Supplementary information for

Computational Exploration of the Electrochemical Oxidation Mechanism of Thiocyanate Catalyzed by Cobalt-Phthalocyanines

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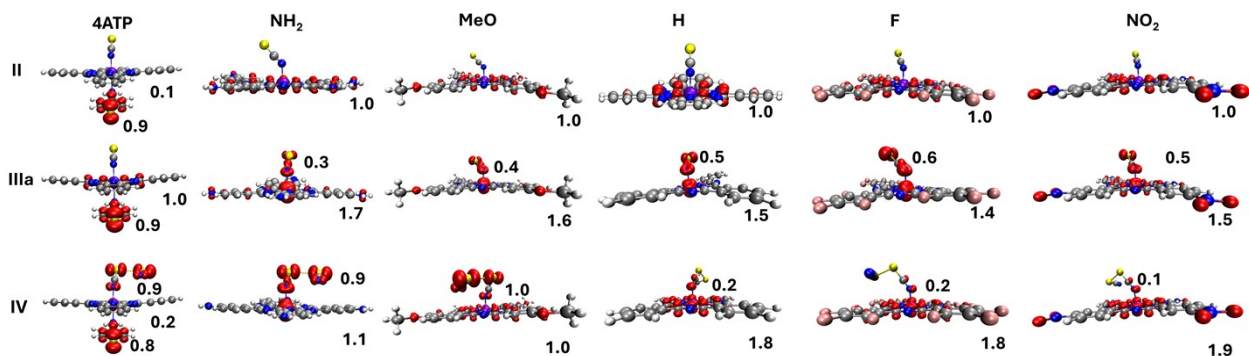
Figure S1. Graphical representation of the spin density evolution along the reaction mechanism for the open shell intermediate states (II, IIIa, and IV) considering the complexes formed through the Co–N binding mode (spin densities are represented by the red isosurface).

Figure S2. Graphical representation of the spin density evolution along the reaction mechanism for the open shell intermediate states (II, IIIa, and IV) considering the complexes formed through the Co–S binding mode (spin densities are represented by the red isosurface).
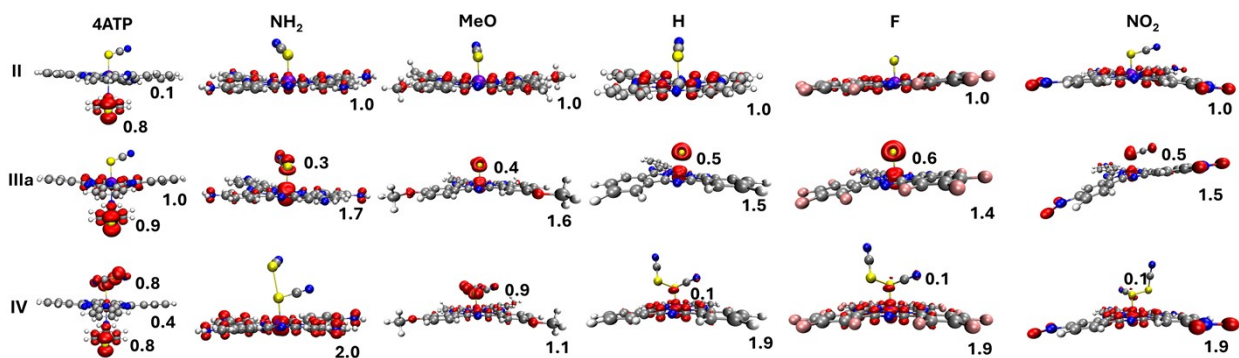
After the first electron-oxidation process (**II**) for both, Co–N and Co–S binding modes (Figures S1 and S2), the unpaired electron is delocalized along the Pc moiety, with exception of the 4ATP-CoPc complex, where it is delocalized at the 4ATP ligand, explaining the differences in the oxidation potential behavior of this system with respect to the rest of the series. The second oxidation to form **IIIa** for the case of the triplet state, leads to the activation of the system towards

2

the dimerization process by localizing the unpaired electron at the SCN$^\bullet$. The addition of the second SCN$^-$ molecule to generate **IV** shows that for the systems for which the S–S bond is formed, corresponding to complexes formed by the Co–N binding mode (R= H, F, NO$_2$), the spin density is delocalized in the Pc moiety. Meanwhile, for the complexes where no S–S bond is formed, the spin density is mainly localized in the (SCN)$_2^{\bullet\,-}$, denoting the radical nature of the dimer intermediate. According to these results, to form the (SCN)$_2$ dimer, the system has to be capable of transferring the unpaired electron to the macrocycle after the addition of the second SCN$^-$ molecule, which is only viable by electron-withdrawing groups, and in a minor extent, by the system without substituents. When electron-donor functionalization is used on the CoPc system, it is not possible to generate the (SCN)$_2$ dimer, as it is not possible to transfer the unpaired electron to the macrocycle, which seems to be a requisite to form the S–S bond.

Binding mode Co-SCN (all energies are in hartree)

4-ATP - Stage I

E = -4225.36673164

G = -4224.915671

S	-2.894592	1.152947	-1.169993
C	-4.065275	0.856012	-0.017497
N	-4.919380	0.651144	0.788415
Co	-0.879536	0.529320	-0.052894
C	-2.047076	-1.980152	1.033051
C	-2.289624	-3.378948	0.679080
C	-1.817161	-3.539163	-0.646392
C	-1.278273	-2.241188	-1.049596
N	-1.435671	-1.327065	-0.022481
C	-1.752325	1.994712	2.377446
C	-2.451010	1.796131	3.646225
C	-2.749693	0.413797	3.723222
C	-2.246092	-0.184199	2.488098
N	-1.645182	0.788464	1.705605
C	0.416944	3.003332	-1.087773
C	0.604273	4.417381	-0.765549
C	-0.055224	4.634587	0.469086
C	-0.612727	3.343196	0.868385

```
N   -0.309607    2.384459   -0.084643

C   -0.087825   -0.914317   -2.533126

C    0.722316   -0.759950   -3.739962

C    1.194742    0.574863   -3.733319

C    0.655898    1.193347   -2.522013

N   -0.091537    0.268525   -1.813531

N   -0.679289   -2.057785   -2.217791

N   -2.404914   -1.470096    2.204305

N   -1.288843    3.178138    1.997426

N    0.884890    2.460893   -2.205524

C   -0.074828    5.903959    1.070750

C    2.053874    1.047610   -4.737613

C    1.106409   -1.665219   -4.741223

C   -1.887023   -4.779953   -1.300370

C   -2.855180   -4.453310    1.385106

C   -3.422911   -0.125499    4.831676

C   -2.814096    2.678017    4.677668

C    1.261916    5.463509   -1.433949

C    1.242573    6.733846   -0.832414

H    1.748193    7.577030   -1.328184

C    0.582844    6.951203    0.402365

C    2.433488    0.143771   -5.746679

C    1.969468   -1.193795   -5.746274
```

H	2.298258	-1.877986	-6.543826
C	-2.452731	-5.856137	-0.594286
C	-2.930651	-5.694799	0.729377
H	-3.366881	-6.559589	1.253072
C	-3.487548	2.138995	5.787594
H	-3.789261	2.801376	6.613823
C	-3.787365	0.756508	5.863814
H	1.773393	5.292807	-2.393032
H	-0.587820	6.071133	2.029668
H	2.425765	2.082992	-4.728440
H	0.760389	-2.708749	-4.727651
H	-1.511578	-4.902855	-2.327183
H	-3.221833	-4.327751	2.414838
H	3.110598	0.478376	-6.547976
H	0.586684	7.959702	0.844318
H	-2.525686	-6.843466	-1.076216
H	-3.656204	-1.199221	4.888087
H	-4.316173	0.368439	6.748228
H	-2.581596	3.751676	4.616423
C	1.517911	-2.313877	0.308866
C	2.149593	-3.205444	-0.555108
C	3.014467	-2.759935	-1.612554
C	3.277052	-1.347374	-1.658515

C	2.656724	-0.454355	-0.790537
S	3.676262	-3.849676	-2.778577
H	0.824519	-2.683081	1.081426
H	1.957341	-4.285846	-0.460585
H	3.964899	-0.970105	-2.431340
H	2.846401	0.627575	-0.873546
C	1.736801	-0.920647	0.180024
N	0.929366	-0.002319	0.884476
H	0.604279	-0.359565	1.793908
H	1.377860	0.915266	1.018291

4-ATP - Stage II

E = -4225.208924

G = -4224.758244

S	-2.849785	1.100068	-1.084042
C	-4.053800	0.481982	-0.097851
N	-4.939331	0.058554	0.572929
Co	-0.925576	0.429244	-0.020008
C	-2.175586	-2.027016	1.096252
C	-2.524344	-3.399521	0.732376
C	-2.092937	-3.579584	-0.604437

C	-1.461924	-2.323668	-1.006105
N	-1.538467	-1.409536	0.032416
C	-1.735646	1.948915	2.398582
C	-2.399265	1.776389	3.689349
C	-2.726731	0.402060	3.789394
C	-2.276473	-0.220283	2.546328
N	-1.677855	0.732460	1.738259
C	0.416489	2.860386	-1.108381
C	0.619418	4.277882	-0.816986
C	-0.030031	4.528617	0.416593
C	-0.598515	3.253357	0.848940
N	-0.312599	2.273140	-0.087028
C	-0.196679	-1.066866	-2.487137
C	0.667618	-0.971956	-3.661638
C	1.200752	0.341326	-3.659812
C	0.636919	1.012569	-2.492695
N	-0.154875	0.123142	-1.781060
N	-0.855776	-2.173647	-2.174829
N	-2.479598	-1.502487	2.275246
N	-1.258246	3.116712	1.991300
N	0.880520	2.283849	-2.209264
C	-0.030897	5.809786	0.992442
C	2.156783	0.742839	-4.606504

C	1.077088	-1.923505	-4.605875
C	-2.280351	-4.800212	-1.273179
C	-3.162425	-4.432676	1.437784
C	-3.376815	-0.112251	4.923077
C	-2.708911	2.676325	4.722466
C	1.285716	5.300949	-1.511673
C	1.283618	6.583432	-0.936768
H	1.795388	7.410281	-1.453059
C	0.634177	6.834320	0.297088
C	2.580045	-0.213559	-5.543250
C	2.050506	-1.529133	-5.541447
H	2.410856	-2.254016	-6.287066
C	-2.919881	-5.834542	-0.568220
C	-3.354282	-5.653466	0.767840
H	-3.850864	-6.486203	1.289461
C	-3.358071	2.162144	5.858052
H	-3.617753	2.838285	6.687250
C	-3.686878	0.787723	5.957177
H	1.789857	5.103868	-2.469407
H	-0.535418	6.002919	1.950801
H	2.577667	1.758892	-4.594626
H	0.677497	-2.947932	-4.594094
H	-1.941299	-4.938790	-2.310496

H -3.497702 -4.291000 2.475896

H 3.344789 0.055476 -6.287728

H 0.652118 7.851921 0.717019

H -3.087432 -6.804436 -1.061624

H -3.632504 -1.179634 4.997211

H -4.195633 0.420250 6.861792

H -2.454240 3.743609 4.643237

C 1.740859 -2.079478 -0.203674

C 2.543938 -2.593400 -1.216139

C 3.452834 -1.753310 -1.940102

C 3.564364 -0.383001 -1.535559

C 2.754728 0.133820 -0.529915

S 4.354890 -2.363130 -3.273200

H 1.028040 -2.725442 0.330537

H 2.469781 -3.655082 -1.494096

H 4.281284 0.267137 -2.058113

H 2.812169 1.196995 -0.251358

C 1.805904 -0.699897 0.108960

N 0.836546 -0.128800 0.965920

H 0.512447 -0.780198 1.696517

H 1.155955 0.747653 1.405930

4-ATP - Stage III-a

E = -4225.020580

G = -4224.568346

S	-2.855606	1.082102	-1.065374
C	-4.044016	0.265300	-0.214768
N	-4.912778	-0.300162	0.366441
Co	-0.927020	0.391067	-0.010573
C	-2.238502	-2.029549	1.098575
C	-2.666325	-3.376569	0.714636
C	-2.227938	-3.568904	-0.615571
C	-1.514252	-2.347406	-0.993564
N	-1.556125	-1.435965	0.051311
C	-1.683977	1.918117	2.414858
C	-2.298170	1.746904	3.733665
C	-2.653907	0.382433	3.832443
C	-2.266071	-0.236894	2.563309
N	-1.674616	0.709299	1.740955
C	0.372712	2.819799	-1.144425
C	0.537683	4.251661	-0.887111
C	-0.082055	4.505368	0.357953
C	-0.601744	3.219338	0.828380
N	-0.317983	2.229858	-0.096909

C	-0.181449	-1.134434	-2.447924
C	0.716686	-1.065466	-3.599530
C	1.243257	0.250231	-3.615197
C	0.640887	0.946325	-2.478866
N	-0.158024	0.068795	-1.762649
N	-0.873056	-2.224625	-2.145194
N	-2.511960	-1.508807	2.287457
N	-1.220418	3.086263	1.993394
N	0.850787	2.231726	-2.230949
C	-0.104944	5.790549	0.914335
C	2.217936	0.637057	-4.541104
C	1.149883	-2.037911	-4.507144
C	-2.476340	-4.764561	-1.301364
C	-3.372469	-4.371103	1.402661
C	-3.273955	-0.130522	4.978511
C	-2.548227	2.644854	4.779001
C	1.156581	5.273866	-1.617786
C	1.131698	6.570291	-1.063569
H	1.605041	7.400558	-1.609367
C	0.511780	6.824058	0.179346
C	2.677566	-0.346519	-5.441220
C	2.152314	-1.661424	-5.424815
H	2.534563	-2.401702	-6.143173

C   -3.192112   -5.766753   -0.614454

C   -3.631474   -5.573838   0.713362

H   -4.185965   -6.378307   1.219994

C   -3.168559   2.131934   5.937026

H   -3.381169   2.806726   6.780102

C   -3.524344   0.769286   6.035236

H   1.641977   5.073431   -2.584065

H   -0.585626   5.986124   1.883969

H   2.632569   1.655132   -4.545825

H   0.748895   -3.061253   -4.485989

H   -2.130303   -4.914370   -2.334433

H   -3.710749   -4.220504   2.438149

H   3.458730   -0.089167   -6.171713

H   0.510999   7.848312   0.582090

H   -3.412251   -6.717997   -1.122476

H   -3.554210   -1.191417   5.051428

H   -4.008154   0.403109   6.953475

H   -2.274394   3.706928   4.699178

C   1.880577   -1.978103   -0.306104

C   2.735858   -2.365362   -1.331348

C   3.614524   -1.417493   -1.951863

C   3.648795   -0.082493   -1.431120

C   2.788543   0.304384   -0.409820

S   4.559854   -1.853569   -3.319689

H   1.189934   -2.702788   0.150558

H   2.724671   -3.402375   -1.697261

H   4.343960   0.645324   -1.874422

H   2.786387   1.339975   -0.037650

C   1.864278   -0.627408   0.121722

N   0.840652   -0.181671   0.987277

H   0.523532   -0.917164   1.637809

H   1.103291   0.659690   1.523747

4-ATP - Stage III-b

E = -4225.022492

G = -4224.567891

S   -2.878399   1.147189   -1.009525

C   -4.050341   0.039717   -0.556855

N   -4.912152   -0.721249   -0.255780

Co   -0.974314   0.351180   -0.012612

C   -2.361169   -2.026052   1.092436

C   -2.789658   -3.377392   0.729473

C   -2.294851   -3.614891   -0.573626

C   -1.564973   -2.408735   -0.962433

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N   -1.638542   -1.464721    0.063744

C   -1.618338    1.879807    2.443706

C   -2.239534    1.728429    3.762372

C   -2.694707    0.392086    3.837100

C   -2.349425   -0.232622    2.559231

N   -1.693837    0.689416    1.749684

C    0.342802    2.763628   -1.181969

C    0.577448    4.181000   -0.900957

C    0.050093    4.424237    0.388313

C   -0.505038    3.152595    0.853993

N   -0.312831    2.174779   -0.106622

C   -0.238292   -1.213729   -2.442454

C    0.644134   -1.168007   -3.576132

C    1.153810    0.164868   -3.638326

C    0.538417    0.889033   -2.520570

N   -0.220661    0.018003   -1.777636

N   -0.910270   -2.308879   -2.100655

N   -2.658028   -1.482700    2.270953

N   -1.087079    3.025185    2.037994

N    0.751108    2.180684   -2.295121

C    0.119753    5.694263    0.979033

C    2.169503    0.506510   -4.520166

C    1.123239   -2.191857   -4.426840
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C   -2.526401   -4.831009   -1.232590

