000	21.257119000000
H	74.300795000000	90.653835000000	22.992254000000
H	73.933273000000	91.963083000000	21.864690000000
H	76.998373000000	80.678321000000	37.015251000000
H	75.194658000000	78.623303000000	38.018273000000
H	76.897866000000	78.447691000000	37.594212000000
H	75.660039000000	78.430747000000	36.333669000000
H	76.396526000000	82.738168000000	36.758213000000
H	75.718897000000	82.546506000000	39.200245000000
H	74.183946000000	83.270773000000	38.772115000000
H	73.663723000000	83.680663000000	36.453609000000
H	75.788247000000	90.848979000000	38.325396000000
H	73.265212000000	84.887114000000	34.615766000000
H	72.608327000000	82.659001000000	33.602551000000
H	73.807384000000	82.918747000000	32.368534000000
H	72.579983000000	84.875829000000	31.530677000000
H	71.473197000000	84.806328000000	32.883061000000
H	70.681579000000	82.578753000000	32.132716000000
H	71.777643000000	82.632794000000	30.774257000000
H	70.601422000000	84.600453000000	29.860203000000
H	75.651541000000	84.818051000000	32.940084000000
H	69.579257000000	84.681815000000	31.276121000000
H	69.623223000000	82.496640000000	29.328303000000
H	68.734003000000	82.495311000000	30.671053000000
H	75.904771000000	86.753387000000	31.512456000000
H	77.499721000000	88.089283000000	32.795961000000
H	77.237759000000	86.528416000000	33.505238000000

H	75.588975000000	86.389351000000	35.557104000000
H	77.254220000000	90.062684000000	34.146422000000
H	75.001329000000	87.481625000000	37.682709000000
H	76.685353000000	91.137273000000	36.287817000000
H	68.920132000000	91.866379000000	26.594989000000
H	70.243428000000	93.007944000000	26.570525000000
H	71.303247000000	91.707958000000	24.915218000000
H	74.058871000000	88.729891000000	32.215766000000
H	75.344009000000	91.031755000000	29.854137000000
H	75.988318000000	91.794693000000	32.155984000000
H	74.445862000000	91.286346000000	32.768292000000
H	74.514855000000	93.751158000000	32.299883000000
H	73.287051000000	92.960497000000	31.344445000000
H	77.149776000000	94.654253000000	29.641123000000
H	72.779344000000	90.534164000000	31.094962000000
H	76.604433000000	94.908850000000	31.291095000000
H	77.303655000000	93.356647000000	30.807935000000
H	71.086080000000	89.959811000000	29.867986000000
H	71.993138000000	87.670755000000	28.092246000000
H	70.958572000000	89.616965000000	27.044952000000
H	70.442741000000	87.811163000000	28.905822000000
H	71.918249000000	87.063153000000	32.128239000000
H	70.567150000000	87.785653000000	31.357531000000
H	69.888648000000	90.232217000000	22.667822000000
H	70.513200000000	87.870637000000	22.487360000000
H	69.156836000000	88.018041000000	23.587166000000
H	72.288041000000	87.734822000000	26.003390000000
H	71.804947000000	89.214568000000	25.377702000000
H	72.521987000000	89.602642000000	23.798117000000

1LFD-N27, symmetry C1, imaginary frequency=0, HF = -3651.8785

C	72.257650000000	90.732248000000	22.148218000000
O	71.511702000000	91.049237000000	21.216231000000
C	73.764697000000	90.971269000000	22.062248000000
N	71.822766000000	90.148204000000	23.263306000000
C	70.412694000000	89.833317000000	23.470200000000
C	69.810582000000	90.410240000000	24.748376000000
O	68.757697000000	89.960256000000	25.199238000000
C	70.195686000000	88.312252000000	23.426234000000
C	70.983704000000	87.561257000000	24.498238000000
N	70.490007000000	91.391440000000	25.336092000000
C	69.990484000000	92.011049000000	26.552252000000
C	70.527666000000	91.449245000000	27.857339000000
O	70.415764000000	92.088286000000	28.899227000000
N	71.099745000000	90.252174000000	27.811087000000
C	71.648648000000	89.633346000000	29.008318000000
C	73.119704000000	89.982246000000	29.192218000000
O	73.905699000000	89.881253000000	28.250240000000
C	71.492662000000	88.112259000000	28.944260000000
C	72.140718000000	87.411247000000	30.126225000000
N	71.460701000000	87.422258000000	31.267241000000
O	73.246698000000	86.883252000000	30.018239000000
N	73.485700000000	90.376244000000	30.410243000000
C	74.872699000000	90.714253000000	30.723239000000
C	75.626700000000	89.443254000000	31.095239000000
O	76.746699000000	89.214254000000	30.636240000000
C	74.939700000000	91.733253000000	31.861239000000
C	74.349698000000	93.080253000000	31.489241000000
S	75.047698000000	93.694254000000	29.933239000000
C	76.671699000000	94.236253000000	30.469240000000

N	74.996698000000	88.623253000000	31.929239000000
C	75.565699000000	87.351253000000	32.365239000000
C	74.495699000000	86.532254000000	33.069239000000
O	73.414699000000	87.035254000000	33.391239000000
C	76.768699000000	87.551253000000	33.310240000000
C	76.443699000000	88.202254000000	34.647240000000
C	75.811698000000	87.484254000000	35.665240000000
O	75.582197000000	84.620956000000	38.496319000000
C	76.750700000000	89.546254000000	34.886240000000
C	75.487700000000	88.085254000000	36.881240000000
C	76.430698000000	90.158254000000	36.099240000000
C	75.797699000000	89.421254000000	37.090240000000
N	74.797699000000	85.257254000000	33.272240000000
C	73.914699000000	84.346254000000	33.975240000000
C	74.831699000000	83.479253000000	34.826240000000
O	75.798699000000	82.908254000000	34.326240000000
C	73.107699000000	83.488254000000	33.002240000000
C	72.076699000000	84.258254000000	32.192240000000
C	71.178699000000	83.309254000000	31.419240000000
C	70.132699000000	84.061254000000	30.615240000000
N	69.145699000000	83.147254000000	29.959240000000
N	74.559698000000	83.443254000000	36.124240000000
C	75.366699000000	82.674253000000	37.060239000000
C	75.039699000000	81.185254000000	37.102240000000
O	73.874699000000	80.791254000000	37.078240000000
C	75.220699000000	83.253254000000	38.470240000000
N	76.084699000000	80.367254000000	37.162240000000
C	75.943699000000	78.917254000000	37.261240000000
O	75.472938000000	90.010150000000	38.287261000000
H	74.188340000000	90.241729000000	21.381375000000

H	74.266793000000	90.892025000000	23.019319000000
H	73.930341000000	91.954169000000	21.643488000000
H	76.990401000000	80.735631000000	36.983922000000
H	75.192806000000	78.678538000000	37.999270000000
H	76.893811000000	78.501243000000	37.566267000000
H	75.649073000000	78.485094000000	36.312800000000
H	76.393888000000	82.809772000000	36.750402000000
H	75.855793000000	82.676431000000	39.136293000000
H	74.192962000000	83.122785000000	38.800131000000
H	73.721956000000	83.858018000000	36.462710000000
H	75.770190000000	90.908623000000	38.294355000000
H	73.258801000000	84.941633000000	34.592309000000
H	72.603654000000	82.715240000000	33.581168000000
H	73.802019000000	82.973853000000	32.345830000000
H	72.574358000000	84.931482000000	31.508036000000
H	71.467594000000	84.861303000000	32.860329000000
H	70.676427000000	82.633512000000	32.109484000000
H	71.772498000000	82.688394000000	30.751163000000
H	70.597971000000	84.655369000000	29.837908000000
H	75.653688000000	84.875497000000	32.933145000000
H	69.573419000000	84.738088000000	31.251564000000
H	69.626695000000	82.519745000000	29.342649000000
H	68.699609000000	82.580797000000	30.655724000000
H	75.899089000000	86.808833000000	31.489599000000
H	77.495034000000	88.144033000000	32.773344000000
H	77.231489000000	86.583473000000	33.483246000000
H	75.595404000000	86.440971000000	35.545486000000
H	77.249602000000	90.118092000000	34.124072000000
H	75.016552000000	87.520428000000	37.663100000000
H	76.680526000000	91.192565000000	36.265406000000

H	68.915766000000	91.909734000000	26.577960000000
H	70.228699000000	93.065069000000	26.545239000000
H	71.283088000000	91.779450000000	24.879676000000
H	74.055065000000	88.786227000000	32.197482000000
H	75.338273000000	91.087045000000	29.831217000000
H	75.982996000000	91.849672000000	32.133294000000
H	74.440774000000	91.341513000000	32.745580000000
H	74.509464000000	93.806616000000	32.276985000000
H	73.281772000000	93.015508000000	31.321532000000
H	77.144629000000	94.709319000000	29.618343000000
H	72.775066000000	90.579394000000	31.076319000000
H	76.599032000000	94.964174000000	31.268276000000
H	77.298109000000	93.411808000000	30.785342000000
H	71.072349000000	90.024970000000	29.832451000000
H	71.986717000000	87.734482000000	28.059446000000
H	71.388559000000	89.888457000000	26.934160000000
H	70.435788000000	87.872597000000	28.886615000000
H	71.915775000000	87.121236000000	32.105572000000
H	70.563602000000	87.844336000000	31.336199000000
H	69.882922000000	90.278475000000	22.640837000000
H	70.498648000000	87.969509000000	22.443796000000
H	69.142750000000	88.103369000000	23.546060000000
H	72.496576000000	89.840390000000	23.926612000000
S	70.756010000000	85.745926000000	24.427561000000
C	71.631801000000	85.411866000000	23.000972000000
N	72.214623000000	85.177505000000	22.052703000000
H	75.542471000000	84.932816000000	39.389782000000
H	72.046984000000	87.749516000000	24.457265000000
H	70.623375000000	87.814917000000	25.487769000000

1LFD-Y31, symmetry C1, imaginary frequency=0, HF = -3705.7518

C	72.263000000000	90.677000000000	22.171000000000
O	71.517000000000	90.994001000000	21.239000000000
C	73.770000000000	90.915999000000	22.085000000000
H	74.163502000000	90.339365000000	21.256966000000
H	74.300816000000	90.653595000000	22.992175000000
H	73.933298000000	91.963142000000	21.864968000000
N	71.828000000000	90.093000000000	23.286000000000
C	70.418000000000	89.777999000000	23.492999000000
C	69.816000000000	90.355000000000	24.771000000000
O	68.763000000000	89.905000000000	25.222000000000
C	70.201000000000	88.257000000000	23.449000000000
C	70.989000000000	87.506000000000	24.521000000000
N	71.676000000000	88.237000000000	25.396000000000
O	70.969000000000	86.276000000000	24.559000000000
H	69.888647000000	90.232226000000	22.667838000000
H	70.513166000000	87.870612000000	22.487358000000
H	69.156838000000	88.018073000000	23.587242000000
H	72.287042000000	87.734907000000	26.004407000000
H	71.802904000000	89.214877000000	25.379543000000
H	72.521889000000	89.603558000000	23.799129000000
N	70.495000000000	91.336000000000	25.359000000000
C	69.996000000000	91.956000000000	26.575000000000
C	70.533000000000	91.394000000000	27.880000000000
O	70.421000000000	92.033000000000	28.922000000000
H	68.920128000000	91.866460000000	26.595022000000
H	70.243452000000	93.007932000000	26.570573000000
H	71.303065000000	91.708170000000	24.915088000000
N	71.105000000000	90.197000000000	27.834000000000
C	71.654000000000	89.578000000000	29.031000000000
C	73.125000000000	89.927000000000	29.215000000000