C   -3.532398   -4.346785   1.417894

C   -3.347363   -0.095843   4.977881

C   -2.419398   2.621829   4.826767

C   1.196066   5.197988   -1.641330

C   1.264986   6.474894   -1.052237

H   1.740151   7.300384   -1.603978

C   0.735548   6.719031   0.236175

C   2.746447   -0.556572   -5.286992

C   2.179325   -1.875890   -5.274707

H   2.620564   -2.644129   -5.926000

C   -3.276655   -5.804488   -0.546731

C   -3.770960   -5.566589   0.756888

H   -4.353386   -6.351582   1.263075

C   -3.072384   2.134356   5.975823

H   -3.232485   2.806472   6.832724

C   -3.528526   0.798497   6.050316

H   1.608992   5.005933   -2.642430

H   -0.290132   5.880667   1.982435

H   2.584439   1.523084   -4.569850

H   0.703882   -3.206777   -4.380489

H   -2.139253   -5.014815   -2.245510

H   -3.914302   -4.160484   2.432216

H   3.513873   -0.314192   -6.038348

H   0.808428   7.730123   0.665109

H   -3.483275   -6.770241   -1.032870

H   -3.703147   -1.135058   5.032172

H   -4.035439   0.452516   6.964039

H   -2.066396   3.661634   4.766645

C   2.030205   -1.793253   -0.497263

C   2.910959   -1.947983   -1.563864

C   3.636777   -0.822747   -2.072034

C   3.533465   0.429238   -1.379438

C   2.680534   0.573949   -0.294987

S   4.541233   -0.917194   -3.532090

H   1.420909   -2.637806   -0.141744

H   3.020622   -2.924980   -2.056263

H   4.118407   1.287179   -1.741662

H   2.583600   1.541021   0.220626

C   1.861546   -0.515998   0.094424

N   0.797246   -0.280273   0.984206

H   0.493942   -1.120024   1.500702

H   0.978046   0.495763   1.639515

4-ATP - Stage IV

E = -4716.085907

G = -4715.632820

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S    -3.008538    1.169375   -0.841736

C    -4.173484    0.223066   -0.093898

N    -5.024134   -0.425016    0.419412

Co   -1.056844    0.406647    0.046669

C    -2.310793   -2.035900    1.198005

C    -2.699904   -3.398068    0.837101

C    -2.275188   -3.594086   -0.499006

C    -1.621007   -2.353744   -0.910567

N    -1.677264   -1.431162    0.122315

C    -1.689841    1.908341    2.532679

C    -2.278947    1.730654    3.858160

C    -2.657103    0.368928    3.948916

C    -2.304203   -0.243765    2.669959

N    -1.718779    0.703383    1.846808

C     0.216572    2.847207   -1.112317

C     0.453202    4.258312   -0.816942

C    -0.078927    4.491793    0.474532

C    -0.626431    3.216247    0.932111

N    -0.434465    2.250164   -0.042341

C    -0.404183   -1.103895   -2.435541
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C	0.420576	-1.008457	-3.635589
C	0.924898	0.315592	-3.671239
C	0.375782	0.996896	-2.500047
N	-0.364299	0.101061	-1.747329
N	-1.019549	-2.221594	-2.082799
N	-2.562539	-1.514023	2.389376
N	-1.202151	3.069030	2.117195
N	0.610775	2.275399	-2.239921
C	-0.012783	5.761003	1.071617
C	1.836016	0.723245	-4.652481
C	0.814359	-1.967170	-4.579677
C	-2.497679	-4.809521	-1.165392
C	-3.362221	-4.411384	1.547783
C	-3.259517	-0.145440	5.108072
C	-2.489584	2.618760	4.925343
C	1.068534	5.285718	-1.550065
C	1.133616	6.557015	-0.953730
H	1.607584	7.387934	-1.498586
C	0.600691	6.791054	0.337437
C	2.255788	-0.243943	-5.583382
C	1.750480	-1.569409	-5.549065
H	2.104019	-2.297281	-6.294815
C	-3.164286	-5.824025	-0.456029

C	-3.589588	-5.627968	0.880349
H	-4.108561	-6.445012	1.404820
C	-3.091491	2.104461	6.087039
H	-3.273624	2.771297	6.943858
C	-3.470432	0.742911	6.177202
H	1.482273	5.101191	-2.552428
H	-0.425918	5.940892	2.075079
H	2.233177	1.748264	-4.673204
H	0.429546	-2.996515	-4.541688
H	-2.165689	-4.959042	-2.203369
H	-3.691619	-4.257858	2.585971
H	2.989638	0.029770	-6.356386
H	0.669752	7.799947	0.772613
H	-3.360518	-6.789717	-0.946917
H	-3.554634	-1.202920	5.175596
H	-3.939862	0.375339	7.102679
H	-2.196243	3.676409	4.852864
C	1.786106	-1.906154	-0.424376
C	2.623467	-2.248583	-1.479648
C	3.458718	-1.266801	-2.108910
C	3.460803	0.060098	-1.564570
C	2.622881	0.403172	-0.509157
S	4.404744	-1.658743	-3.489986

H   1.125744   -2.656381   0.036190

H   2.633984   -3.278707   -1.864813

H   4.119851   0.816280   -2.015651

H   2.605699   1.430512   -0.114981

C   1.744993   -0.566032   0.032905

N   0.738654   -0.168400   0.943508

H   0.449534   -0.930414   1.576146

H   1.001031   0.659384   1.500745

S   -3.522107   -0.096584   -3.470045

C   -2.489388   0.924930   -4.255848

N   -1.751838   1.670251   -4.829680

4-ATP - Stage V

E = -4716.074757

G = -4715.617535

S   -3.096150   1.013645   -0.841577

C   -4.151441   0.271723   0.233368

N   -4.952810   -0.227239   0.956048

Co   -1.061079   0.413884   0.035790

C   -2.139480   -2.077651   1.234204

C   -2.529086   -3.442879   0.876810

C	-2.269271	-3.582432	-0.507687
C	-1.674716	-2.318438	-0.944591
N	-1.623911	-1.433957	0.122786
C	-1.780234	1.916728	2.485667
C	-2.346263	1.723434	3.820502
C	-2.569712	0.332823	3.962174
C	-2.168991	-0.280782	2.695163
N	-1.684474	0.690215	1.839967
C	0.222621	2.851409	-1.097837
C	0.398912	4.276081	-0.822266
C	-0.259633	4.529780	0.405056
C	-0.789614	3.244110	0.860353
N	-0.501534	2.263670	-0.064899
C	-0.514295	-1.042430	-2.485028
C	0.373949	-0.977162	-3.655938
C	0.936843	0.343823	-3.648099
C	0.404320	1.008530	-2.484976
N	-0.403272	0.122098	-1.765900
N	-1.176278	-2.145766	-2.157871
N	-2.334655	-1.574373	2.444838
N	-1.399254	3.099593	2.034093
N	0.693619	2.268771	-2.183847
C	-0.292916	5.817268	0.962385

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C    1.938148    0.727920   -4.563886

C    0.840206   -1.955638   -4.521076

C   -2.546017   -4.779194   -1.185161

C   -3.082466   -4.493104    1.624559

C   -3.105885   -0.203487    5.142163

C   -2.647708    2.620213    4.857008

C    1.038427    5.303163   -1.533285

C    1.002889    6.594928   -0.978008

H    1.493948    7.426131   -1.507046

C    0.346823    6.848102    0.250433

C    2.437584   -0.259791   -5.410157

C    1.936411   -1.607696   -5.357455

H    2.303053   -2.338113   -6.094328

C   -3.102193   -5.833154   -0.437259

C   -3.365452   -5.692607    0.945969

H   -3.799933   -6.539001    1.499802

C   -3.184022    2.084337    6.041901

H   -3.435357    2.757209    6.876121

C   -3.408800    0.694277    6.182468

H    1.547648    5.103724   -2.487702

H   -0.803567    6.012678    1.916881

H    2.343839    1.749115   -4.564659

H    0.440767   -2.979242   -4.509808
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H	-2.340083	-4.886425	-2.260380
H	-3.285397	-4.382305	2.699930
H	3.246620	-0.027291	-6.117648
H	0.337595	7.872190	0.654305
H	-3.338149	-6.785734	-0.936158
H	-3.282759	-1.283840	5.248858
H	-3.830404	0.309824	7.123936
H	-2.474011	3.700551	4.744527
C	1.580654	-2.016031	-0.423769
C	2.255594	-2.497445	-1.537178
C	3.142160	-1.653197	-2.287501
C	3.358413	-0.315808	-1.821072
C	2.655993	0.175339	-0.724221
S	3.876487	-2.231597	-3.728452
H	0.895571	-2.664543	0.141655
H	2.107350	-3.536001	-1.867185
H	4.067141	0.329397	-2.359949
H	2.783120	1.217352	-0.394956
C	1.717266	-0.652022	-0.060710
N	0.826941	-0.102647	0.884420
H	0.566736	-0.768937	1.627537
H	1.164438	0.777269	1.303420
S	-2.049400	0.516017	-4.953159

C   -2.139041   1.837171   -3.972312

N   -2.195043   2.801680   -3.263194

NH$_2$ - Stage I

E = -3761.574596

G = -3761.167950

S   -1.919256   0.645052   -0.735458

C   -1.959495   2.251000   -0.258486

N   -2.036557   3.394223   0.060321

Co   0.072567   -0.081258   0.004862

C   -0.193604   1.218273   2.685396

C   -0.757429   0.990918   3.999155

C   -1.362096   -0.291076   3.966294

C   -1.122430   -0.818423   2.620895

N   -0.398142   0.090791   1.873982

C   1.443549   2.347117   -1.038311

C   1.766303   3.706344   -0.665882

C   1.403731   3.852975   0.697627

C   0.856989   2.559746   1.112125

N   0.909687   1.659838   0.063949

C   0.598873   -1.494528   -2.578789

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C    1.170027    -1.271791    -3.889886

C    1.638162     0.066592    -3.907905

C    1.351494     0.613831    -2.579625

N    0.756060    -0.347163    -1.785310

C   -1.288264    -2.526746     1.056159

C   -1.693754    -3.857121     0.656531

C   -1.234286    -4.041856    -0.672474

C   -0.555687    -2.797983    -1.043556

N   -0.584011    -1.906703     0.012010

N   -1.547277    -2.021649     2.252368

N    0.390505     2.353909     2.338231

N    1.652900     1.864997    -2.254090

N   -0.002384    -2.624729    -2.238384

C    2.245147     0.628375    -5.031780

C   -1.434310    -5.233423    -1.370958

C   -2.381471    -4.896413     1.317339

C   -2.011403    -0.836909     5.074714

C   -0.807859     1.766274     5.176035

C    1.582717     5.050401     1.391040

C    2.327272     4.792729    -1.369741

C    1.305985    -2.083694    -5.035181

C    1.908077    -1.539200    -6.169340

H    2.025867    -2.149923    -7.078427
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C    2.387600   -0.184957   -6.194359

C   -2.129433   -6.289042   -0.711234

C   -2.595378   -6.092999    0.633722

H   -3.131838   -6.920669    1.124040

C   -2.063087   -0.062839    6.270613

C   -1.455442    1.238851    6.293340

H   -1.511105    1.823523    7.225221

C    2.506712    5.999791   -0.695679

H    2.934703    6.867853   -1.221623

C    2.143536    6.155328    0.686424

H    0.945433   -3.123454   -5.040127

H    2.602757    1.669131   -5.034758

H   -1.070359   -5.366883   -2.400924

H   -2.744092   -4.770977    2.348836

H   -2.476783   -1.833503    5.037487

H   -0.349700    2.766069    5.217269

H    1.294387    5.153746    2.448026

H    2.611731    4.696925   -2.428515

N   -2.660824   -0.557352    7.394266

H   -2.835832    0.061509    8.187659

H   -3.219988   -1.409979    7.334144

N   -2.333241   -7.484421   -1.335851

H   -2.950333   -8.180341   -0.914652
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H	-2.120353	-7.581602	-2.329828
N	2.991294	0.304381	-7.315701
H	3.208949	1.299942	-7.381939
H	2.957564	-0.229818	-8.185443
N	2.356644	7.346784	1.315534
H	1.974051	7.502645	2.249431
H	2.616228	8.169562	0.769172

NH$_2$ - Stage II

E = -3761.406857

G = -3760.999619

S	-1.905571	0.662249	-0.743547
C	-1.959722	2.249426	-0.204930
N	-2.050191	3.378924	0.153550
Co	0.072513	-0.080719	0.001539
C	-0.207374	1.218549	2.680417
C	-0.780522	1.000821	3.985080
C	-1.389144	-0.278913	3.950438
C	-1.143194	-0.813062	2.602596
N	-0.412114	0.095472	1.862800
C	1.443150	2.348752	-1.036286

C	1.769929	3.701830	-0.666186
C	1.419892	3.843699	0.700658
C	0.867696	2.547199	1.117392
N	0.913697	1.653829	0.063550
C	0.581804	-1.483318	-2.590365
C	1.140644	-1.261110	-3.900580
C	1.618534	0.073436	-3.915265
C	1.341411	0.621224	-2.578843
N	0.744467	-0.341958	-1.789277
C	-1.307578	-2.520567	1.041422
C	-1.703447	-3.850381	0.650489
C	-1.230873	-4.040993	-0.672639
C	-0.557467	-2.789629	-1.050988
N	-0.600288	-1.896623	0.001442
N	-1.572280	-2.011097	2.238766
N	0.396868	2.349897	2.337888
N	1.647299	1.867377	-2.257486
N	-0.012025	-2.620458	-2.244871
C	2.219067	0.637468	-5.033160
C	-1.412792	-5.231414	-1.364472
C	-2.387510	-4.890119	1.317085
C	-2.046638	-0.820829	5.047171
C	-0.833146	1.781387	5.160148

C	1.600841	5.031639	1.396414
C	2.326601	4.789194	-1.374373
C	1.264240	-2.072946	-5.048839
C	1.861668	-1.530675	-6.184229
H	1.972239	-2.137736	-7.096041
C	2.346402	-0.178564	-6.205720
C	-2.109184	-6.291964	-0.696349
C	-2.586188	-6.093110	0.643860
H	-3.116912	-6.922896	1.135551
C	-2.103164	-0.036453	6.246332
C	-1.489092	1.261961	6.273793
H	-1.547758	1.846371	7.205005
C	2.511767	5.993988	-0.701386
H	2.936205	6.863597	-1.226521
C	2.157308	6.143943	0.683156
H	0.898580	-3.110491	-5.051842
H	2.585204	1.674886	-5.036391
H	-1.039108	-5.372668	-2.389586
H	-2.756008	-4.758255	2.345281
H	-2.515240	-1.815608	5.012034
H	-0.367944	2.777517	5.200268
H	1.323968	5.134103	2.456237
H	2.603065	4.693167	-2.434838

N	-2.733600	-0.519882	7.343227
H	-2.786205	0.031716	8.201871
H	-3.171806	-1.442847	7.329179
N	-2.313193	-7.472154	-1.328125
H	-2.805205	-8.236987	-0.862145
H	-1.972170	-7.620071	-2.279824
N	2.918011	0.326362	-7.324780
H	3.265309	1.287095	-7.345741
H	3.010775	-0.244262	-8.167365
N	2.344516	7.328069	1.312017
H	2.090896	7.442704	2.295232
H	2.730090	8.130908	0.811102

NH$_2$ - Stage III-a

E = -3761.216507

G = -3760.807811

S	-2.078409	0.752670	-0.793631
C	-2.007367	2.354800	-0.335539
N	-1.963828	3.498874	-0.007821
Co	0.029777	-0.066863	-0.009141
C	-0.191890	1.203234	2.684636