O	73.911000000000	89.826000000000	28.273000000000
C	71.498000000000	88.057000000000	28.967000000000
C	72.146000000000	87.356000000000	30.149000000000
N	71.466000000000	87.367000000000	31.290000000000
O	73.252000000000	86.828000000000	30.041000000000
H	71.086181000000	89.959662000000	29.868135000000
H	71.993049000000	87.670593000000	28.092259000000
H	70.955774000000	89.616067000000	27.046118000000
H	70.442747000000	87.811250000000	28.906053000000
H	71.915271000000	87.058070000000	32.127794000000
H	70.566206000000	87.783728000000	31.357619000000
N	73.491000000000	90.321000000000	30.433000000000
C	74.878000000000	90.659000000000	30.746000000000
C	75.632000000000	89.388000000000	31.118000000000
O	76.752000000000	89.159000000000	30.659000000000
C	74.945000000000	91.678000000000	31.884000000000
C	74.355000000000	93.025000000000	31.512000000000
S	75.053000000000	93.639000000000	29.956000000000
C	76.677000000000	94.181000000000	30.492000000000
H	75.344493000000	91.031696000000	29.854312000000
H	75.988409000000	91.795294000000	32.155840000000
H	74.444862000000	91.287181000000	32.768052000000
H	74.514685000000	93.750627000000	32.300210000000
H	73.287035000000	92.960569000000	31.345075000000
H	77.149399000000	94.655368000000	29.641522000000
H	72.778938000000	90.540165000000	31.092812000000
H	76.604308000000	94.907885000000	31.291916000000
H	77.304195000000	93.356622000000	30.806959000000
N	75.002000000000	88.568000000000	31.952000000000
C	75.571000000000	87.296000000000	32.388000000000

C	74.501000000000	86.477000000000	33.092000000000
O	73.420000000000	86.980000000000	33.414000000000
C	76.774000000000	87.496000000000	33.333000000000
C	76.449000000000	88.147000000000	34.670000000000
C	75.816999000000	87.429000000000	35.688000000000
C	76.756001000000	89.491000000000	34.909000000000
C	75.493001000000	88.030000000000	36.904000000000
C	76.435999000000	90.103000000000	36.122000000000
C	75.803000000000	89.366000000000	37.113000000000
S	75.447726000000	90.126144000000	38.698073000000
H	75.909975000000	86.753276000000	31.514962000000
H	77.500900000000	88.089856000000	32.798488000000
H	77.234894000000	86.529467000000	33.513657000000
H	75.600509000000	86.386208000000	35.566325000000
H	77.253436000000	90.063672000000	34.147172000000
H	75.022948000000	87.449671000000	37.674608000000
H	76.685410000000	91.134038000000	36.288791000000
H	74.053946000000	88.722267000000	32.203539000000
N	74.803000000000	85.202000000000	33.295000000000
C	73.920000000000	84.291000000000	33.998000000000
C	74.837000000000	83.424000000000	34.849000000000
O	75.804000000000	82.853000000000	34.349000000000
C	73.113000000000	83.433000000000	33.025000000000
C	72.082000000000	84.203000000000	32.215000000000
C	71.184000000000	83.254000000000	31.442000000000
C	70.138000000000	84.006000000000	30.638000000000
N	69.151000000000	83.092000000000	29.982000000000
H	73.264074000000	84.886595000000	34.614797000000
H	72.609040000000	82.660304000000	33.604269000000
H	73.807162000000	82.918023000000	32.368845000000

H	72.579581000000	84.875781000000	31.530226000000
H	71.472958000000	84.806062000000	32.883155000000
H	70.681757000000	82.578840000000	32.132852000000
H	71.777695000000	82.632759000000	30.774298000000
H	70.601402000000	84.600414000000	29.860080000000
H	75.652098000000	84.815607000000	32.943738000000
H	69.579160000000	84.681830000000	31.276020000000
H	69.624134000000	82.494604000000	29.330780000000
H	68.732761000000	82.497045000000	30.671832000000
N	74.565000000000	83.388000000000	36.147000000000
C	75.372000000000	82.619000000000	37.083000000000
C	75.045000000000	81.130000000000	37.125000000000
O	73.880000000000	80.736000000000	37.101000000000
C	75.226000000000	83.198000000000	38.493000000000
O	75.601000000000	84.562000000000	38.522000000000
H	76.399025000000	82.754618000000	36.772957000000
H	75.853610000000	82.615407000000	39.160875000000
H	74.196201000000	83.077559000000	38.819660000000
H	75.569205000000	84.866983000000	39.418285000000
H	73.714587000000	83.781057000000	36.480507000000
N	76.090000000000	80.312000000000	37.185000000000
C	75.949000000000	78.862000000000	37.284000000000
H	76.995863000000	80.680074000000	37.006925000000
H	75.197512000000	78.623331000000	38.021395000000
H	76.898875000000	78.446166000000	37.589889000000
H	75.655212000000	78.429908000000	36.335319000000
C	73.871507000000	90.731016000000	38.414852000000
N	72.824216000000	91.150389000000	38.270724000000
1LFD-N29, symmetry C1, imaginary frequency=0, HF = -3651.8413			
C	72.263000000000	90.677000000000	22.171000000000

O	71.517000000000	90.994001000000	21.239000000000
C	73.770000000000	90.915999000000	22.085000000000
N	71.828000000000	90.093000000000	23.286000000000
C	70.418000000000	89.777999000000	23.492999000000
C	69.816000000000	90.355000000000	24.771000000000
O	68.763000000000	89.905000000000	25.222000000000
C	70.201000000000	88.257000000000	23.449000000000
C	70.989000000000	87.506000000000	24.521000000000
N	71.676000000000	88.237000000000	25.396000000000
O	70.969000000000	86.276000000000	24.559000000000
N	70.495000000000	91.335999000000	25.359000000000
C	69.996001000000	91.956000000000	26.575000000000
C	70.532997000000	91.393999000000	27.880001000000
O	70.420999000000	92.033000000000	28.922000000000
N	71.104988000000	90.197002000000	27.834006000000
C	71.653994000000	89.578001000000	29.030986000000
C	73.125000000000	89.927000000000	29.214985000000
O	73.911000000000	89.826001000000	28.273000000000
C	71.498058000000	88.057026000000	28.967019000000
C	72.145961000000	87.355971000000	30.149004000000
N	73.491002000000	90.321000000000	30.432998000000
C	74.877997000000	90.658998000000	30.745999000000
C	75.631985000000	89.388015000000	31.118002000000
O	76.752003000000	89.159003000000	30.659005000000
C	74.944999000000	91.678000000000	31.884000000000
C	74.355000000000	93.025000000000	31.512000000000
S	75.053000000000	93.639000000000	29.956000000000
C	76.677000000000	94.181000000000	30.492000000000
N	75.002031000000	88.567991000000	31.951994000000
C	75.570985000000	87.295990000000	32.387999000000