C	-0.708753	0.960493	4.002053
C	-1.311725	-0.326108	3.971627
C	-1.117403	-0.838713	2.604343
N	-0.419473	0.089601	1.855221
C	1.397283	2.375678	-1.040056
C	1.689129	3.734315	-0.686707
C	1.329978	3.878678	0.679103
C	0.804118	2.566209	1.105759
N	0.862050	1.680068	0.056792
C	0.608320	-1.488862	-2.568396
C	1.212221	-1.284772	-3.854543
C	1.693533	0.052405	-3.870602
C	1.367205	0.621241	-2.551303
N	0.741130	-0.336489	-1.773661
C	-1.350017	-2.516051	1.022692
C	-1.772315	-3.828912	0.625331
C	-1.299450	-4.017989	-0.699160
C	-0.594447	-2.772462	-1.065735
N	-0.647706	-1.885295	-0.017651
N	-1.575394	-2.020157	2.238226
N	0.370297	2.355660	2.336487
N	1.643875	1.873849	-2.249740
N	-0.013136	-2.619005	-2.242374

C   2.318276   0.602544   -4.972981

C   -1.501465   -5.192013   -1.399460

C   -2.478863   -4.859423   1.287114

C   -1.930770   -0.881400   5.074715

C   -0.728398   1.738245   5.183309

C   1.489831   5.065508   1.367040

C   2.232438   4.825103   -1.404375

C   1.358060   -2.117682   -4.988463

C   1.986428   -1.594436   -6.110623

H   2.123393   -2.209800   -7.012694

C   2.474091   -0.239013   -6.132234

C   -2.228316   -6.245697   -0.734418

C   -2.703707   -6.051076   0.606587

H   -3.252638   -6.873983   1.088638

C   -1.947337   -0.101091   6.285544

C   -1.341291   1.205802   6.309969

H   -1.375464   1.777037   7.249984

C   2.394929   6.036848   -0.742863

H   2.807006   6.910478   -1.270134

C   2.033245   6.186380   0.639555

H   0.985811   -3.152188   -4.982968

H   2.684034   1.639644   -4.986410

H   -1.129404   -5.337923   -2.424417

H	-2.843877	-4.724721	2.315808
H	-2.399249	-1.876175	5.049283
H	-0.270207	2.737348	5.211035
H	1.213309	5.174235	2.426250
H	2.515348	4.721573	-2.462093
N	-2.531552	-0.597426	7.390045
H	-2.554211	-0.056976	8.259900
H	-2.964979	-1.525294	7.381516
N	-2.451841	-7.405519	-1.381490
H	-2.964683	-8.167623	-0.929988
H	-2.112569	-7.545503	-2.336711
N	3.073183	0.246873	-7.233171
H	3.422636	1.209217	-7.258422
H	3.192245	-0.336866	-8.066279
N	2.194885	7.366706	1.266624
H	1.939642	7.475391	2.251817
H	2.574430	8.176798	0.769251

NH$_2$ - Stage III-b

E = -3761.225200

G = -3760.815035

S	-1.830666	0.701480	-0.782660
C	-2.186882	1.953203	0.277404
N	-2.492204	2.848792	0.994400
Co	0.094985	-0.078153	-0.013065
C	-0.216644	1.227115	2.654637
C	-0.857265	1.048600	3.925924
C	-1.483303	-0.223149	3.885333
C	-1.178015	-0.791852	2.558200
N	-0.400911	0.101071	1.840160
C	1.468931	2.353307	-1.043837
C	1.866358	3.676332	-0.656031
C	1.545956	3.805606	0.719522
C	0.927960	2.527049	1.121712
N	0.922788	1.657352	0.045498
C	0.573744	-1.462812	-2.618571
C	1.071751	-1.223945	-3.943191
C	1.534855	0.116429	-3.963408
C	1.305385	0.652972	-2.607714
N	0.736874	-0.326377	-1.812888
C	-1.281121	-2.520244	1.020466
C	-1.624194	-3.866071	0.658328
C	-1.113992	-4.072141	-0.649010
C	-0.485596	-2.798272	-1.052434

N	-0.573733	-1.891606	-0.012683
N	-1.593964	-1.989260	2.203813
N	0.443499	2.340337	2.330931
N	1.633383	1.885621	-2.282166
N	0.034349	-2.625999	-2.250028
C	2.080694	0.697515	-5.093007
C	-1.238674	-5.277356	-1.314380
C	-2.290087	-4.910743	1.339198
C	-2.202194	-0.732409	4.950797
C	-0.954235	1.857885	5.080599
C	1.784626	4.965307	1.432917
C	2.461106	4.750933	-1.356241
C	1.157171	-2.028240	-5.102444
C	1.698892	-1.471120	-6.255819
H	1.778657	-2.067020	-7.177610
C	2.165448	-0.112882	-6.282457
C	-1.915542	-6.348823	-0.627122
C	-2.431334	-6.135832	0.696026
H	-2.943999	-6.971824	1.195227
C	-2.308197	0.086562	6.132487
C	-1.675187	1.375544	6.167689
H	-1.774277	1.979300	7.082479
C	2.713248	5.931587	-0.666117

H	3.169139	6.791308	-1.180102
C	2.384802	6.068660	0.725484
H	0.803397	-3.069473	-5.096274
H	2.438024	1.737767	-5.104166
H	-0.839865	-5.433753	-2.327657
H	-2.687609	-4.762099	2.353823
H	-2.683194	-1.721064	4.915774
H	-0.473561	2.846152	5.121057
H	1.527862	5.063451	2.498078
H	2.713349	4.660983	-2.422932
N	-3.002786	-0.366998	7.194140
H	-3.092425	0.198936	8.042107
H	-3.451787	-1.286254	7.172087
N	-2.055548	-7.542071	-1.236663
H	-2.527706	-8.319064	-0.766835
H	-1.685811	-7.694658	-2.178380
N	2.682101	0.414446	-7.409645
H	3.015064	1.381800	-7.429976
H	2.749418	-0.142659	-8.265547
N	2.629026	7.220769	1.379358
H	2.391507	7.320656	2.369685
H	3.048159	8.019397	0.895724

NH$_2$ - Stage IV

E = -4252.282899

G = -4251.874422

S	-1.744796	-0.193078	-0.121605
C	-2.218106	0.945408	1.030239
N	-2.556881	1.745049	1.837087
Co	0.565556	0.136364	-0.038490
C	0.676869	0.443934	2.912725
C	0.721907	-0.337801	4.123066
C	0.731715	-1.702292	3.731440
C	0.716183	-1.705867	2.266139
N	0.692451	-0.396421	1.789090
C	0.243818	3.087451	-0.325427
C	0.087967	4.290124	0.452002
C	0.246949	3.913808	1.810685
C	0.470051	2.461661	1.806514
N	0.479181	1.988640	0.507660
C	0.737481	-0.142113	-2.997213
C	0.648219	0.635303	-4.208552
C	0.420695	1.980333	-3.815726
C	0.398651	1.978171	-2.349964

N	0.613406	0.688553	-1.873932
C	0.795741	-2.826575	0.242302
C	0.888916	-4.036664	-0.533879
C	0.958019	-3.637254	-1.893636
C	0.884326	-2.168985	-1.890732
N	0.802643	-1.703805	-0.591777
N	0.741193	-2.825957	1.571484
N	0.602139	1.769043	2.923567
N	0.198741	3.080654	-1.654680
N	0.876900	-1.462726	-3.008083
C	0.264695	3.006817	-4.736692
C	1.063205	-4.552868	-2.931671
C	0.930089	-5.405176	-0.187388
C	0.756081	-2.739433	4.653776
C	0.733364	0.017811	5.490192
C	0.169609	4.831070	2.849231
C	-0.154439	5.637796	0.106828
C	0.722359	0.288801	-5.576187
C	0.571340	1.298845	-6.519342
H	0.624659	1.068292	-7.594486
C	0.341232	2.666093	-6.126971
C	1.099152	-5.946189	-2.589342
C	1.032188	-6.343918	-1.209659

H	1.062411	-7.419196	-0.975518
C	0.767775	-2.389331	6.043477
C	0.757039	-1.002252	6.434119
H	0.766491	-0.764715	7.508990
C	-0.241369	6.577114	1.129972
H	-0.435861	7.635385	0.897330
C	-0.083942	6.201940	2.508897
H	0.894978	-0.751137	-5.889375
H	0.086004	4.047417	-4.428480
H	1.115963	-4.239222	-3.984786
H	0.879172	-5.725487	0.863639
H	0.762432	-3.795382	4.346238
H	0.723112	1.072230	5.802020
H	0.292058	4.534153	3.901361
H	-0.277572	5.940618	-0.943413
N	0.788151	-3.354545	6.988194
H	0.796155	-3.113039	7.982310
H	0.794439	-4.343325	6.725608
N	1.195377	-6.878719	-3.564305
H	1.219851	-7.874684	-3.334019
H	1.241234	-6.603867	-4.548075
N	0.197811	3.622284	-7.069970
H	0.035578	4.597423	-6.806380

H	0.249112	3.387754	-8.064465
N	-0.174516	7.134455	3.484374
H	-0.068605	6.874227	4.467480
H	-0.358055	8.114185	3.256244
S	-4.406988	-0.627667	-0.528626
C	-4.728602	0.937907	-0.989361
N	-4.969052	2.059878	-1.315889

NH$_2$ - Stage V

E = -4252.291563

G = -4251.880616

S	-1.708482	-0.116993	-0.215765
C	-2.162603	0.618954	1.229801
N	-2.480355	1.148059	2.243025
Co	0.575495	0.134910	-0.069631
C	0.645975	0.432483	2.895718
C	0.653586	-0.341148	4.107042
C	0.656100	-1.702649	3.713242
C	0.676034	-1.702842	2.235730
N	0.674219	-0.404015	1.768780
C	0.238001	3.079879	-0.355865

C	0.091764	4.283443	0.417698
C	0.249603	3.907820	1.775203
C	0.462616	2.446009	1.775165
N	0.464964	1.975262	0.477463
C	0.764007	-0.134260	-3.038771
C	0.669081	0.633721	-4.251908
C	0.427482	1.973603	-3.858299
C	0.402320	1.969897	-2.381224
N	0.629181	0.691131	-1.913515
C	0.812604	-2.820871	0.213449
C	0.934594	-4.027928	-0.558976
C	1.028150	-3.626958	-1.915266
C	0.935177	-2.152314	-1.914965
N	0.829507	-1.691754	-0.618066
N	0.718873	-2.824733	1.542784
N	0.592481	1.763832	2.895953
N	0.194435	3.072770	-1.688073
N	0.926914	-1.457279	-3.036878
C	0.267879	2.999659	-4.772659
C	1.161076	-4.534554	-2.950803
C	0.980379	-5.396744	-0.214068
C	0.648894	-2.740330	4.627612
C	0.639882	0.007174	5.475572

C	0.179052	4.820387	2.811961
C	-0.142950	5.632634	0.072931
C	0.754060	0.295936	-5.620398
C	0.598301	1.307091	-6.564958
H	0.659399	1.078199	-7.639868
C	0.354216	2.665315	-6.171585
C	1.203787	-5.933873	-2.609482
C	1.112630	-6.334580	-1.234472
H	1.147789	-7.409676	-1.001042
C	0.635091	-2.395256	6.027083
C	0.631735	-1.015090	6.420319
H	0.620467	-0.778949	7.495298
C	-0.222828	6.574795	1.094918
H	-0.410478	7.633942	0.861613
C	-0.066438	6.199068	2.471034
H	0.939273	-0.741020	-5.937156
H	0.078650	4.037980	-4.462002
H	1.231173	-4.218760	-4.002349
H	0.909616	-5.718640	0.835321
H	0.649800	-3.795769	4.317279
H	0.635336	1.060737	5.791204
H	0.300369	4.523025	3.864184
H	-0.265914	5.935192	-0.977399

N	0.624559	-3.375567	6.954187
H	0.610817	-3.151067	7.952178
H	0.624320	-4.359713	6.675314
N	1.329017	-6.854119	-3.588690
H	1.359255	-7.852354	-3.367219
H	1.390068	-6.569994	-4.569350
N	0.202559	3.634581	-7.098592
H	0.032839	4.603913	-6.819892
H	0.257385	3.416665	-8.096506
N	-0.147350	7.122313	3.452013
H	-0.041004	6.853519	4.433163
H	-0.323884	8.105714	3.232308
S	-4.493284	-0.391826	-0.644577
C	-4.806364	1.227686	-0.455941
N	-5.036854	2.391629	-0.314162

MeO - Stage I

E = -3998.025146

G = -3997.561816

S	-1.806643	0.662617	-0.712896
C	-1.890639	2.206996	-0.062090

N   -2.009032   3.307015   0.370341

Co   0.140807   -0.109440   0.023765

C   -0.071816   1.227022   2.684044

C   -0.644795   1.035925   4.006114

C   -1.298881   -0.220992   3.984304

C   -1.080580   -0.773083   2.648203

N   -0.325011   0.105906   1.888898

C   1.542598   2.274689   -1.064674

C   1.907628   3.634496   -0.707859

C   1.581317   3.793896   0.662178

C   1.011560   2.520740   1.097694

N   1.014013   1.614529   0.049462

C   0.603119   -1.561206   -2.544427

C   1.163062   -1.365096   -3.871339

C   1.652570   -0.035644   -3.910097

C   1.392267   0.534299   -2.589053

N   0.786061   -0.408346   -1.775571

C   -1.288701   -2.493604   1.106420

C   -1.719044   -3.830198   0.731516

C   -1.253868   -4.048504   -0.589556

C   -0.556347   -2.826113   -0.985126

N   -0.572908   -1.912989   0.056107

N   -1.538269   -1.965802   2.293498

N	0.556239	2.335098	2.328922
N	1.722577	1.780153	-2.278271
N	-0.005851	-2.678726	-2.182618
C	2.256948	0.494841	-5.052401
C	-1.473250	-5.254831	-1.259156
C	-2.424906	-4.834730	1.414150
C	-1.970534	-0.722086	5.102139
C	-0.659586	1.828431	5.165520
C	1.794050	4.998741	1.336019
C	2.463915	4.698407	-1.437468
C	1.267435	-2.197168	-4.998114
C	1.868443	-1.681857	-6.155661
H	1.955709	-2.321682	-7.044028
C	2.362484	-0.345785	-6.186394
C	-2.185166	-6.265142	-0.569473
C	-2.657933	-6.051694	0.757573
H	-3.208881	-6.845214	1.279870
C	-1.983776	0.077735	6.269711
C	-1.332071	1.344428	6.297065
H	-1.351669	1.954747	7.209906
C	2.677380	5.918604	-0.780871
H	3.103690	6.761167	-1.341551
C	2.344699	6.072412	0.596437

H	0.889548	-3.230184	-4.981043
H	2.641867	1.523825	-5.093931
H	-1.113033	-5.437251	-2.281761
H	-2.787983	-4.678961	2.440907
H	-2.479951	-1.696341	5.098080
H	-0.157610	2.806934	5.193479
H	1.539834	5.135462	2.396812
H	2.721102	4.587176	-2.501292
O	2.520866	7.233624	1.286185
O	2.957178	0.210377	-7.278621
O	-2.374999	-7.425956	-1.256871
O	-2.652087	-0.446402	7.335091
C	-2.711105	0.309353	8.549365
H	-3.224990	1.282371	8.395814
H	-3.293979	-0.303604	9.261290
H	-1.696296	0.488624	8.964462
C	-3.076767	-8.497699	-0.617674
H	-2.548936	-8.836569	0.299431
H	-4.116415	-8.203791	-0.358814
H	-3.102459	-9.324576	-1.351108
C	3.102555	-0.582012	-8.462164
H	2.115138	-0.895026	-8.863847
H	3.608750	0.065719	-9.201400

H	3.726866	-1.481379	-8.272987
C	3.043085	8.373645	0.595122
H	2.382077	8.674756	-0.245576
H	3.081339	9.189504	1.340255
H	4.067014	8.180145	0.209927

MeO - Stage II

E = -3997.842932

G = -3997.380408

S	-1.769213	0.694905	-0.723979
C	-1.939885	2.130466	0.128807
N	-2.116736	3.155424	0.701174
Co	0.156145	-0.113619	0.021055
C	-0.058771	1.213964	2.681748
C	-0.644265	1.031596	3.996054
C	-1.308734	-0.217736	3.969232
C	-1.083742	-0.774890	2.631057
N	-0.315632	0.101004	1.878871
C	1.554091	2.272697	-1.059995
C	1.927261	3.626728	-0.700646
C	1.619629	3.776740	0.672934

C	1.043643	2.500134	1.107031
N	1.031990	1.602966	0.050224
C	0.602964	-1.551332	-2.554007
C	1.152088	-1.352750	-3.881675
C	1.647629	-0.027286	-3.917104
C	1.393143	0.541821	-2.589278
N	0.786154	-0.404207	-1.778632
C	-1.284777	-2.493125	1.091224
C	-1.700929	-3.833407	0.724613
C	-1.220790	-4.057620	-0.588137
C	-0.534485	-2.825137	-0.990847
N	-0.567050	-1.907763	0.047012
N	-1.546388	-1.961747	2.278031
N	0.591517	2.316340	2.335507
N	1.725868	1.783456	-2.280435
N	0.007429	-2.678699	-2.188124
C	2.246961	0.507081	-5.053165
C	-1.416079	-5.265503	-1.249996
C	-2.399851	-4.838328	1.412381
C	-1.994509	-0.713015	5.073594
C	-0.659350	1.826572	5.152962
C	1.838338	4.970032	1.353191
C	2.475700	4.692599	-1.432058

C	1.246464	-2.183141	-5.009799
C	1.844844	-1.667112	-6.169213
H	1.924432	-2.303877	-7.060227
C	2.344501	-0.335440	-6.196683
C	-2.124131	-6.284544	-0.552167
C	-2.611135	-6.065745	0.766265
H	-3.155652	-6.861144	1.291882
C	-2.010169	0.093035	6.246935
C	-1.346623	1.350849	6.280069
H	-1.367878	1.962298	7.191853
C	2.698516	5.909747	-0.771076
H	3.117577	6.755330	-1.332254
C	2.383031	6.054414	0.608789
H	0.863178	-3.213825	-4.993236
H	2.636502	1.534101	-5.093922
H	-1.044567	-5.454045	-2.267198
H	-2.773844	-4.676143	2.433882
H	-2.514279	-1.681488	5.066647
H	-0.147534	2.799519	5.183021
H	1.598242	5.101151	2.417764
H	2.718488	4.586841	-2.499508
O	-2.690979	-0.427165	7.293923
O	-2.284693	-7.443375	-1.231593

O	2.935489	0.224956	-7.276943
O	2.561827	7.199470	1.306122
C	3.077336	8.355012	0.629355
H	2.406257	8.663163	-0.199744
H	3.118818	9.156038	1.389356
H	4.097153	8.163993	0.234292
C	3.082068	-0.553690	-8.473279
H	2.092535	-0.855834	-8.875991
H	3.592238	0.103551	-9.200352
H	3.701938	-1.456022	-8.287921
C	-2.974267	-8.531149	-0.599202
H	-4.020936	-8.252144	-0.355727
H	-2.972207	-9.357239	-1.333051
H	-2.448252	-8.852597	0.324325
C	-2.761993	0.318930	8.517231
H	-3.266959	1.295051	8.359421
H	-3.358056	-0.298381	9.213313
H	-1.749691	0.485850	8.941488

MeO - Stage III-a

E = -3997.631789

G = -3997.169644

S	-1.986430	0.776077	-0.781685
C	-1.937195	2.336336	-0.194642
N	-1.900870	3.448279	0.227101
Co	0.070939	-0.081943	0.003850
C	-0.063290	1.214272	2.694512
C	-0.563285	0.990737	4.028215
C	-1.221584	-0.265298	4.007035
C	-1.069789	-0.788527	2.639945
N	-0.354583	0.110057	1.876247
C	1.485947	2.303508	-1.067725
C	1.806397	3.670039	-0.731116
C	1.472531	3.833932	0.635160
C	0.935429	2.538963	1.086612
N	0.952826	1.638511	0.043622
C	0.638228	-1.569683	-2.524597
C	1.250756	-1.398199	-3.818190
C	1.744110	-0.069264	-3.858046
C	1.421274	0.529843	-2.553081
N	0.782985	-0.402205	-1.759169
C	-1.350340	-2.475340	1.078262
C	-1.798402	-3.796284	0.700274
C	-1.319611	-4.020282	-0.612841

C	-0.591784	-2.799998	-1.001009
N	-0.637129	-1.884792	0.027802
N	-1.565563	-1.960944	2.283378
N	0.528706	2.343161	2.330034
N	1.713019	1.786288	-2.270352
N	0.001777	-2.681429	-2.176680
C	2.378848	0.447221	-4.973644
C	-1.540671	-5.210434	-1.285973
C	-2.525666	-4.788802	1.379450
C	-1.846388	-0.787727	5.125922
C	-0.525458	1.767745	5.201270
C	1.656630	5.033981	1.300085
C	2.342137	4.736472	-1.474482
C	1.387589	-2.254079	-4.927440
C	2.029514	-1.761957	-6.069161
H	2.149116	-2.413909	-6.944338
C	2.523726	-0.425653	-6.101247
C	-2.288792	-6.219911	-0.596687
C	-2.772949	-6.002400	0.721553
H	-3.342375	-6.786749	1.236907
C	-1.801498	-0.000658	6.322455
C	-1.145229	1.264187	6.350254
H	-1.124975	1.853553	7.276309

C	2.526624	5.969271	-0.833269
H	2.934450	6.815219	-1.401610
C	2.190027	6.125383	0.539073
H	1.002755	-3.283630	-4.902338
H	2.762300	1.475813	-5.025816
H	-1.170591	-5.402936	-2.302923
H	-2.894976	-4.624799	2.402136
H	-2.364797	-1.756725	5.128024
H	-0.022170	2.745034	5.220129
H	1.404712	5.178313	2.360145
H	2.605958	4.615108	-2.535056
O	-2.416618	-0.548140	7.378770
O	-2.479193	-7.352342	-1.293204
O	3.146112	0.116949	-7.155289
O	2.331897	7.271153	1.223992
C	2.842254	8.437562	0.554637
H	2.181909	8.724493	-0.289556
H	2.850705	9.238637	1.314726
H	3.872633	8.256642	0.184975
C	3.346171	-0.664194	-8.347971
H	2.371633	-0.969615	-8.780759
H	3.879588	-0.001266	-9.051495
H	3.962814	-1.559695	-8.128435

C	-3.218076	-8.433104	-0.697681
H	-4.253882	-8.114461	-0.459726
H	-3.236214	-9.236276	-1.455405
H	-2.711905	-8.792840	0.221929
C	-2.435412	0.150683	8.637395
H	-2.959127	1.123068	8.534336
H	-2.988578	-0.504253	9.333114
H	-1.402678	0.311817	9.008470

MeO - Stage III-b

E = -3997.645337

G = -3997.181886

S	-1.761246	0.726553	-0.729399
C	-1.992703	2.066725	0.253633
N	-2.206636	3.024695	0.920892
Co	0.154288	-0.112415	0.014552
C	-0.068841	1.211991	2.674504
C	-0.679239	1.048229	3.972864
C	-1.351127	-0.196360	3.943545
C	-1.102659	-0.769842	2.610436
N	-0.318384	0.098657	1.868350

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C    1.564891     2.271231    -1.056967

C    1.969670     3.608066    -0.690974

C    1.674866     3.751719     0.685352

C    1.066560     2.481330     1.113151

N    1.033630     1.596950     0.047514

C    0.574683    -1.533625    -2.572464

C    1.095266    -1.328811    -3.903876

C    1.598388    -0.006811    -3.937497

C    1.368623     0.556887    -2.596720

N    0.766569    -0.392490    -1.788118

C   -1.281872    -2.496050     1.081556

C   -1.668542    -3.843034     0.731386

C   -1.183097    -4.069615    -0.578270

C   -0.525298    -2.820187    -0.997232

N   -0.576415    -1.899026     0.034741

N   -1.560075    -1.956472     2.265374

N    0.607960     2.306032     2.335954

N    1.717550     1.789536    -2.287269

N   -0.001376    -2.672743    -2.197866

C    2.180773     0.532119    -5.072750

C   -1.347609    -5.282359    -1.226375

C   -2.344729    -4.855532     1.433578

C   -2.059701    -0.677359     5.031859
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C	-0.708692	1.856287	5.122238
C	1.919850	4.927872	1.373773
C	2.535981	4.668073	-1.420295
C	1.164476	-2.155134	-5.038666
C	1.745408	-1.637123	-6.205008
H	1.804927	-2.267301	-7.102016
C	2.253626	-0.310126	-6.230168
C	-2.033185	-6.316828	-0.509306
C	-2.525518	-6.096193	0.805163
H	-3.049452	-6.898382	1.340808
C	-2.093729	0.147377	6.203495
C	-1.421493	1.398965	6.240123
H	-1.456396	2.019172	7.145339
C	2.789839	5.875032	-0.753248
H	3.222763	6.716276	-1.310039
C	2.486163	6.013188	0.628434
H	0.774200	-3.182906	-5.019549
H	2.578352	1.555899	-5.115706
H	-0.973998	-5.476476	-2.241710
H	-2.722984	-4.687093	2.452263
H	-2.586791	-1.641787	5.026885
H	-0.188334	2.824464	5.150859
H	1.690430	5.058245	2.440774

H	2.767632	4.563695	-2.490148
O	-2.799588	-0.360785	7.226409
O	-2.156305	-7.475434	-1.176867
O	2.829812	0.256601	-7.302487
O	2.686884	7.135543	1.337174
C	3.223652	8.299158	0.684305
H	2.553441	8.631752	-0.135059
H	3.280661	9.079553	1.463558
H	4.237016	8.091031	0.283302
C	2.963762	-0.501996	-8.517187
H	1.967003	-0.788399	-8.911562
H	3.472553	0.167304	-9.233098
H	3.578160	-1.409976	-8.345807
C	-2.811975	-8.588641	-0.545169
H	-3.866802	-8.338943	-0.308096
H	-2.776474	-9.412805	-1.279336
H	-2.275920	-8.883851	0.380469
C	-2.912211	0.388125	8.448816
H	-3.411253	1.361992	8.265392
H	-3.530410	-0.230525	9.122975
H	-1.912297	0.554670	8.899979

MeO - Stage IV

E = -4488.718421

G = -4488.252670

S	-1.636211	-0.251755	-0.076229
C	-2.240724	0.883455	1.002822
N	-2.696227	1.673288	1.760524
Co	0.555498	0.076007	-0.012888
C	0.644419	0.439443	2.949147
C	0.763007	-0.316205	4.179272
C	0.874614	-1.677128	3.806731
C	0.837899	-1.707199	2.339718
N	0.724844	-0.422537	1.845110
C	0.314574	3.031886	-0.360826
C	0.095539	4.243535	0.399393
C	0.113117	3.870609	1.764803
C	0.357688	2.423622	1.792144
N	0.473194	1.940054	0.504443
C	0.695878	-0.258070	-2.973388
C	0.614847	0.498887	-4.203164
C	0.492162	1.859447	-3.830752
C	0.493325	1.884899	-2.362244
N	0.652964	0.604536	-1.868305

C	0.907317	-2.866656	0.335399
C	0.997649	-4.094996	-0.426449
C	0.958107	-3.725524	-1.792556
C	0.848281	-2.261298	-1.819900
N	0.831913	-1.766923	-0.530266
N	0.911576	-2.841124	1.659302
N	0.466215	1.750166	2.927951
N	0.353560	3.012076	-1.683820
N	0.784097	-1.580555	-2.953406
C	0.385704	2.875717	-4.770425
C	1.027578	-4.665485	-2.813440
C	1.108006	-5.443932	-0.051022
C	0.996460	-2.692760	4.747842
C	0.770639	0.059936	5.532428
C	-0.077901	4.794287	2.784761
C	-0.127358	5.577930	0.022149
C	0.623800	0.123298	-5.557577
C	0.514386	1.128938	-6.527489
H	0.517041	0.853096	-7.590168
C	0.400928	2.495351	-6.144632
C	1.132779	-6.035588	-2.432294
C	1.172843	-6.414050	-1.061755
H	1.255696	-7.473024	-0.784122

C	1.000242	-2.311608	6.121136
C	0.890700	-0.945499	6.502835
H	0.897641	-0.667838	7.565069
C	-0.330726	6.529629	1.031213
H	-0.512211	7.576548	0.754232
C	-0.307614	6.148039	2.402203
H	0.712046	-0.931487	-5.855860
H	0.287235	3.935289	-4.495639
H	0.999056	-4.393857	-3.878073
H	1.141912	-5.739796	1.007597
H	1.081798	-3.753623	4.473330
H	0.684603	1.114782	5.831304
H	-0.067588	4.519653	3.848886
H	-0.149893	5.873837	-1.036531
S	-2.724302	1.121199	-2.384376
C	-2.867065	2.565769	-1.592260
N	-2.990466	3.611369	-1.029280
O	-0.499259	7.007676	3.425586
O	0.297977	3.514944	-7.022052
O	1.186251	-6.912618	-3.457248
O	1.109910	-3.331888	6.999358
C	1.275795	-8.317116	-3.172378
H	0.392706	-8.661049	-2.594259

H	1.297709	-8.822549	-4.154445
H	2.205101	-8.549895	-2.611620
C	1.102320	-3.046809	8.406357
H	0.152957	-2.555694	8.706505
H	1.191434	-4.024884	8.912264
H	1.962307	-2.402894	8.685788
C	-0.752320	8.391455	3.139545
H	-1.677067	8.509064	2.536992
H	-0.883111	8.882586	4.120470
H	0.105358	8.849816	2.604222
C	0.309384	3.232806	-8.430141
H	-0.549549	2.588800	-8.712079
H	0.220719	4.212059	-8.933654
H	1.260020	2.743177	-8.728099

MeO - Stage V

E = -4488.721313

G = -4488.252212

S	-1.695843	-0.377325	0.063141
C	-2.173203	0.320079	1.510143
N	-2.559840	0.780430	2.534246

Co	0.469364	0.089914	-0.034231
C	0.642415	0.472212	2.911072
C	0.717799	-0.281786	4.145386
C	0.817203	-1.643507	3.777911
C	0.814298	-1.675515	2.306996
N	0.731509	-0.386083	1.808661
C	0.069634	3.030618	-0.392594
C	-0.025698	4.262088	0.371112
C	0.129851	3.904158	1.728296
C	0.324884	2.447887	1.751735
N	0.292050	1.943114	0.469999
C	0.556443	-0.241336	-2.992870
C	0.465971	0.501790	-4.228333
C	0.234976	1.852492	-3.871295
C	0.149783	1.875161	-2.394829
N	0.407894	0.596158	-1.896595
C	0.906148	-2.830965	0.305301
C	1.042994	-4.060329	-0.449230
C	1.011938	-3.695985	-1.815794
C	0.843747	-2.233765	-1.849163
N	0.804063	-1.739153	-0.550299
N	0.892655	-2.808121	1.634925
N	0.498381	1.788471	2.887341

N	0.045655	3.004743	-1.714154
N	0.751290	-1.563092	-2.975424
C	0.164418	2.863258	-4.815805
C	1.120575	-4.633597	-2.832265
C	1.188949	-5.402875	-0.066913
C	0.893209	-2.659491	4.719071
C	0.693836	0.097567	5.496397
C	0.080423	4.841604	2.752471
C	-0.235034	5.597463	0.001802
C	0.593067	0.126151	-5.578181
C	0.505413	1.124380	-6.556072
H	0.600458	0.851062	-7.615042
C	0.303131	2.484184	-6.184270
C	1.262544	-6.001588	-2.445007
C	1.297052	-6.374406	-1.074106
H	1.408036	-7.429554	-0.791706
C	0.862266	-2.275793	6.095260
C	0.766721	-0.908757	6.472024
H	0.745648	-0.629133	7.533430
C	-0.291084	6.568021	1.015680
H	-0.458420	7.618196	0.742627
C	-0.136661	6.201035	2.379721
H	0.763929	-0.921981	-5.863458

H	-0.004854	3.916757	-4.553098
H	1.096429	-4.366338	-3.898145
H	1.216033	-5.694511	0.992991
H	0.968278	-3.722069	4.448242
H	0.617031	1.154256	5.790773
H	0.197314	4.574903	3.812294
H	-0.361475	5.885047	-1.052005
S	-2.679974	1.579800	-2.805278
C	-2.815789	2.382824	-1.376312
N	-2.866253	2.984396	-0.342494
O	-0.180244	7.077099	3.407257
O	0.226251	3.499040	-7.067473
O	1.354765	-6.875253	-3.467214
O	0.927716	-3.296804	6.971767
C	1.482221	-8.277556	-3.182097
H	0.602626	-8.646080	-2.614053
H	1.529971	-8.780639	-4.164300
H	2.411626	-8.482029	-2.610860
C	0.888294	-3.015204	8.379958
H	-0.060444	-2.508671	8.654438
H	0.947753	-3.996111	8.884275
H	1.751413	-2.385771	8.681049
C	-0.393706	8.468766	3.127818