C	74.501000000000	86.477003000000	33.092000000000
O	73.420001000000	86.980000000000	33.414002000000
C	76.774000000000	87.495997000000	33.333001000000
C	76.449000000000	88.147003000000	34.669998000000
C	75.816999000000	87.429000000000	35.688000000000
C	76.756001000000	89.491000000000	34.909000000000
C	75.493001000000	88.030000000000	36.904000000000
C	76.436001000000	90.102999000000	36.122001000000
C	75.803000000000	89.366000000000	37.113001000000
N	74.802998000000	85.202001000000	33.295001000000
C	73.920001000000	84.290999000000	33.998001000000
C	74.837000000000	83.424000000000	34.848999000000
O	75.804000000000	82.853000000000	34.349000000000
C	73.113000000000	83.433001000000	33.025000000000
C	72.082000000000	84.202999000000	32.215000000000
C	71.184000000000	83.254001000000	31.442000000000
C	70.138000000000	84.005999000000	30.638000000000
N	69.151000000000	83.092000000000	29.982000000000
N	74.565000000000	83.388000000000	36.147000000000
C	75.372000000000	82.619000000000	37.083000000000
C	75.045000000000	81.130000000000	37.125000000000
O	73.880000000000	80.736000000000	37.101000000000
C	75.226000000000	83.198000000000	38.493000000000
N	76.090000000000	80.312000000000	37.185000000000
C	75.949000000000	78.862000000000	37.284000000000
O	75.478238000000	89.954897000000	38.310021000000
H	74.164086000000	90.337290000000	21.258675000000
H	74.300234000000	90.655662000000	22.993121000000
H	73.933293000000	91.962615000000	21.862469000000
H	76.995334000000	80.680181000000	37.004612000000

H	75.195874000000	78.623545000000	38.019798000000
H	76.898175000000	78.446006000000	37.592110000000
H	75.657179000000	78.429389000000	36.334879000000
H	76.400162000000	82.757195000000	36.778797000000
H	75.845040000000	82.614741000000	39.169026000000
H	74.193350000000	83.101079000000	38.820069000000
H	73.724126000000	83.797705000000	36.483949000000
H	75.771225000000	90.854815000000	38.316507000000
H	73.263194000000	84.886664000000	34.613711000000
H	72.606666000000	82.661556000000	33.603490000000
H	73.805468000000	82.916261000000	32.368536000000
H	72.589634000000	84.872652000000	31.538005000000
H	71.479842000000	84.820196000000	32.876517000000
H	70.681181000000	82.583334000000	32.136253000000
H	71.775373000000	82.631763000000	30.774348000000
H	70.594795000000	84.589110000000	29.850109000000
H	75.660885000000	84.818470000000	32.962862000000
H	69.580563000000	84.683856000000	31.277106000000
H	69.617881000000	82.534913000000	29.291927000000
H	68.768927000000	82.461688000000	30.661168000000
H	75.923883000000	86.762528000000	31.517875000000
H	77.500992000000	88.088298000000	32.796378000000
H	77.235588000000	86.527807000000	33.505870000000
H	75.599787000000	86.385993000000	35.568098000000
H	77.257365000000	90.062849000000	34.148200000000
H	75.019277000000	87.466060000000	37.684816000000
H	76.686688000000	91.136957000000	36.288478000000
H	68.920124000000	91.866036000000	26.594888000000
H	70.242919000000	93.008114000000	26.570472000000
H	71.303930000000	91.706756000000	24.915634000000

H	74.134838000000	88.814371000000	32.371606000000
H	75.347472000000	91.032648000000	29.855993000000
H	75.988100000000	91.795054000000	32.156215000000
H	74.445181000000	91.289291000000	32.769602000000
H	74.516105000000	93.749876000000	32.300664000000
H	73.286696000000	92.962507000000	31.345913000000
H	77.149657000000	94.653469000000	29.640670000000
H	72.774754000000	90.584090000000	31.072407000000
H	76.604237000000	94.909658000000	31.290268000000
H	77.303950000000	93.357132000000	30.808687000000
H	71.085215000000	89.947460000000	29.873350000000
H	71.904195000000	87.682712000000	28.042759000000
H	70.941421000000	89.610824000000	27.052218000000
H	70.436510000000	87.834864000000	28.951067000000
H	69.888451000000	90.232399000000	22.668060000000
H	70.513345000000	87.870819000000	22.487343000000
H	69.156777000000	88.018268000000	23.586824000000
H	72.292605000000	87.729567000000	25.994063000000
H	71.805282000000	89.214581000000	25.380494000000
H	72.520907000000	89.598846000000	23.796009000000
C	73.224689000000	85.373387000000	28.642974000000
N	72.902144000000	84.541144000000	27.937181000000
S	73.762030000000	86.595829000000	29.703948000000
O	75.629195000000	84.535792000000	38.458260000000
H	75.600393000000	84.903261000000	39.330897000000
H	71.514224000000	86.575253000000	30.535267000000
H	72.376315000000	88.005911000000	30.975530000000
1LFD-K32, symmetry C1, imaginary frequency=0, HF = -3647.5206			
C	72.263000000000	90.677000000000	22.171000000000
O	71.517000000000	90.994001000000	21.239000000000

C	73.770000000000	90.915999000000	22.085000000000
N	71.828000000000	90.093000000000	23.286000000000
C	70.418000000000	89.777999000000	23.492999000000
C	69.816000000000	90.355000000000	24.771000000000
O	68.763000000000	89.905000000000	25.222000000000
C	70.201000000000	88.257000000000	23.449000000000
C	70.989000000000	87.506000000000	24.521000000000
N	71.676000000000	88.237000000000	25.396000000000
O	70.969000000000	86.276000000000	24.559000000000
N	70.495000000000	91.336000000000	25.359000000000
C	69.996000000000	91.956000000000	26.575000000000
C	70.533000000000	91.394000000000	27.880000000000
O	70.421000000000	92.033000000000	28.922000000000
N	71.105000000000	90.197000000000	27.834000000000
C	71.654000000000	89.578000000000	29.031000000000
C	73.125000000000	89.927000000000	29.215000000000
O	73.911000000000	89.826000000000	28.273000000000
C	71.498000000000	88.057000000000	28.967000000000
C	72.146000000000	87.356000000000	30.149000000000
N	71.466000000000	87.367000000000	31.290000000000
O	73.252000000000	86.828000000000	30.041000000000
N	73.491000000000	90.321000000000	30.433000000000
C	74.878000000000	90.659000000000	30.746000000000
C	75.632000000000	89.388000000000	31.118000000000
O	76.752000000000	89.159000000000	30.659000000000
C	74.945000000000	91.678000000000	31.884000000000
C	74.355000000000	93.025000000000	31.512000000000
S	75.053000000000	93.639000000000	29.956000000000
C	76.677000000000	94.181000000000	30.492000000000
N	75.002000000000	88.568000000000	31.952000000000