H	-1.372259	8.628164	2.628307
H	-0.390070	8.977140	4.108672
H	0.421391	8.875555	2.493162
C	0.360117	3.222552	-8.470803
H	-0.445067	2.542432	-8.818190
H	0.268016	4.198939	-8.979094
H	1.351791	2.776317	-8.692973

H - Stage I

E = -3540.229927

G = -3539.878024

S	-1.846849	0.636103	-0.762555
C	-2.125691	2.020051	0.146029
N	-2.385274	3.006662	0.753304
Co	0.102315	-0.090149	-0.008581
C	-1.272654	-2.515561	1.034715
C	-1.669563	-3.864138	0.643330
C	-1.175036	-4.060775	-0.668503
C	-0.504744	-2.820717	-1.045786
N	-0.560291	-1.912739	0.004677
C	-0.174787	1.214639	2.653157

C	-0.767838	1.003189	3.969295
C	-1.382856	-0.270850	3.929949
C	-1.129771	-0.809661	2.597863
N	-0.384342	0.097663	1.851929
C	1.415982	2.347928	-1.070229
C	1.769021	3.711408	-0.689978
C	1.448499	3.838630	0.682746
C	0.889294	2.556326	1.095909
N	0.895178	1.667924	0.026843
C	0.610934	-1.496313	-2.585895
C	1.163443	-1.267757	-3.917013
C	1.604243	0.077174	-3.940833
C	1.325531	0.625116	-2.617777
N	0.749855	-0.349417	-1.810951
N	0.046655	-2.641792	-2.236540
N	-1.551415	-2.007746	2.225097
N	0.434274	2.341410	2.320321
N	1.615197	1.874974	-2.289865
C	1.665332	5.041587	1.375273
C	2.186926	0.634468	-5.091578
C	1.290369	-2.097552	-5.043827
C	-1.371118	-5.274407	-1.348740
C	-2.373518	-4.876532	1.317086

C	-2.063749	-0.787689	5.045032
C	-0.817523	1.802846	5.123350
C	2.319399	4.783055	-1.413252
C	2.533312	5.987506	-0.722658
H	2.957666	6.851319	-1.257248
C	2.211373	6.114832	0.651783
C	2.312731	-0.193998	-6.219076
C	1.871567	-1.540706	-6.195229
H	1.987193	-2.160025	-7.098069
C	-2.077599	-6.285830	-0.676809
C	-2.571814	-6.089628	0.636911
H	-3.120303	-6.905653	1.132149
C	-1.500507	1.288121	6.237908
H	-1.561674	1.886262	7.160136
C	-2.114716	0.011408	6.199286
H	2.567334	4.682876	-2.480227
H	1.413096	5.138483	2.441516
H	2.528901	1.679772	-5.107792
H	0.947230	-3.142384	-5.023714
H	-0.984826	-5.425269	-2.367560
H	-2.754169	-4.723657	2.337731
H	2.762054	0.208230	-7.140138
H	2.392105	7.074934	1.159365

H   -2.251351   -7.250612   -1.177931

H   -2.540136   -1.778617   5.012569

H   -2.642095   -0.358428   7.092131

H   -0.340800   2.793708   5.150967

H - Stage II

E = -3540.036491

G = -3539.685720

S   -1.842548   0.656026   -0.762976

C   -2.116148   2.020329   0.175480

N   -2.363911   2.993510   0.808156

Co   0.106024   -0.090997   -0.009167

C   -1.285471   -2.504673   1.026480

C   -1.695237   -3.851910   0.631589

C   -1.202640   -4.048730   -0.677827

C   -0.520879   -2.810017   -1.051077

N   -0.571666   -1.901931   -0.001294

C   -0.163026   1.208665   2.650275

C   -0.743394   0.992250   3.974672

C   -1.362197   -0.276747   3.934336

C   -1.123828   -0.808740   2.593446

N   -0.382680   0.098107   1.844088

C   1.408275   2.345595   -1.072668

C   1.744467   3.718311   -0.698621

C   1.427004   3.845368   0.671978

C   0.885007   2.553968   1.090386

N   0.895606   1.662110   0.024942

C   0.611881   -1.495464   -2.581689

C   1.183880   -1.274932   -3.909393

C   1.629783   0.065296   -3.932184

C   1.333680   0.619532   -2.612103

N   0.746021   -0.348778   -1.807285

N   0.039029   -2.638486   -2.238684

N   -1.558702   -2.001741   2.219949

N   0.442874   2.337504   2.319122

N   1.615175   1.872585   -2.291011

C   1.627267   5.047267   1.362121

C   2.227945   0.618885   -5.071127

C   1.319853   -2.110666   -5.024956

C   -1.403272   -5.253801   -1.362546

C   -2.404585   -4.854502   1.304718

C   -2.033300   -0.799693   5.046801

C   -0.775715   1.786632   5.127399

C   2.275505   4.788880   -1.429055

C	2.474238	6.003583	-0.740025
H	2.883339	6.870385	-1.280757
C	2.156889	6.130195	0.629608
C	2.366953	-0.218597	-6.197688
C	1.922247	-1.558066	-6.174634
H	2.047046	-2.182827	-7.071966
C	-2.120376	-6.265483	-0.690122
C	-2.611879	-6.069426	0.618374
H	-3.166587	-6.880993	1.113048
C	-1.451826	1.265228	6.250390
H	-1.500078	1.859576	7.175313
C	-2.069036	-0.003587	6.210717
H	2.521564	4.688878	-2.496092
H	1.378128	5.144040	2.428720
H	2.573015	1.662746	-5.087276
H	0.971896	-3.153494	-5.005930
H	-1.017372	-5.405447	-2.380989
H	-2.784285	-4.701655	2.325303
H	2.830622	0.179982	-7.112683
H	2.324425	7.093345	1.135005
H	-2.299689	-7.226759	-1.195077
H	-2.514429	-1.787856	5.013483
H	-2.589188	-0.378220	7.105270

H   -0.295694   2.775439   5.155734

H - Stage III-a

E = -3539.807726

G = -3539.458916

S   -2.048935   0.815221   -0.867392

C   -2.169467   2.204691   0.044104

N   -2.235664   3.199315   0.692963

Co   -0.017361   -0.036994   -0.050843

C   -1.477590   -2.401412   0.971625

C   -2.045313   -3.669217   0.508127

C   -1.515973   -3.891824   -0.783900

C   -0.655760   -2.747831   -1.079811

N   -0.671027   -1.855501   -0.026010

C   -0.056367   1.184848   2.666582

C   -0.386555   0.846235   4.049247

C   -1.068769   -0.391260   4.002340

C   -1.096932   -0.795261   2.595146

N   -0.465044   0.149515   1.816734

C   1.260726   2.387644   -1.132818

C   1.391053   3.809287   -0.819348

C	1.092257	3.942042	0.556323
C	0.764563	2.599564	1.036731
N	0.855648	1.686685	0.005013
C	0.704326	-1.549494	-2.514194
C	1.506048	-1.410301	-3.728115
C	1.924878	-0.060787	-3.776177
C	1.391487	0.579031	-2.571623
N	0.695228	-0.340644	-1.814348
N	0.045712	-2.649790	-2.204850
N	-1.661648	-1.929177	2.189177
N	0.470367	2.335459	2.306226
N	1.554855	1.870943	-2.310674
C	1.138250	5.180409	1.200485
C	2.685404	0.432410	-4.838147
C	1.831140	-2.315038	-4.743742
C	-1.814201	-5.048270	-1.510566
C	-2.892266	-4.596071	1.120237
C	-1.562249	-0.999871	5.158636
C	-0.178867	1.523102	5.254978
C	1.744960	4.912794	-1.601050
C	1.772084	6.174413	-0.960121
H	2.030935	7.069540	-1.544985
C	1.476932	6.304920	0.409656

C   3.031418   -0.483110   -5.862730

C   2.614560   -1.826119   -5.816143

H   2.898808   -2.509115   -6.630260

C   -2.686682   -5.982877   -0.903492

C   -3.213848   -5.761612   0.382225

H   -3.885030   -6.510991   0.827548

C   -0.663384   0.905522   6.432237

H   -0.509125   1.401224   7.402172

C   -1.340225   -0.327591   6.385027

H   1.986852   4.807957   -2.668423

H   0.914492   5.280328   2.272189

H   2.999023   1.485107   -4.882463

H   1.493708   -3.360822   -4.711573

H   -1.387949   -5.226526   -2.508196

H   -3.291132   -4.431957   2.131511

H   3.634996   -0.133465   -6.713544

H   1.508487   7.300522   0.876652

H   -2.952741   -6.901999   -1.446417

H   -2.101707   -1.956938   5.120270

H   -1.707919   -0.778315   7.318829

H   0.340532   2.491449   5.288969

H - Stage III-b

E = -3539.823858

G = -3539.472726

S	-1.827854	0.681289	-0.790168
C	-2.115097	2.020762	0.177624
N	-2.360586	2.981133	0.830132
Co	0.108450	-0.086051	-0.009897
C	-1.358206	-2.455693	1.001776
C	-1.919696	-3.728399	0.547750
C	-1.446018	-3.922797	-0.767817
C	-0.619454	-2.758082	-1.083026
N	-0.590000	-1.884428	-0.004547
C	-0.089536	1.189767	2.660361
C	-0.506517	0.902247	4.033080
C	-1.111033	-0.372558	4.004044
C	-1.032454	-0.834576	2.617885
N	-0.378435	0.108031	1.835607
C	1.333465	2.364233	-1.103728
C	1.498863	3.781872	-0.785247
C	1.170660	3.921566	0.580787
C	0.793037	2.589519	1.050589
N	0.889870	1.668164	0.016414

C	0.676566	-1.521704	-2.543632
C	1.408266	-1.362719	-3.801203
C	1.878991	-0.032142	-3.820831
C	1.430913	0.580273	-2.570310
N	0.753959	-0.353096	-1.795889
N	0.012090	-2.624614	-2.239369
N	-1.542302	-1.991821	2.226604
N	0.431551	2.350387	2.301560
N	1.634114	1.856837	-2.287407
C	1.239300	5.156691	1.229875
C	2.603677	0.473400	-4.903251
C	1.643279	-2.238937	-4.863447
C	-1.763613	-5.069709	-1.499958
C	-2.727153	-4.675255	1.182942
C	-1.651481	-0.954007	5.153752
C	-0.422108	1.647258	5.211689
C	1.910142	4.873094	-1.554711
C	1.965984	6.132722	-0.908557
H	2.271825	7.018906	-1.484285
C	1.638859	6.271205	0.452106
C	2.857545	-0.412728	-5.979243
C	2.388890	-1.738073	-5.959511
H	2.600698	-2.399725	-6.812502

C   -2.595106   -6.027353   -0.868703

C   -3.065719   -5.834742   0.442298

H   -3.707195   -6.599442   0.904964

C   -0.957942   1.060200   6.384786

H   -0.905352   1.613168   7.334348

C   -1.558587   -0.210651   6.356420

H   2.174674   4.762761   -2.616099

H   0.991010   5.261404   2.295735

H   2.959411   1.513393   -4.922804

H   1.266680   -3.271687   -4.852334

H   -1.384551   -5.224895   -2.520227

H   -3.084782   -4.529809   2.212321

H   3.429657   -0.053541   -6.847555

H   1.693551   7.263724   0.923397

H   -2.873812   -6.940580   -1.415242

H   -2.130459   -1.943216   5.128183

H   -1.968462   -0.636726   7.284140

H   0.037537   2.645750   5.230333

H - Stage IV

E = -4030.902133

G = -4030.550412

S	-1.721466	0.731953	-0.767513
C	-2.471094	1.454517	0.576660
N	-2.944572	1.999829	1.510905
Co	0.343616	-0.055487	0.082314
C	-0.954337	-2.507179	1.163836
C	-1.371717	-3.851348	0.765719
C	-0.930156	-4.027894	-0.566416
C	-0.259065	-2.785596	-0.946912
N	-0.286623	-1.886957	0.114265
C	0.022448	1.279108	2.722110
C	-0.560848	1.069721	4.047888
C	-1.100835	-0.235770	4.041660
C	-0.826403	-0.787495	2.714390
N	-0.141520	0.141753	1.943046
C	1.714871	2.366948	-0.970581
C	2.110708	3.721845	-0.583019
C	1.723331	3.877739	0.767029
C	1.096414	2.616252	1.163566
N	1.107674	1.724915	0.099432
C	0.835880	-1.455170	-2.499149
C	1.409834	-1.240785	-3.828200
C	1.892204	0.087389	-3.842524

C	1.606606	0.643129	-2.518849
N	0.974472	-0.308224	-1.729349
N	0.266796	-2.599711	-2.148521
N	-1.210585	-2.006603	2.363516
N	0.601932	2.419913	2.376801
N	1.940201	1.880857	-2.182652
C	1.954288	5.071720	1.461311
C	2.508271	0.629645	-4.976993
C	1.525610	-2.073022	-4.948320
C	-1.174794	-5.216276	-1.266794
C	-2.071825	-4.858015	1.443319
C	-1.751482	-0.764022	5.163183
C	-0.652630	1.893699	5.176114
C	2.744553	4.754070	-1.285639
C	2.977762	5.959985	-0.591077
H	3.470765	6.795613	-1.110488
C	2.589924	6.115918	0.756725
C	2.626500	-0.204683	-6.108886
C	2.144425	-1.530754	-6.094750
H	2.253290	-2.153836	-6.995346
C	-1.877972	-6.232359	-0.587659
C	-2.318094	-6.056499	0.742405
H	-2.864963	-6.870937	1.241083

C   -1.308156   1.366495   6.309165

H   -1.401837   1.984489   7.214959

C   -1.847681   0.062682   6.302754

H   3.045789   4.631600   -2.336126

H   1.651328   5.191371   2.511630

H   2.883294   1.663299   -4.986164

H   1.149898   -3.106369   -4.935662

H   -0.832880   -5.350383   -2.303234

H   -2.415536   -4.718945   2.478511

H   3.103559   0.186309   -7.020309

H   2.786702   7.070587   1.267737

H   -2.089321   -7.180824   -1.104318

H   -2.172119   -1.779993   5.155648

H   -2.353968   -0.316107   7.203515

H   -0.233751   2.910384   5.178766

S   -3.080264   -1.047995   -1.010321

C   -4.237909   -0.339127   -2.007809

N   -5.082811   0.102969   -2.709044

H - Stage V

E = -4030.910372

G = -4030.552815

S	-1.544177	0.836960	-1.063995
C	-1.818199	2.239960	-0.189524
N	-2.044225	3.254757	0.383741
Co	0.231674	-0.043939	-0.065356
C	-1.294647	-2.425730	0.900627
C	-1.574583	-3.828218	0.538569
C	-0.971273	-4.035989	-0.719389
C	-0.322366	-2.779605	-1.081297
N	-0.494542	-1.836096	-0.093183
C	-0.193438	1.270922	2.555363
C	-0.799344	1.061059	3.869697
C	-1.409314	-0.209376	3.827968
C	-1.164522	-0.739499	2.481158
N	-0.405052	0.181612	1.740566
C	1.714457	2.321386	-1.028894
C	2.045980	3.696474	-0.649366
C	1.602951	3.859104	0.680222
C	1.000470	2.583388	1.072693
N	1.101395	1.664938	0.027358
C	0.922981	-1.508543	-2.560930
C	1.590612	-1.313320	-3.850263
C	2.082203	0.009186	-3.846817

C	1.708047	0.583585	-2.552188
N	1.031494	-0.350469	-1.788260
N	0.326057	-2.635752	-2.237730
N	-1.536690	-1.947241	2.118239
N	0.452876	2.395742	2.255491
N	2.004265	1.832543	-2.224418
C	1.760699	5.068663	1.363226
C	2.776628	0.536543	-4.939603
C	1.775251	-2.161090	-4.946680
C	-1.041505	-5.275054	-1.372525
C	-2.247720	-4.853754	1.206244
C	-2.081129	-0.735652	4.933594
C	-0.846081	1.861585	5.017029
C	2.665430	4.736878	-1.348233
C	2.823236	5.964905	-0.666418
H	3.300040	6.810953	-1.183659
C	2.380706	6.127230	0.661430
C	2.964869	-0.313790	-6.052895
C	2.475031	-1.634830	-6.056167
H	2.639252	-2.269160	-6.940125
C	-1.729844	-6.310990	-0.710985
C	-2.315717	-6.105301	0.556812
H	-2.839249	-6.938631	1.049337

C   -1.526628   1.338608   6.137560

H   -1.587117   1.935642   7.059840

C   -2.129843   0.064724   6.096887

H   3.009944   4.608658   -2.384390

H   1.414269   5.193055   2.399213

H   3.157702   1.567770   -4.935504

H   1.392082   -3.191566   -4.947515

H   -0.572059   -5.431660   -2.354343

H   -2.713006   -4.691484   2.188948

H   3.504012   0.064203   -6.934509

H   2.518613   7.097545   1.161627

H   -1.808237   -7.299675   -1.187448

H   -2.556942   -1.726135   4.898801

H   -2.651699   -0.313276   6.988978

H   -0.373825   2.854037   5.043912

S   -3.796744   -1.755372   -0.036719

C   -3.773480   -0.492562   1.013276

N   -3.694297   0.389479   1.818260

F - Stage I

E = -5126.687302

G = -5126.483510

S	-1.836196	0.633526	-0.768212
C	-2.114054	2.013526	0.146497
N	-2.369029	2.997238	0.759845
Co	0.113348	-0.093591	-0.005434
C	-1.285471	-2.505709	1.028812
C	-1.685045	-3.850977	0.636607
C	-1.161960	-4.059611	-0.666171
C	-0.479663	-2.826636	-1.037248
N	-0.555202	-1.916012	0.006656
C	-0.167978	1.213121	2.651056
C	-0.760399	1.002458	3.965140
C	-1.392038	-0.267377	3.920297
C	-1.142208	-0.804262	2.588984
N	-0.387899	0.099426	1.851653
C	1.396289	2.351218	-1.078329
C	1.730655	3.718763	-0.703979
C	1.425072	3.841579	0.676359
C	0.885543	2.555006	1.094350
N	0.893529	1.671140	0.024537
C	0.651957	-1.512146	-2.566224
C	1.215300	-1.288718	-3.891246
C	1.626347	0.069208	-3.927917

C	1.330462	0.623272	-2.613367
N	0.767136	-0.355319	-1.806106
N	0.093582	-2.658753	-2.217447
N	-1.574419	-1.996116	2.214026
N	0.440896	2.338737	2.320661
N	1.598787	1.878838	-2.295784
C	1.632209	5.049221	1.355454
C	2.203273	0.615463	-5.082052
C	1.374263	-2.119101	-5.008458
C	-1.354446	-5.276912	-1.332412
C	-2.402552	-4.859034	1.293848
C	-2.071045	-0.772017	5.037251
C	-0.805447	1.789806	5.122955
C	2.251728	4.801915	-1.424095
C	2.455620	6.015969	-0.743543
F	2.943956	7.075847	-1.394879
C	2.149847	6.138177	0.630861
C	2.360299	-0.217578	-6.204479
C	1.954847	-1.570939	-6.166362
F	2.126386	-2.328968	-7.253703
C	-2.077991	-6.287422	-0.673833
C	-2.597613	-6.080451	0.623940
F	-3.279367	-7.067386	1.213468

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C   -1.489238    1.283967    6.243415

F   -1.555392    2.000801    7.369382

C   -2.116122    0.018252    6.199953

F    2.552535    4.733081   -2.724429

F    1.356723    5.209899    2.653096

F    2.602298    1.888251   -5.163094

F    1.003111   -3.402795   -5.018705

F   -0.879154   -5.518492   -2.557958

F   -2.908353   -4.708075    2.521604

F    2.901746    0.265089   -7.326953

F    2.356678    7.310488    1.238110

F   -2.284513   -7.463621   -1.274001

F   -2.678981   -1.962087    5.043283

F   -2.756647   -0.424104    7.286389

F   -0.225997    2.990923    5.207925
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F - Stage II

E = -5126.488087

G = -5126.284414

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S   -1.832239    0.653004   -0.770589

C   -2.102973    2.020379    0.164001
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N    -2.345807    2.995520    0.795179

Co    0.115971   -0.094077   -0.005608

C    -1.300424   -2.494855    1.020890

C    -1.714166   -3.835860    0.623756

C    -1.192621   -4.044721   -0.677253

C    -0.497454   -2.816136   -1.043034

N    -0.567778   -1.905826    0.000991

C    -0.158104    1.208167    2.648747

C    -0.734475    0.990795    3.970097

C    -1.368053   -0.275671    3.925431

C    -1.136365   -0.804252    2.586236

N    -0.389156    0.100895    1.844421

C     1.389541    2.348976   -1.080585

C     1.705597    3.723782   -0.712550

C     1.401564    3.847214    0.665968

C     0.880036    2.553780    1.089374

N     0.893977    1.666236    0.023144

C     0.654614   -1.512642   -2.561111

C     1.238880   -1.297541   -3.879608

C     1.654277    0.056756   -3.916112

C     1.340552    0.617226   -2.607138

N     0.764223   -0.355280   -1.802277

N     0.086515   -2.656465   -2.219016
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N	-1.582021	-1.990847	2.210209
N	0.447431	2.336089	2.319791
N	1.600702	1.875986	-2.296437
C	1.591169	5.056257	1.341576
C	2.245076	0.599119	-5.061222
C	1.408284	-2.133808	-4.986865
C	-1.391095	-5.255034	-1.348081
C	-2.437739	-4.836309	1.279298
C	-2.034580	-0.786766	5.043228
C	-0.762821	1.772696	5.128371
C	2.206553	4.807942	-1.439485
C	2.395199	6.035213	-0.761235
F	2.863731	7.090845	-1.422507
C	2.092091	6.157609	0.608161
C	2.416183	-0.242869	-6.185124
C	2.009489	-1.590196	-6.146212
F	2.189768	-2.357164	-7.218999
C	-2.125738	-6.268835	-0.689666
C	-2.642683	-6.062211	0.603298
F	-3.329722	-7.036794	1.194726
C	-1.437018	1.259653	6.261543
F	-1.482184	1.973165	7.384074
C	-2.064929	0.000525	6.218251

F   2.504445   4.742557   -2.733259

F   1.318575   5.219810   2.631983

F   2.645898   1.863503   -5.145288

F   1.036120   -3.409626   -5.000016

F   -0.920327   -5.498788   -2.567043

F   -2.941401   -4.688986   2.500480

F   2.971388   0.239839   -7.294215

F   2.278803   7.327087   1.215295

F   -2.334706   -7.434425   -1.297402

F   -2.642980   -1.968434   5.052678

F   -2.692366   -0.452460   7.301192

F   -0.184727   2.966259   5.215553

F - Stage III-a

E = -5126.255379

G = -5126.053405

S   -2.064445   0.774559   -0.814595

C   -2.132659   2.224813   0.002404

N   -2.171735   3.258399   0.590007

Co   0.001355   -0.056911   -0.043531

C   -1.397556   -2.458069   0.990609

C   -1.833681   -3.790021   0.582828

C   -1.302681   -4.004039   -0.713047

C   -0.575957   -2.791174   -1.065360

N   -0.663710   -1.875021   -0.033950

C   -0.118381   1.187481   2.662023

C   -0.602895   0.922839   4.009538

C   -1.284496   -0.318396   3.953222

C   -1.150266   -0.799802   2.582243

N   -0.441384   0.117385   1.831533

C   1.318577   2.365834   -1.100317

C   1.585006   3.754190   -0.744571

C   1.296377   3.874404   0.637213

C   0.832930   2.563579   1.075505

N   0.850398   1.678654   0.013242

C   0.660114   -1.527709   -2.549253

C   1.329787   -1.338655   -3.828488

C   1.737906   0.017793   -3.870054

C   1.334435   0.607386   -2.598244

N   0.710821   -0.346370   -1.815957

N   0.065321   -2.659796   -2.218948

N   -1.644725   -1.966913   2.191900

N   0.467660   2.321203   2.327502

N   1.554749   1.881186   -2.306419

C 1.458731   5.089602   1.305206

C 2.384958   0.541618   -4.989760

C 1.565209   -2.197580   -4.905524

C -1.500226   -5.212792   -1.384829

C -2.566234   -4.783737   1.233453

C -1.914286   -0.844972   5.081913

C -0.545726   1.664245   5.192270

C 2.038543   4.847663   -1.484641

C 2.197634   6.092517   -0.813120

F 2.618043   7.151014   -1.490797

C 1.913006   6.210862   0.555641

C 2.631126   -0.328601   -6.089512

C 2.231369   -1.673481   -6.047164

F 2.476441   -2.464594   -7.081917

C -2.250447   -6.228661   -0.730088

C -2.775420   -6.017442   0.553577

F -3.470348   -6.977690   1.145989

C -1.184285   1.134352   6.346556

F -1.139464   1.810127   7.485782

C -1.859333   -0.095228   6.290887

F 2.320877   4.787350   -2.774351

F 1.204307   5.253543   2.591565

F 2.778042   1.799643   -5.083865

F   1.202762   -3.467794   -4.914768

F   -1.022120   -5.462781   -2.590923

F   -3.073709   -4.639410   2.444920

F   3.248887   0.138974   -7.163962

F   2.065655   7.381082   1.159124

F   -2.456303   -7.385710   -1.343200

F   -2.566148   -1.994709   5.084292

F   -2.448286   -0.570129   7.378644

F   0.075875   2.825890   5.291568

F - Stage III-b

E = -5126.272042

G = -5126.067037

S   -1.836556   0.684766   -0.762290

C   -2.088992   2.037167   0.197504

N   -2.309957   3.002818   0.850619

Co   0.111425   -0.092773   -0.009500

C   -1.327858   -2.479124   1.008968

C   -1.768073   -3.808337   0.601473

C   -1.248717   -4.017936   -0.698616

C   -0.528365   -2.801889   -1.054284

N	-0.587245	-1.894166	-0.007335
C	-0.127342	1.195165	2.650925
C	-0.671738	0.964117	3.982843
C	-1.317661	-0.294179	3.936534
C	-1.123266	-0.806855	2.585675
N	-0.386842	0.101006	1.837181
C	1.360512	2.352907	-1.092288
C	1.641783	3.737225	-0.734247
C	1.355581	3.857189	0.646897
C	0.874679	2.552248	1.081656
N	0.893328	1.661479	0.018556
C	0.656864	-1.515534	-2.557395
C	1.280409	-1.314046	-3.859486
C	1.696834	0.038191	-3.897177
C	1.343274	0.612057	-2.604999
N	0.746819	-0.352041	-1.805533
N	0.074180	-2.654150	-2.222735
N	-1.593291	-1.982914	2.205280
N	0.471378	2.326357	2.320823
N	1.582234	1.877619	-2.305249
C	1.528343	5.069389	1.318058
C	2.318531	0.571023	-5.028149
C	1.481753	-2.161889	-4.950210

C	-1.461183	-5.220084	-1.376459
C	-2.502833	-4.800866	1.252922
C	-1.972166	-0.809391	5.057461
C	-0.674501	1.736858	5.145457
C	2.106250	4.827838	-1.472163
C	2.278362	6.069334	-0.797471
F	2.710042	7.124639	-1.472969
C	1.994020	6.187961	0.571257
C	2.527993	-0.286521	-6.144489
C	2.121877	-1.628739	-6.104108
F	2.332228	-2.411380	-7.153008
C	-2.212416	-6.235255	-0.720916
C	-2.725363	-6.028845	0.568284
F	-3.422928	-6.988049	1.160206
C	-1.338716	1.218695	6.292750
F	-1.351920	1.925888	7.413579
C	-1.978503	-0.028764	6.247730
F	2.386230	4.768844	-2.762351
F	1.276546	5.231661	2.604949
F	2.718428	1.827271	-5.116191
F	1.112357	-3.430435	-4.965074
F	-0.995905	-5.465826	-2.588690
F	-3.002264	-4.658053	2.467966

F   3.117202   0.190877   -7.231658

F   2.159175   7.354873   1.177730

F   -2.430089   -7.387425   -1.339218

F   -2.591476   -1.976603   5.067966

F   -2.593105   -0.491519   7.327225

F   -0.089364   2.918128   5.235784

F - Stage IV

E = -5617.355062

G = -5617.150502

S   -1.793622   0.810549   -0.815944

C   -2.551354   1.472033   0.555588

N   -3.025552   1.981300   1.508976

Co   0.316302   -0.041543   0.072572

C   -0.999799   -2.484097   1.150320

C   -1.390906   -3.835152   0.763350

C   -0.939785   -4.016523   -0.569103

C   -0.292281   -2.768692   -0.958097

N   -0.342694   -1.864729   0.095745

C   -0.041278   1.308820   2.697067

C   -0.636462   1.105584   4.014274

C   -1.182734   -0.201978   4.006081

C   -0.894946   -0.758544   2.688072

N   -0.204397   0.169322   1.923600

C   1.696128   2.373222   -0.978693

C   2.109776   3.717171   -0.586244

C   1.709192   3.879103   0.763587

C   1.059950   2.630537   1.151630

N   1.071288   1.743334   0.086297

C   0.786071   -1.436484   -2.512681

C   1.335202   -1.215132   -3.846537

C   1.828516   0.113595   -3.859045

C   1.569325   0.659825   -2.530001

N   0.940895   -0.293824   -1.742926

N   0.227515   -2.583959   -2.160597

N   -1.267599   -1.981563   2.344487

N   0.550233   2.443385   2.358362

N   1.918230   1.890764   -2.191041

C   1.961480   5.069136   1.451987

C   2.420974   0.650816   -5.005313

C   1.424546   -2.027272   -4.980429

C   -1.168978   -5.216186   -1.250320

C   -2.075749   -4.851551   1.436390

C   -1.834116   -0.718091   5.129721

C	-0.735876	1.920187	5.145564
C	2.771500	4.741908	-1.268524
C	3.029734	5.947929	-0.575020
F	3.655686	6.946378	-1.195170
C	2.629994	6.109522	0.764560
C	2.512065	-0.167288	-6.155978
C	2.019962	-1.485936	-6.143897
F	2.119100	-2.229903	-7.244087
C	-1.860049	-6.246558	-0.572065
C	-2.307055	-6.066691	0.751141
F	-2.954608	-7.057146	1.361005
C	-1.392998	1.400935	6.286248
F	-1.506425	2.148304	7.382646
C	-1.936492	0.102756	6.277354
F	3.166102	4.638291	-2.534378
F	1.604907	5.268597	2.717612
F	2.897131	1.891112	-5.066671
F	0.976304	-3.278884	-5.017578
F	-0.767604	-5.431851	-2.499355
F	-2.517703	-4.728111	2.684226
F	3.065758	0.313595	-7.267377
F	2.883614	7.258534	1.388207
F	-2.092704	-7.404074	-1.187319

F   -2.361637   -1.938276   5.170991

F   -2.551347   -0.355543   7.365975

F   -0.242244   3.153843   5.201140

S   -3.045583   -0.980686   -1.106437

C   -4.237800   -0.301974   -2.091283

N   -5.105103   0.107851   -2.782663

F - Stage V

E = -5617.354297

G = -5617.148327

S   -1.595550   0.658780   -0.812590

C   -2.633780   0.701130   0.512820

N   -3.364220   0.729980   1.446330

Co   0.375710   -0.071080   0.187500

C   -0.761260   -2.548950   1.341760

C   -0.936370   -3.967280   1.032690

C   -0.592470   -4.120120   -0.332910

C   -0.201780   -2.795570   -0.806200

N   -0.253810   -1.884590   0.236910

C   -0.142270   1.359900   2.709920

C   -0.934550   1.243150   3.929500

C	-1.419490	-0.087440	3.962320
C	-0.914940	-0.736280	2.756590
N	-0.175890	0.165830	2.004740
C	1.885880	2.252000	-0.843470
C	2.474810	3.511420	-0.397690
C	2.027440	3.709200	0.931160
C	1.189440	2.556240	1.257060
N	1.165760	1.670980	0.194300
C	0.532100	-1.365410	-2.462860
C	0.742320	-1.016120	-3.861810
C	1.323040	0.275550	-3.866610
C	1.440950	0.675580	-2.467400
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N	0.079130	-2.544890	-2.074140
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N	1.974240	1.828470	-2.091740
C	2.363930	4.863150	1.638350
C	1.640400	0.917530	-5.064120
C	0.447590	-1.679120	-5.053110
C	-0.695430	-5.359150	-0.968670
C	-1.386320	-5.051180	1.786280
C	-2.208080	-0.539880	5.021610