C	75.571000000000	87.296000000000	32.388000000000
C	74.501000000000	86.477000000000	33.092000000000
O	73.420000000000	86.980000000000	33.414000000000
C	76.774000000000	87.496000000000	33.333000000000
O	75.791193000000	84.492830000000	38.570095000000
C	76.449000000000	88.147000000000	34.670000000000
C	75.816999000000	87.429000000000	35.688000000000
C	76.756001000000	89.491000000000	34.909000000000
C	75.493001000000	88.030000000000	36.904000000000
C	76.435999000000	90.103000000000	36.122000000000
C	75.803000000000	89.366000000000	37.113000000000
N	74.803000000000	85.202000000000	33.295000000000
C	73.920000000000	84.291000000000	33.998000000000
C	74.837000000000	83.424000000000	34.849000000000
O	75.804000000000	82.853000000000	34.349000000000
C	73.113000000000	83.433000000000	33.025000000000
C	72.082000000000	84.203000000000	32.215000000000
N	74.565000000000	83.388000000000	36.147000000000
C	75.372000000000	82.619000000000	37.083000000000
C	75.045000000000	81.130000000000	37.125000000000
O	73.880000000000	80.736000000000	37.101000000000
C	75.226000000000	83.198000000000	38.493000000000
N	76.090000000000	80.312000000000	37.185000000000
C	75.949000000000	78.862000000000	37.284000000000
O	75.478239000000	89.954896000000	38.310022000000
H	74.163575000000	90.338807000000	21.257375000000
H	74.300627000000	90.653949000000	22.992367000000
H	73.933370000000	91.963018000000	21.864370000000
H	76.997356000000	80.681209000000	37.017082000000
H	75.198065000000	78.622620000000	38.021746000000

H	76.899153000000	78.446293000000	37.588986000000
H	75.654870000000	78.430426000000	36.335243000000
H	76.400307000000	82.755151000000	36.778342000000
H	75.728806000000	82.527378000000	39.183819000000
H	74.173213000000	83.214748000000	38.764079000000
H	73.711086000000	83.774212000000	36.479940000000
H	75.773406000000	90.854107000000	38.316896000000
H	73.264937000000	84.886118000000	34.616331000000
H	72.610361000000	82.658136000000	33.600975000000
H	73.807463000000	82.925930000000	32.364506000000
H	72.553241000000	84.883981000000	31.526607000000
H	71.404397000000	84.744050000000	32.858523000000
H	75.663994000000	84.822613000000	32.965083000000
H	75.904189000000	86.752730000000	31.512559000000
H	77.498966000000	88.089153000000	32.794865000000
H	77.238700000000	86.528849000000	33.505699000000
H	75.603407000000	86.384904000000	35.569238000000
H	77.254524000000	90.062877000000	34.146724000000
H	75.024703000000	87.465396000000	37.687901000000
H	76.685691000000	91.137254000000	36.287992000000
H	68.920153000000	91.866041000000	26.594822000000
H	70.243288000000	93.008007000000	26.570497000000
H	71.304852000000	91.706031000000	24.916663000000
H	74.057579000000	88.729537000000	32.211158000000
H	75.344208000000	91.031381000000	29.854075000000
H	75.988253000000	91.794771000000	32.156396000000
H	74.445484000000	91.286373000000	32.768107000000
H	74.514717000000	93.751218000000	32.299902000000
H	73.287149000000	92.960180000000	31.344134000000
H	77.149849000000	94.654044000000	29.641031000000

H	72.778784000000	90.532594000000	31.094900000000
H	76.604628000000	94.909024000000	31.291011000000
H	77.303662000000	93.356679000000	30.808084000000
H	71.086228000000	89.958488000000	29.868642000000
H	71.994678000000	87.670304000000	28.093346000000
H	70.945345000000	89.612394000000	27.050640000000
H	70.444624000000	87.804576000000	28.906832000000
H	71.916979000000	87.076590000000	32.132325000000
H	70.533052000000	87.706731000000	31.336420000000
H	69.888539000000	90.232356000000	22.668005000000
H	70.512759000000	87.870777000000	22.487164000000
H	69.156895000000	88.018202000000	23.587828000000
H	72.279698000000	87.734096000000	26.010912000000
H	71.797517000000	89.215590000000	25.385849000000
H	72.521105000000	89.604077000000	23.800895000000
S	71.092346000000	83.006586000000	31.234101000000
C	70.026843000000	84.113827000000	30.492001000000
N	69.311487000000	84.854428000000	30.008343000000
H	75.708680000000	84.813794000000	39.457444000000
1LFD-N54, symmetry C1, imaginary frequency=0, HF = -2459.0988			
N	73.431134000000	75.462328000000	27.906028000000
C	72.042132000000	75.281329000000	28.332022000000
C	71.511135000000	76.547327000000	29.002029000000
O	70.412136000000	77.009333000000	28.693027000000
C	71.926135000000	74.108333000000	29.311029000000
C	72.113135000000	72.752330000000	28.641026000000
O	72.270131000000	72.695330000000	27.401028000000
O	72.096134000000	71.734332000000	29.367027000000
N	72.308135000000	77.095330000000	29.918029000000
C	71.960129000000	78.310331000000	30.651028000000

C	71.669131000000	79.462330000000	29.686026000000
O	70.764133000000	80.265329000000	29.924027000000
C	73.094138000000	78.671324000000	31.620026000000
C	72.930139000000	79.987330000000	32.364033000000
C	71.660127000000	80.049327000000	33.213024000000
C	71.695138000000	79.101323000000	34.394027000000
N	70.561133000000	79.374335000000	35.333029000000
N	72.414140000000	79.506323000000	28.581026000000
C	72.232135000000	80.533329000000	27.559033000000
C	71.340126000000	80.053333000000	26.408024000000
O	71.277129000000	80.688330000000	25.353029000000
C	73.584134000000	81.001331000000	27.019025000000
C	74.279132000000	81.988329000000	27.902030000000
C	74.072133000000	83.313327000000	28.093028000000
N	75.338130000000	81.646326000000	28.715030000000
C	75.755132000000	82.717333000000	29.368028000000
N	75.004131000000	83.741327000000	29.009027000000
N	70.658130000000	78.929313000000	26.625046000000
C	69.751132000000	78.342334000000	25.642059000000
C	70.405138000000	78.000349000000	24.308024000000
O	69.985137000000	78.486334000000	23.255028000000
C	68.544090000000	79.255299000000	25.418959000000
C	67.756175000000	79.493347000000	26.689051000000
N	71.442134000000	77.169325000000	24.368031000000
C	72.167128000000	76.721339000000	23.183029000000
C	72.148139000000	75.193331000000	23.199031000000
O	73.180134000000	74.535327000000	23.043029000000
C	73.608143000000	77.245325000000	23.208014000000
C	73.803128000000	78.765330000000	23.256030000000
C	75.278134000000	79.091325000000	23.387032000000