C	-1.223920	2.141210	4.958540
C	3.262460	4.466160	-1.044170
C	3.611860	5.641900	-0.329620
F	4.363670	6.568110	-0.914910
C	3.171800	5.835640	0.989190
C	1.343120	0.248280	-6.282250
C	0.760340	-1.027830	-6.276630
F	0.485760	-1.628990	-7.428360
C	-1.144150	-6.468570	-0.205190
C	-1.483760	-6.317120	1.148430
F	-1.900080	-7.370420	1.842310
C	-2.031650	1.690010	6.034240
F	-2.337850	2.525180	7.021340
C	-2.513940	0.371040	6.066360
F	3.695750	4.329220	-2.288930
F	1.963530	5.101760	2.879400
F	2.188470	2.122070	-5.122910
F	-0.103750	-2.879410	-5.099350
F	-0.396130	-5.548620	-2.245870
F	-1.726780	-4.959550	3.064360
F	1.617970	0.839580	-7.439050
F	3.513060	6.942740	1.638670
F	-1.245710	-7.663410	-0.777940

F   -2.684980   -1.774860   5.099260

F   -3.270850   -0.025670   7.083700

F   -0.790560   3.394380   4.974810

S   -3.677780   0.938370   -2.548040

C   -2.896550   -0.104410   -3.578880

N   -2.344140   -0.859930   -4.316690

NO$_2$ - Stage I

E = -4357.750929

G = -4357.408450

S   -1.850355   0.660453   -0.781452

C   -2.160652   1.993993   0.189370

N   -2.437631   2.945944   0.841906

Co   0.094129   -0.083882   -0.014939

C   -0.198233   1.214692   2.644912

C   -0.793304   1.001025   3.958769

C   -1.409829   -0.272415   3.912082

C   -1.157465   -0.808012   2.577744

N   -0.410287   0.102589   1.840036

C   1.408280   2.356029   -1.066141

C   1.759378   3.718466   -0.683056

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C    1.431685    3.841174    0.688762

C    0.870540    2.557830    1.098684

N    0.879151    1.676661    0.025453

C    0.602889   -1.480042   -2.594181

C    1.161279   -1.251095   -3.921696

C    1.605794    0.093162   -3.938584

C    1.322885    0.640644   -2.615387

N    0.739020   -0.335377   -1.818097

C   -1.303078   -2.502827    1.009893

C   -1.704121   -3.848009    0.613442

C   -1.198507   -4.042382   -0.694853

C   -0.520947   -2.803705   -1.066499

N   -0.584696   -1.900567   -0.014179

N   -1.583623   -2.000683    2.201828

N    0.413319    2.341902    2.319379

N    1.615035    1.886634   -2.285508

N    0.036821   -2.626255   -2.251581

C    2.191829    0.657686   -5.076308

C   -1.388812   -5.244318   -1.384173

C   -2.420145   -4.855690    1.282276

C   -2.091661   -0.797878    5.014503

C   -0.840535    1.800363    5.113604

C    1.633259    5.035650    1.387648
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C    1.871243   -1.534311   -6.196373

H    1.997976   -2.130880   -7.109340

C    2.307029   -0.188663   -6.189416

C   -2.107366   -6.235747   -0.699071

C   -2.621865   -6.065644    0.607319

H   -3.174043   -6.891517    1.074662

C   -2.126523    0.015705    6.157038

C   -1.520345    1.291691    6.226818

H   -1.594085    1.866712    7.159209

C    2.514309    5.996125   -0.724819

H    2.933741    6.872919   -1.235324

C    2.176148    6.095132    0.645012

H    0.941575   -3.125365   -5.033011

H    2.542717    1.696961   -5.112553

H   -1.004860   -5.416508   -2.397820

H   -2.809844   -4.704525    2.298796

H   -2.574984   -1.783182    5.001830

H   -0.363513    2.789927    5.146182

H    1.381664    5.153757    2.449382

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N   -2.833811   -0.489918    7.349999
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O	-2.855577	0.223678	8.360369
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N	2.399705	7.382776	1.331138
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O	2.874362	8.318107	0.674943

NO$_2$ - Stage II

E = -4357.541389

G = -4357.200524

S	-1.844194	0.681527	-0.778597
C	-2.110839	2.040102	0.168999
N	-2.348745	3.009538	0.810718
Co	0.098683	-0.086461	-0.012979
C	-0.179563	1.205358	2.645937
C	-0.754259	0.981509	3.973976

C	-1.378815	-0.284317	3.924572
C	-1.150765	-0.807585	2.577462
N	-0.411163	0.103211	1.834282
C	1.403531	2.349687	-1.066278
C	1.727968	3.727444	-0.691327
C	1.402535	3.850054	0.677780
C	0.869168	2.553954	1.095215
N	0.887285	1.666791	0.027819
C	0.607615	-1.483690	-2.585089
C	1.192320	-1.264272	-3.909707
C	1.643146	0.074442	-3.924985
C	1.338852	0.628943	-2.605916
N	0.739656	-0.338772	-1.811001
C	-1.322453	-2.489514	1.002742
C	-1.744027	-3.832940	0.598652
C	-1.241024	-4.027151	-0.707139
C	-0.545016	-2.792780	-1.071117
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N	1.620678	1.879730	-2.282592
N	0.026530	-2.623869	-2.251875
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C	-1.441833	-5.219630	-1.403899
C	-2.470250	-4.827347	1.264864
C	-2.046499	-0.818562	5.027690
C	-0.773788	1.770843	5.129867
C	1.577008	5.048193	1.371836
C	2.246078	4.800989	-1.425699
C	1.328548	-2.102326	-5.022818
C	1.937385	-1.558873	-6.168782
H	2.074889	-2.161843	-7.076183
C	2.377115	-0.221469	-6.160356
C	-2.175253	-6.206629	-0.720536
C	-2.686683	-6.037241	0.580018
H	-3.249781	-6.857270	1.044977
C	-2.055408	-0.013099	6.181110
C	-1.441737	1.251758	6.254168
H	-1.494591	1.819232	7.192754
C	2.424374	6.020716	-0.747411
H	2.818952	6.904005	-1.266845
C	2.090888	6.118341	0.616855
H	0.976328	-3.143016	-5.009771
H	2.603314	1.672282	-5.087058
H	-1.058370	-5.392149	-2.417737
H	-2.858628	-4.676805	2.281732

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N   -2.419027   -7.494898   -1.410544

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O   3.391369   1.493629   -7.365119

O   3.123367   -0.433413   -8.358617

N   2.284130   7.420282   1.297461

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O   2.728298   8.360831   0.632139

NO$_2$ - Stage III-a

E = -4357.297662

G = -4356.959284

S   -2.046659   0.787392   -0.810875

C	-2.379550	1.942030	0.343081
N	-2.612403	2.755612	1.178319
Co	-0.032227	-0.041423	-0.066751
C	-0.358251	1.260400	2.572976
C	-1.164810	1.144395	3.793678
C	-1.788101	-0.122875	3.735002
C	-1.337732	-0.750558	2.494072
N	-0.492590	0.126731	1.805269
C	1.494060	2.299415	-1.025253
C	2.109404	3.546612	-0.557013
C	1.807333	3.644647	0.820638
C	0.988338	2.481103	1.150210
N	0.857722	1.666036	0.015347
C	0.413377	-1.397639	-2.663577
C	0.760964	-1.088269	-4.054080
C	1.216705	0.249601	-4.058785
C	1.142338	0.718665	-2.675087
N	0.621985	-0.294491	-1.865117
C	-1.245300	-2.518592	1.005963
C	-1.376383	-3.951738	0.715799
C	-0.846491	-4.142123	-0.581058
C	-0.443066	-2.822768	-1.061774
N	-0.662794	-1.872416	-0.058094

N	-1.654838	-1.980465	2.148956
N	0.410664	2.315879	2.318602
N	1.564600	1.905254	-2.293209
N	0.000900	-2.600513	-2.279717
C	1.648039	0.876437	-5.226872
C	-0.797102	-5.400755	-1.180752
C	-1.879980	-5.012708	1.470233
C	-2.629594	-0.577633	4.749746
C	-1.355990	2.012723	4.869945
C	2.210356	4.738200	1.587876
C	2.838423	4.532367	-1.225356
C	0.724981	-1.861306	-5.217002
C	1.143910	-1.241845	-6.415185
H	1.129009	-1.788834	-7.367365
C	1.585912	0.089767	-6.395326
C	-1.294370	-6.463332	-0.400243
C	-1.827874	-6.298939	0.887707
H	-2.199791	-7.178323	1.430654
C	-2.826405	0.317258	5.820507
C	-2.218954	1.579953	5.900893
H	-2.422480	2.218448	6.771040
C	3.268145	5.642117	-0.464882
H	3.844265	6.453659	-0.929364

C   2.948752   5.721164   0.900382

H   0.384716   -2.905927   -5.210535

H   2.013301   1.911292   -5.253321

H   -0.396342   -5.569574   -2.188827

H   -2.299654   -4.864681   2.474892

H   -3.113712   -1.562688   4.731870

H   -0.864249   2.993929   4.919224

H   1.971589   4.843095   2.654293

H   3.064155   4.461657   -2.298354

N   -3.722450   -0.106497   6.926313

O   -3.887929   0.676253   7.864427

O   -4.247248   -1.219904   6.838273

N   -1.244593   -7.832228   -0.975072

O   -1.702305   -8.756343   -0.299499

O   -0.745575   -7.960039   -2.096239

N   2.016768   0.709749   -7.675039

O   2.382938   1.887593   -7.641150

O   1.982064   0.013138   -8.691552

N   3.407099   6.909545   1.665282

O   3.104379   6.968511   2.859937

O   4.059729   7.764333   1.062342

NO$_2$ - Stage III-b

E = -4357.313535

G = -4356.972294

S	-1.857645	0.714023	-0.774817
C	-2.068117	2.091301	0.157124
N	-2.263836	3.068991	0.800634
Co	0.078126	-0.099033	-0.021295
C	-0.339783	1.238398	2.583402
C	-1.165778	1.131354	3.791751
C	-1.804941	-0.125783	3.721536
C	-1.334313	-0.759746	2.489256
N	-0.476083	0.098846	1.809665
C	1.571458	2.253420	-0.995348
C	2.152114	3.518852	-0.530835
C	1.803514	3.635946	0.831762
C	1.009076	2.451027	1.159127
N	0.930760	1.611132	0.053592
C	0.436063	-1.422951	-2.643106
C	0.754458	-1.097964	-4.037765
C	1.236354	0.229337	-4.031430
C	1.209278	0.671904	-2.636511
N	0.701668	-0.333312	-1.825412

C	-1.222026	-2.543686	1.028881
C	-1.357782	-3.975462	0.735363
C	-0.847928	-4.159731	-0.568660
C	-0.437701	-2.836144	-1.041245
N	-0.626719	-1.894371	-0.038936
N	-1.638110	-2.002041	2.159973
N	0.417508	2.293100	2.329869
N	1.652103	1.856804	-2.253320
N	-0.006338	-2.610306	-2.269396
C	1.640892	0.872278	-5.199609
C	-0.812161	-5.412798	-1.176178
C	-1.858108	-5.037677	1.489986
C	-2.659877	-0.574553	4.726039
C	-1.359018	2.000560	4.866286
C	2.157724	4.749408	1.590475
C	2.874925	4.509654	-1.197063
C	0.661117	-1.844727	-5.213629
C	1.051921	-1.208256	-6.414266
H	0.991529	-1.734920	-7.376094
C	1.521446	0.112249	-6.382749
C	-1.302743	-6.480251	-0.393501
C	-1.817828	-6.322538	0.900530
H	-2.184404	-7.203356	1.444670

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C   -2.856907    0.320631    5.799067

C   -2.238262    1.575271    5.888819

H   -2.441550    2.213607    6.759126

C    3.257415    5.644239   -0.444686

H    3.828963    6.459821   -0.907628

C    2.896594    5.738624    0.906599

H    0.298366   -2.881828   -5.217516

H    2.024494    1.900699   -5.217634

H   -0.427782   -5.577896   -2.191219

H   -2.264800   -4.893009    2.500511

H   -3.154502   -1.554245    4.701786

H   -0.853326    2.974212    4.924720

H    1.882152    4.868999    2.646397

H    3.133357    4.425136   -2.261710

N   -3.766782   -0.098054    6.896399

O   -3.920188    0.676492    7.842932

O   -4.312755   -1.199633    6.792132

N   -1.264290   -7.845873   -0.977785

O   -1.709436   -8.774169   -0.299884

O   -0.785721   -7.966190   -2.108701

N    1.915424    0.753265   -7.664035

O    2.283995    1.930000   -7.620354

O    1.849246    0.074244   -8.690629
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N   3.301975   6.951504   1.663360

O   2.964581   7.020922   2.848149

O   3.948071   7.813788   1.064450

NO₂ - Stage IV

E = -4848.408648

G = -4848.066038

S   -2.094044   0.681223   -0.976726

C   -2.047940   2.376015   -0.836459

N   -1.966305   3.551919   -0.778315

Co   0.077632   -0.086859   -0.042256

C   -0.357500   1.241758   2.580407

C   -0.865448   0.982484   3.929845

C   -1.321985   -0.355609   3.930136

C   -1.095030   -0.871738   2.579058

N   -0.502057   0.107864   1.791830

C   1.468686   2.334640   -1.042504

C   1.758613   3.723320   -0.675168

C   1.253733   3.898267   0.633197

C   0.682914   2.610019   1.032122

N   0.818669   1.692055   0.001447

C	0.599315	-1.459499	-2.624468
C	1.259939	-1.260831	-3.917862
C	1.817538	0.037327	-3.880068
C	1.473921	0.597673	-2.571536
N	0.756639	-0.332070	-1.832694
C	-1.258701	-2.542261	0.985959
C	-1.715048	-3.865774	0.553831
C	-1.308038	-4.003136	-0.792829
C	-0.608082	-2.765167	-1.141971
N	-0.614882	-1.896881	-0.059229
N	-1.454338	-2.093158	2.216357
N	0.154086	2.410308	2.228942
N	1.799182	1.832154	-2.221889
N	-0.048931	-2.575222	-2.326595
C	2.518172	0.568186	-4.963469
C	-1.579798	-5.157329	-1.528384
C	-2.414152	-4.879232	1.220054
C	-1.874376	-0.943769	5.068845
C	-0.942385	1.787854	5.072678
C	1.348800	5.119482	1.300641
C	2.381570	4.766330	-1.370718
C	1.383206	-2.083742	-5.043655
C	2.087937	-1.569035	-6.147554

H	2.219978	-2.162694	-7.061846
C	2.633321	-0.272805	-6.086071
C	-2.288012	-6.163505	-0.844986
C	-2.704527	-6.049332	0.494807
H	-3.252949	-6.880204	0.957951
C	-1.938724	-0.121674	6.208766
C	-1.491175	1.213134	6.233287
H	-1.577447	1.789783	7.163745
C	2.484463	6.008514	-0.717913
H	2.958636	6.868402	-1.209219
C	1.972702	6.158404	0.584789
H	0.947315	-3.092055	-5.072659
H	2.954309	1.575413	-4.958905
H	-1.270365	-5.287160	-2.573409
H	-2.728159	-4.771846	2.267647
H	-2.237592	-1.979229	5.091078
H	-0.589383	2.828410	5.070632
H	0.964252	5.277157	2.316442
H	2.774501	4.628928	-2.387733
N	-2.509256	-0.694969	7.448818
O	-2.567514	0.028283	8.448266
O	-2.896130	-1.868073	7.414885
N	-2.609373	-7.408854	-1.578165

O	-3.228402	-8.292623	-0.976935
O	-2.239237	-7.495710	-2.754044
N	3.364612	0.239626	-7.267227
O	3.842581	1.377192	-7.198565
O	3.457151	-0.495265	-8.255558
N	2.094619	7.480114	1.240637
O	1.643451	7.598147	2.385097
O	2.639102	8.392151	0.610315
S	-3.511136	0.209990	0.609917
C	-4.920455	0.099929	-0.317523
N	-5.942373	0.002707	-0.903204

NO_2 - Stage V

E = -4848.408742

G = -4848.063814

S	-1.849544	0.765111	-0.705354
C	-2.175351	1.979760	0.412421
N	-2.403351	2.846946	1.186146
Co	0.086141	-0.009199	-0.023162
C	-0.069627	1.225980	2.669979
C	-0.579908	0.972837	4.020110