C	73.219139000000	79.415332000000	22.014026000000
H	71.607694000000	77.070667000000	22.327926000000
H	71.188899000000	74.707339000000	23.367196000000
H	74.125462000000	76.847944000000	22.340740000000
H	74.101760000000	76.791242000000	24.065065000000
H	73.283054000000	79.166844000000	24.119233000000
H	71.776627000000	76.891809000000	25.262537000000
H	75.838958000000	78.728859000000	22.529127000000
H	75.434067000000	80.163951000000	23.451120000000
H	75.715926000000	78.642330000000	24.275396000000
H	72.145047000000	79.293716000000	21.958338000000
H	73.417587000000	80.483200000000	22.006687000000
H	73.662223000000	78.995229000000	21.112901000000
H	72.206681000000	70.957400000000	28.823271000000
S	66.285779000000	78.416705000000	26.953234000000
C	66.973112000000	76.856816000000	27.042641000000
N	67.382408000000	75.795975000000	27.091861000000
H	68.362447000000	79.458036000000	27.581741000000
H	67.284889000000	80.468601000000	26.666322000000
H	73.744376000000	74.614643000000	27.471313000000
H	73.495863000000	76.176088000000	27.204569000000
H	71.366022000000	75.091379000000	27.508015000000
H	70.942199000000	74.105489000000	29.772196000000
H	72.648497000000	74.198104000000	30.116208000000
H	71.034541000000	78.141776000000	31.178882000000
H	74.024417000000	78.707046000000	31.055601000000
H	73.198304000000	77.849760000000	32.322975000000
H	72.939362000000	80.808601000000	31.655942000000
H	73.799591000000	80.121842000000	33.001683000000
H	73.217675000000	76.700551000000	30.024997000000

H	70.778562000000	79.882253000000	32.606199000000
H	71.566889000000	81.061500000000	33.600660000000
H	72.617337000000	79.211951000000	34.954328000000
H	71.621499000000	78.062302000000	34.094164000000
H	69.690564000000	79.267584000000	34.847322000000
H	70.604915000000	80.327924000000	35.638258000000
H	69.432262000000	77.406481000000	26.082155000000
H	67.910577000000	78.842443000000	24.646580000000
H	68.910286000000	80.198901000000	25.043301000000
H	70.675983000000	78.490987000000	27.516639000000
H	71.710598000000	81.358501000000	28.020034000000
H	73.407449000000	81.447394000000	26.050580000000
H	74.242493000000	80.152689000000	26.864775000000
H	73.368802000000	83.998657000000	27.668052000000
H	76.563933000000	82.760851000000	30.064904000000
H	75.088694000000	84.678852000000	29.330366000000
H	73.199745000000	78.901966000000	28.502518000000

C₆₀, HF=-131.9069122

C	3.356821000000	-0.806068000000	1.175626000000
C	2.445279000000	-1.595085000000	2.017690000000
C	1.897046000000	-2.684773000000	1.232257000000
C	2.440031000000	-2.574077000000	-0.108432000000
C	3.353234000000	-1.422868000000	-0.163935000000
C	3.349724000000	-0.620310000000	-1.298501000000
C	3.349526000000	0.847978000000	-1.163040000000
C	3.352818000000	1.429374000000	0.099206000000
C	3.356587000000	0.577930000000	1.303291000000
C	2.444981000000	1.199413000000	2.275504000000
C	1.620246000000	0.441222000000	3.077178000000

C	1.620426000000	-0.996610000000	2.944590000000
C	0.252794000000	-1.457435000000	3.155509000000
C	-0.250470000000	-2.500542000000	2.429286000000
C	0.598530000000	-3.123165000000	1.437069000000
C	-0.255310000000	-3.470742000000	0.322123000000
C	0.243137000000	-3.345508000000	-0.944563000000
C	1.610630000000	-2.887986000000	-1.162637000000
C	1.607355000000	-2.054269000000	-2.341470000000
C	2.433579000000	-0.953622000000	-2.399321000000
C	1.885427000000	0.272183000000	-2.948366000000
C	2.433349000000	1.376954000000	-2.184312000000
C	1.606902000000	2.448279000000	-1.925978000000
C	1.610088000000	3.052353000000	-0.614547000000
C	2.439500000000	2.550883000000	0.364398000000
C	1.896541000000	2.414327000000	1.702702000000
C	0.597955000000	2.807661000000	1.984174000000
C	-0.250835000000	2.013611000000	2.845451000000
C	0.252545000000	0.855362000000	3.368714000000
C	-0.597168000000	-0.315598000000	3.419071000000
C	-1.903118000000	-0.273743000000	2.963540000000
C	-2.449360000000	-1.386153000000	2.200744000000
C	-1.627037000000	-2.467604000000	1.938466000000
C	-1.629911000000	-3.073882000000	0.621235000000
C	-2.454805000000	-2.568606000000	-0.368000000000
C	-1.914294000000	-2.426859000000	-1.711620000000
C	-0.609887000000	-2.802381000000	-1.980571000000
C	0.237936000000	-2.004469000000	-2.840911000000
C	-0.265544000000	-0.853214000000	-3.379395000000
C	0.585215000000	0.316051000000	-3.425635000000
C	-0.265683000000	1.456845000000	-3.165923000000

C	0.237493000000	2.490359000000	-2.425989000000
C	-0.610454000000	3.117395000000	-1.434268000000
C	0.242495000000	3.462143000000	-0.316441000000
C	-0.256046000000	3.353527000000	0.951751000000
C	-1.630787000000	2.908548000000	1.173208000000
C	-1.627182000000	2.070706000000	2.356711000000
C	-2.448781000000	0.959185000000	2.416317000000
C	-3.337652000000	0.618772000000	1.297877000000
C	-3.337953000000	-0.846638000000	1.162939000000
C	-3.340495000000	-1.428090000000	-0.100063000000
C	-3.344145000000	-0.578479000000	-1.301671000000
C	-2.460875000000	-1.209108000000	-2.291608000000
C	-1.640482000000	-0.442434000000	-3.100357000000
C	-1.640311000000	1.001587000000	-2.966616000000
C	-2.460268000000	1.606938000000	-2.030877000000
C	-1.914777000000	2.698785000000	-1.238462000000
C	-2.456179000000	2.593098000000	0.108281000000
C	-3.341403000000	1.422011000000	0.162929000000
C	-3.343807000000	0.806068000000	-1.173630000000
C	0.326099000000	0.001098000000	0.000465000000
N	1.429727000000	0.000038000000	-0.000385000000
C	-1.030031000000	-0.000076000000	-0.000365000000
H	-1.316170000000	0.828836000000	0.566747000000
H	-1.313712000000	0.076110000000	-1.002613000000
H	-1.313629000000	-0.906723000000	0.433755000000
C ₈₀ , HF=-3161.0352842			
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C	-0.144906000000	-2.303031000000	-3.271222000000
C	-1.342359000000	-1.589851000000	-3.476960000000
C	1.093371000000	-1.641819000000	-3.539533000000

C	1.025069000000	-3.609440000000	-1.571318000000
C	3.076602000000	-2.644017000000	-0.619605000000
C	2.248278000000	-2.879342000000	-1.769610000000
C	2.265199000000	-1.929273000000	-2.769887000000
C	1.118580000000	-0.276283000000	-3.842298000000
C	-0.069410000000	0.462752000000	-3.965128000000
C	-1.311926000000	-0.233648000000	-3.828446000000
C	-0.042692000000	1.821902000000	-3.577362000000
C	2.357749000000	0.301544000000	-3.283621000000
C	3.188909000000	1.947707000000	-1.737241000000
C	2.378844000000	1.652476000000	-2.805063000000
C	1.161302000000	2.427273000000	-2.991446000000
C	3.886957000000	-1.423996000000	-0.483835000000
C	3.851146000000	-0.427415000000	-1.470166000000
C	3.050579000000	-0.693577000000	-2.642946000000
C	3.941417000000	0.918561000000	-1.052041000000
C	-1.168876000000	2.444122000000	-3.035167000000
C	-2.385355000000	1.717757000000	-2.804211000000
C	-2.457640000000	0.403566000000	-3.253392000000
C	-3.155744000000	2.079095000000	-1.649253000000
C	-0.704892000000	3.416753000000	-2.092179000000
C	-0.642895000000	4.011630000000	0.245690000000
C	-1.405524000000	3.677180000000	-0.939204000000
C	-2.672585000000	3.017785000000	-0.746614000000
C	2.771388000000	2.928677000000	-0.748632000000
C	1.521839000000	3.629078000000	-0.894193000000
C	0.763807000000	3.382065000000	-2.102504000000
C	0.819874000000	3.994079000000	0.232129000000
C	-3.917794000000	1.076749000000	-0.908697000000
C	-3.922595000000	-0.272536000000	-1.308016000000

C	-3.203705000000	-0.606714000000	-2.514915000000
C	-3.965247000000	-1.259511000000	-0.294410000000
C	-3.890940000000	1.434764000000	0.462565000000
C	-3.051969000000	0.743577000000	2.638710000000
C	-3.842747000000	0.444234000000	1.470779000000
C	-3.922000000000	-0.904498000000	1.076102000000
C	-1.062355000000	3.614699000000	1.487083000000
C	-2.301812000000	2.873014000000	1.677921000000
C	-3.118903000000	2.648536000000	0.583695000000
C	-2.321380000000	1.917341000000	2.742202000000
C	-3.254105000000	-2.505606000000	-0.447191000000
C	-2.498897000000	-2.764338000000	-1.576086000000
C	-2.527761000000	-1.812773000000	-2.645901000000
C	-1.287208000000	-3.560650000000	-1.436453000000
C	-2.772894000000	-2.900240000000	0.863552000000
C	-0.765556000000	-3.387396000000	2.125633000000
C	-1.527242000000	-3.613357000000	1.003017000000
C	-0.832900000000	-3.979154000000	-0.213485000000
C	-2.322578000000	-0.299283000000	3.346690000000
C	-2.337664000000	-1.616846000000	2.907096000000
C	-3.175959000000	-1.942685000000	1.786319000000
C	-1.143743000000	-2.394824000000	3.086305000000
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C	1.393358000000	-3.693233000000	0.833198000000
C	0.627641000000	-4.026483000000	-0.262620000000
C	2.664640000000	-3.047408000000	0.634577000000
C	1.179232000000	-2.479066000000	2.942290000000
C	2.485318000000	-0.407472000000	3.182827000000
C	2.421815000000	-1.757978000000	2.704835000000
C	3.169829000000	-2.087324000000	1.603261000000

C	-1.128067000000	0.286103000000	3.875785000000
C	1.299281000000	0.222850000000	3.793130000000
C	0.085435000000	-0.464075000000	3.963133000000
C	0.031852000000	-1.824146000000	3.580269000000
C	0.120204000000	3.333272000000	2.302565000000
C	1.321366000000	1.587742000000	3.488387000000
C	0.103699000000	2.303290000000	3.271742000000
C	-1.112372000000	1.641203000000	3.523498000000
C	3.222280000000	2.508145000000	0.487336000000
C	2.472869000000	1.825781000000	2.672063000000
C	2.453413000000	2.776315000000	1.671313000000
C	1.255288000000	3.559694000000	1.524013000000
C	3.937280000000	-1.090885000000	0.885858000000
C	3.196678000000	0.557330000000	2.513898000000
C	3.933591000000	0.258073000000	1.307184000000
C	3.972781000000	1.253734000000	0.318914000000
C	0.350013000000	0.006676000000	0.002630000000
N	1.477386000000	0.025319000000	0.016000000000
C	-1.084234000000	-0.021518000000	-0.021782000000
H	-1.426633000000	-0.784424000000	0.646304000000
H	-1.457253000000	0.932878000000	0.287603000000
H	-1.405834000000	-0.236782000000	-1.019379000000
C ₁₄₀ , HF=-131.9069122			
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C	-3.633044000000	0.466173000000	4.055914000000
C	-4.127361000000	-3.473326000000	1.043033000000
C	-1.089476000000	4.593611000000	2.776600000000
C	-1.619094000000	0.304281000000	5.153289000000
C	-1.129811000000	4.870796000000	-2.194309000000

C	1.152710000000	4.864429000000	2.211197000000
C	-3.653260000000	0.940263000000	-3.933213000000
C	0.328985000000	3.941104000000	-3.696624000000
C	0.958904000000	-4.869583000000	-2.276487000000
C	-0.982436000000	-4.864263000000	2.289765000000
C	3.342483000000	-0.937018000000	-4.200238000000
C	-0.610202000000	-3.941147000000	-3.665999000000
C	5.192898000000	1.798057000000	-0.472597000000
C	2.547643000000	1.197447000000	-4.636719000000
C	3.928534000000	-0.466736000000	3.768752000000
C	4.195901000000	3.475153000000	0.729641000000
C	1.297218000000	-4.594835000000	2.683548000000
C	2.004534000000	-0.305390000000	5.014554000000
C	-4.560953000000	-0.933901000000	-2.645904000000
C	-4.260987000000	-2.317692000000	-2.270001000000
C	-4.671975000000	-1.383606000000	2.270005000000
C	-3.785195000000	-1.855272000000	3.307636000000
C	-2.145569000000	2.468790000000	4.192298000000
C	-0.774681000000	2.825442000000	4.411788000000
C	-0.539162000000	5.297349000000	0.495832000000
C	0.565460000000	5.295949000000	-0.478286000000
C	-2.046607000000	3.177345000000	-3.707015000000
C	-1.606358000000	2.098309000000	-4.566942000000
C	0.574437000000	-5.296896000000	0.450475000000
C	-0.601063000000	-5.294560000000	-0.437175000000
C	1.757404000000	-3.175542000000	-3.853672000000
C	1.252080000000	-2.094870000000	-4.676376000000
C	4.347529000000	0.936996000000	-2.984780000000
C	4.076964000000	2.320739000000	-2.586464000000
C	4.830481000000	1.384722000000	1.910419000000

C	4.024923000000	1.855405000000	3.012454000000
C	2.457347000000	-2.468987000000	4.016446000000
C	1.106756000000	-2.825956000000	4.338768000000
C	-3.928956000000	-0.446621000000	-3.749410000000
C	-4.675442000000	-2.730467000000	-1.043957000000
C	-4.888294000000	-2.248153000000	1.185289000000
C	-3.348911000000	-0.921132000000	4.216243000000
C	-2.540257000000	1.207251000000	4.648996000000
C	-0.308698000000	3.947262000000	3.718327000000
C	-0.205409000000	5.171522000000	1.800396000000
C	0.231437000000	5.166993000000	-1.781606000000
C	-1.070161000000	4.129632000000	-3.344065000000
C	-2.456665000000	1.042071000000	-4.704453000000
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C	-0.366414000000	-5.166644000000	-1.762280000000
C	0.811063000000	-4.128046000000	-3.418985000000
C	2.091804000000	-1.039393000000	-4.879679000000
C	3.631664000000	0.450322000000	-4.038182000000
C	4.584327000000	2.732760000000	-1.394096000000
C	4.963527000000	2.249753000000	0.812754000000
C	3.658522000000	0.920685000000	3.951580000000
C	2.886468000000	-1.208679000000	4.444941000000
C	0.589248000000	-3.945931000000	3.680299000000
C	-5.366302000000	-0.426017000000	-0.349439000000
C	-2.468866000000	-2.455466000000	-4.000241000000
C	-4.342654000000	0.956360000000	3.000040000000
C	-3.153827000000	-3.867561000000	1.955643000000
C	-2.375246000000	4.150590000000	2.422676000000
C	-0.244774000000	0.576749000000	5.232115000000
C	-2.188511000000	4.714353000000	-1.275368000000

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C	5.323753000000	0.428145000000	-0.755548000000
C	2.157996000000	2.458073000000	-4.174948000000
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C	3.293100000000	3.868099000000	1.713242000000
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C	-4.066892000000	2.340076000000	2.603128000000
C	1.616136000000	2.090742000000	4.584932000000
C	-2.810638000000	4.453691000000	1.077296000000
C	2.833385000000	4.440388000000	-1.060150000000
C	-3.272669000000	3.883291000000	-1.695923000000
C	0.246050000000	0.576017000000	-5.214976000000
C	2.883955000000	-4.452755000000	0.858294000000
C	-2.905969000000	-4.438931000000	-0.844561000000
C	3.134343000000	-3.882085000000	-1.941859000000
C	-0.643488000000	-0.573498000000	-5.181094000000
C	4.665563000000	-1.405958000000	-2.255523000000
C	2.395077000000	4.138131000000	-2.405043000000
C	5.364532000000	-0.452711000000	0.364674000000

C	2.061593000000	3.169248000000	3.725554000000
C	4.252256000000	-2.339782000000	2.286139000000
C	-1.264861000000	-2.091946000000	4.693086000000
C	-5.071887000000	0.026880000000	-1.680371000000
C	-3.184657000000	-3.072242000000	-2.921605000000
C	-4.930883000000	-0.001531000000	2.077165000000
C	-2.978971000000	-3.058568000000	3.147313000000
C	-2.938441000000	3.088858000000	3.169351000000
C	0.192265000000	1.876176000000	4.891094000000
C	-1.918836000000	4.969944000000	0.098905000000
C	1.942797000000	4.958429000000	-0.081762000000
C	-3.192587000000	3.073676000000	-2.896583000000
C	-0.183546000000	1.875347000000	-4.870323000000
C	1.919834000000	-4.967990000000	-0.049635000000
C	-1.944529000000	-4.958719000000	0.063199000000
C	2.962767000000	-3.071789000000	-3.132545000000
C	-0.189342000000	-1.873747000000	-4.874247000000
C	4.929464000000	-0.024339000000	-2.061230000000
C	2.954855000000	3.075360000000	-3.154673000000
C	5.073237000000	0.001589000000	1.697467000000
C	3.209019000000	3.059043000000	2.914543000000
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