C	-1.226276	-0.282464	3.968637
C	-1.087746	-0.766888	2.595553
N	-0.348656	0.152413	1.847571
C	1.307454	2.445952	-1.097106
C	1.596676	3.833842	-0.728293
C	1.351431	3.933711	0.660138
C	0.885245	2.618474	1.096845
N	0.866928	1.743651	0.012681
C	0.627462	-1.424630	-2.578283
C	1.274469	-1.223323	-3.877396
C	1.701891	0.123596	-3.903344
C	1.326258	0.703127	-2.615116
N	0.711284	-0.263096	-1.825158
C	-1.429444	-2.360639	0.954346
C	-1.964008	-3.646399	0.505957
C	-1.405724	-3.882680	-0.771056
C	-0.603951	-2.702019	-1.099329
N	-0.625911	-1.812583	-0.033826
N	-1.621093	-1.897470	2.184108
N	0.523473	2.366036	2.339955
N	1.543672	1.969099	-2.310908
N	0.022507	-2.555216	-2.255927
C	2.341821	0.672053	-5.016344

C	-1.701287	-5.034464	-1.499982
C	-2.847754	-4.552395	1.105980
C	-1.856710	-0.831485	5.086400
C	-0.530159	1.731200	5.194977
C	1.536157	5.129015	1.356836
C	2.043643	4.927295	-1.478483
C	1.472086	-2.080952	-4.965549
C	2.120407	-1.550048	-6.095858
H	2.307266	-2.169295	-6.983309
C	2.534447	-0.204415	-6.099113
C	-2.590943	-5.931574	-0.883512
C	-3.165959	-5.715765	0.383973
H	-3.859427	-6.463020	0.791786
C	-1.796899	-0.056437	6.258820
C	-1.154827	1.193637	6.335773
H	-1.155505	1.738107	7.289379
C	2.227918	6.145182	-0.797390
H	2.567774	7.043710	-1.329355
C	1.973727	6.220552	0.584951
H	1.136029	-3.126834	-4.945959
H	2.675823	1.716616	-5.060998
H	-1.284866	-5.234860	-2.495263
H	-3.285484	-4.362524	2.095739

H   -2.370958   -1.800978   5.068088

H   -0.030575   2.709104   5.231675

H   1.350731   5.228383   2.434109

H   2.239047   4.847998   -2.556913

N   -2.450312   -0.587988   7.478504

O   -2.394990   0.092302   8.507121

O   -3.014119   -1.683779   7.395723

N   -2.946231   -7.171100   -1.614323

O   -3.740622   -7.950326   -1.079399

O   -2.426263   -7.355179   -2.719519

N   3.208644   0.322111   -7.309002

O   3.567696   1.504058   -7.297264

O   3.374137   -0.447433   -8.260114

N   2.174069   7.520468   1.268484

O   1.950155   7.570559   2.482103

O   2.552137   8.478932   0.588532

S   -4.039379   -0.886439   -0.211639

C   -3.700536   -1.754855   -1.577867

N   -3.423910   -2.375214   -2.557863

Binding mode Co-NCS (all energies are in hartree)

4-ATP - Stage I

E= -4225.364483

G= -4224.912612

N	-2.671147	1.180319	-0.885307
C	-3.675037	1.512628	-0.301519
S	-5.034497	1.964356	0.456843
Co	-0.931372	0.569576	-0.079059
C	-2.252834	-1.880391	0.967846
C	-2.534537	-3.272632	0.616436
C	-1.997480	-3.469974	-0.679172
C	-1.394409	-2.197095	-1.072012
N	-1.562307	-1.266773	-0.061495
C	-1.729815	2.056704	2.370235
C	-2.481364	1.895215	3.614006
C	-2.903215	0.543636	3.650686
C	-2.403428	-0.075290	2.423753
N	-1.690896	0.854365	1.685976
C	0.467608	2.993955	-1.100564
C	0.728815	4.393003	-0.762784
C	0.107064	4.622735	0.489053
C	-0.510272	3.355563	0.878692

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N    -0.272921    2.398916   -0.094039

C    -0.136118   -0.914495   -2.539752

C     0.691762   -0.786904   -3.738436

C     1.180580    0.541869   -3.742506

C     0.640050    1.179448   -2.540981

N    -0.132644    0.276079   -1.834870

N    -0.756568   -2.042774   -2.223917

N    -2.646482   -1.342678    2.115606

N    -1.185367    3.212064    2.011748

N     0.903889    2.441111   -2.225750

C     0.161535    5.882117    1.109208

C     2.057000    0.991559   -4.742169

C     1.074563   -1.708644   -4.724805

C    -2.080406   -4.716397   -1.320901

C    -3.177565   -4.314868    1.304259

C    -3.664274    0.046922    4.721535

C    -2.806865    2.788060    4.648272

C     1.423575    5.415954   -1.429498

C     1.478588    6.676239   -0.809394

H     2.014131    7.501564   -1.303786

C     0.855794    6.906284    0.442176

C     2.435546    0.071205   -5.736923

C     1.954470   -1.260027   -5.725982
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H	2.283346	-1.957941	-6.511516
C	-2.723165	-5.760369	-0.632742
C	-3.265063	-5.561959	0.660942
H	-3.761246	-6.402140	1.171126
C	-3.568366	2.291676	5.720614
H	-3.843591	2.963861	6.548160
C	-3.990982	0.940008	5.756883
H	1.906211	5.235773	-2.401708
H	-0.323257	6.059068	2.080958
H	2.442367	2.022064	-4.740884
H	0.715724	-2.747698	-4.702519
H	-1.655733	-4.868102	-2.324420
H	-3.593895	-4.160946	2.311018
H	3.125294	0.387827	-6.534739
H	0.918112	7.906487	0.898382
H	-2.807308	-6.751384	-1.105197
H	-3.993681	-1.002511	4.746726
H	-4.587117	0.585295	6.612004
H	-2.480093	3.838168	4.617159
C	1.399258	-2.349751	0.269362
C	2.050561	-3.238539	-0.583404
C	3.229691	-1.379981	-1.629360
C	2.591292	-0.490145	-0.770860

C	2.953464	-2.790564	-1.607115
H	0.676347	-2.719598	1.014169
H	2.793894	0.590738	-0.835406
H	1.844804	-4.317905	-0.507126
H	3.944609	-1.001088	-2.376461
S	3.643286	-3.874776	-2.762588
C	1.637934	-0.958522	0.165001
N	0.822617	-0.038818	0.865274
H	0.470072	-0.417283	1.756108
H	1.294875	0.859140	1.045393

4-ATP - Stage II

E= -4225.2072522

G= -4224.755123

N   -2.656422   1.042123   -0.811632

C   -3.655424   1.434873   -0.252810

S   -5.016913   1.968633   0.425249

Co   -0.995376   0.416470   -0.043800

C   -2.465953   -1.941841   1.019548

C   -2.872389   -3.298804   0.657096

C   -2.331050   -3.546604   -0.627927

C   -1.602984   -2.337214   -1.008092

N   -1.704730   -1.394814   0.000836

C   -1.665206   1.954339   2.411754

C   -2.382195   1.830260   3.678859

C   -2.889634   0.508617   3.722493

C   -2.468924   -0.134975   2.480021

N   -1.715902   0.751123   1.728244

C   0.412272   2.796019   -1.157434

C   0.695456   4.199085   -0.860084

C   0.138811   4.456342   0.416500

C   -0.471764   3.203479   0.858520

N   -0.289153   2.228927   -0.107359

C   -0.255141   -1.146952   -2.473638

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C    0.633654   -1.089661   -3.632539

C    1.156981    0.227629   -3.667672

C    0.569149    0.932914   -2.530635

N   -0.231649    0.065818   -1.807163

N   -0.930840   -2.239300   -2.147129

N   -2.813136   -1.377040    2.168028

N   -1.093315    3.086139    2.024015

N    0.825904    2.206895   -2.271405

C    0.237998    5.724207    1.012681

C    2.130638    0.601508   -4.605196

C    1.068331   -2.072040   -4.533659

C   -2.530237   -4.775178   -1.278937

C   -3.631380   -4.271676    1.328098

C   -3.647922    0.054399    4.814237

C   -2.617940    2.736723    4.725759

C    1.369619    5.200993   -1.577418

C    1.467907    6.470383   -0.982116

H    1.987748    7.281144   -1.515598

C    0.909829    6.728267    0.294230

C    2.584923   -0.387694   -5.493712

C    2.061324   -1.706068   -5.458361

H    2.445613   -2.454746   -6.167598

C   -3.290776   -5.748669   -0.608619
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C   -3.833676   -5.500346   0.676114

H   -4.424189   -6.286471   1.171610

C   -3.375266   2.282534   5.818878

H   -3.580777   2.965387   6.657729

C   -3.882820   0.960312   5.862565

H   1.802978   4.998402   -2.568079

H   -0.195023   5.922616   2.004345

H   2.546129   1.619618   -4.620818

H   0.672921   -3.097485   -4.494193

H   -2.106767   -4.966248   -2.276157

H   -4.050728   -4.078288   2.326612

H   3.365395   -0.140519   -6.229201

H   1.005805   7.735016   0.729507

H   -3.469225   -6.723235   -1.088862

H   -4.043647   -0.971579   4.844883

H   -4.473388   0.639722   6.734738

H   -2.225790   3.763845   4.688549

C   1.781530   -2.026936   -0.357663

C   2.668646   -2.420718   -1.354148

C   3.588587   -0.145310   -1.435445

C   2.701432   0.249015   -0.439159

C   3.574381   -1.483034   -1.950020

H   1.068527   -2.744480   0.075707

H   2.695606   1.285269   -0.068813

H   2.666353   -3.458726   -1.717828

H   4.298760   0.578232   -1.861973

S   4.593033   -1.941766   -3.259202

C   1.760812   -0.677815   0.069734

N   0.720158   -0.227467   0.921834

H   0.376271   -0.970570   1.549604

H   0.997582   0.589576   1.487457

4-ATP - Stage III-a

E= -4225.0190481

G= -4224.566833

N	-2.624041	1.031895	-0.828559
C	-3.615621	1.422980	-0.252002
S	-4.963009	1.953292	0.449987
Co	-0.971390	0.404915	-0.035380
C	-2.481206	-1.930387	1.004026
C	-2.931529	-3.271211	0.621183
C	-2.387578	-3.520992	-0.659347
C	-1.611061	-2.330839	-1.015255
N	-1.693311	-1.394600	0.002781
C	-1.636158	1.940502	2.416389
C	-2.329404	1.808764	3.699817
C	-2.842093	0.492129	3.740927
C	-2.447802	-0.142366	2.481269
N	-1.698098	0.742586	1.724962
C	0.401079	2.790323	-1.166577
C	0.635072	4.210844	-0.895187
C	0.084236	4.466460	0.381167
C	-0.479392	3.196597	0.846752
N	-0.274308	2.213880	-0.102985
C	-0.214500	-1.164397	-2.448991

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C    0.695226   -1.116983   -3.593711

C    1.215839    0.200360   -3.631680

C    0.605503    0.913713   -2.509195

N   -0.202246    0.051521   -1.788928

N   -0.915382   -2.246908   -2.138740

N   -2.816490   -1.374129    2.160882

N   -1.082976    3.078206    2.022125

N    0.835703    2.197353   -2.267987

C    0.143537    5.739781    0.961220

C    2.195639    0.573100   -4.557884

C    1.136924   -2.104585   -4.480366

C   -2.615443   -4.730787   -1.327188

C   -3.725141   -4.221151    1.276310

C   -3.582951    0.029785    4.835851

C   -2.540201    2.708663    4.752082

C    1.266797    5.218838   -1.634316

C    1.325279    6.503770   -1.056055

H    1.810399    7.323234   -1.607821

C    0.773828    6.759456    0.218236

C    2.663922   -0.425306   -5.437136

C    2.143464   -1.741604   -5.399158

H    2.532249   -2.493615   -6.101647

C   -3.417032   -5.689054   -0.672924
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C	-3.961966	-5.438773	0.605206
H	-4.582316	-6.209613	1.087246
C	-3.281884	2.246209	5.858641
H	-3.467687	2.923719	6.705864
C	-3.793628	0.930872	5.899879
H	1.698328	5.017007	-2.625538
H	-0.284168	5.936614	1.955094
H	2.606269	1.592600	-4.579584
H	0.739796	-3.128954	-4.442037
H	-2.187210	-4.925499	-2.321265
H	-4.145562	-4.026397	2.273681
H	3.447894	-0.178501	-6.168280
H	0.838039	7.774267	0.639417
H	-3.621688	-6.650789	-1.167510
H	-3.985010	-0.993381	4.863831
H	-4.369922	0.604161	6.778811
H	-2.145311	3.734342	4.715878
C	1.822149	-2.034175	-0.330097
C	2.700952	-2.416179	-1.337972
C	3.609178	-0.131029	-1.409768
C	2.728754	0.249101	-0.402766
C	3.587579	-1.463168	-1.937604
H	1.119795	-2.759926	0.106922

H	2.722875	1.281663	-0.022354
H	2.700531	-3.451902	-1.707683
H	4.311599	0.600400	-1.835355
S	4.556404	-1.889666	-3.292842
C	1.793339	-0.686053	0.101950
N	0.747974	-0.244735	0.950463
H	0.402615	-0.993596	1.571481
H	1.019362	0.569930	1.523281

4-ATP - Stage III-b

E= -4225.0212876

G= -4224.565472

N	-2.635697	1.059975	-0.822334
C	-3.705769	1.192239	-0.268426
S	-5.157044	1.390112	0.395645
Co	-0.966039	0.485376	-0.051569
C	-2.337271	-1.917023	1.022271
C	-2.746736	-3.273011	0.648981
C	-2.292129	-3.475087	-0.674520
C	-1.587869	-2.249544	-1.059871
N	-1.634166	-1.335714	-0.013604
C	-1.699780	2.015112	2.383638
C	-2.396076	1.864439	3.662497
C	-2.814401	0.515659	3.732216
C	-2.373586	-0.117898	2.486297
N	-1.687370	0.798153	1.713706
C	0.445094	2.880498	-1.140743
C	0.688853	4.292813	-0.841898
C	0.062575	4.549885	0.399732
C	-0.535319	3.283429	0.828334
N	-0.297659	2.307230	-0.109346
C	-0.263621	-1.032192	-2.513017

C   0.670710 -0.977347 -3.642958

C   1.231479   0.336203 -3.630278

C   0.630405   1.024011 -2.520273

N   -0.212092   0.150221 -1.822327

N   -0.966812 -2.121827 -2.217668

N   -2.658536 -1.378636   2.191758

N   -1.185114   3.163756   1.984692

N   0.898527   2.294429 -2.230268

C   0.100382   5.821580   0.988703

C   2.286208   0.706086 -4.499376

C   1.164968 -1.963387 -4.485416

C   -2.520542 -4.682266 -1.349132

C   -3.451305 -4.268846   1.340129

C   -3.521762   0.026171   4.838127

C   -2.671259   2.769718   4.697078

C   1.373089   5.300338 -1.536873

C   1.410498   6.579390 -0.949853

H   1.937008   7.396627 -1.466122

C   0.784368   6.835915   0.291836

C   2.824901 -0.286234 -5.310462

C   2.318139 -1.629376 -5.268242

H   2.697346 -2.363634 -5.995945

C   -3.228699 -5.684361 -0.658306

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C    -3.686138   -5.481254    0.664049

H    -4.234948   -6.287838    1.173787

C    -3.380793    2.281351    5.810876

H    -3.616486    2.961524    6.643533

C    -3.798137    0.932493    5.880454

H     1.860722    5.099033   -2.501989

H    -0.386968    6.018712    1.954772

H     2.689120    1.728690   -4.494091

H     0.757384   -2.984078   -4.494985

H    -2.162858   -4.838922   -2.377341

H    -3.803725   -4.109751    2.369744

H     3.674510   -0.065171   -5.972456

H     0.833353    7.848740    0.720152

H    -3.430925   -6.644993   -1.156365

H    -3.848466   -1.022664    4.889401

H    -4.351595    0.585403    6.766398

H    -2.347355    3.819101    4.639192

C     1.541413   -2.136075   -0.215520

C     2.231293   -2.703467   -1.278042

C     3.436075   -0.585449   -1.640042

C     2.711384   -0.004623   -0.602391

C     3.159053   -1.928579   -2.049106

H     0.815750   -2.725438    0.363761
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H	2.867009	1.049142	-0.326238
H	2.047235	-3.750096	-1.560996
H	4.189140	-0.000369	-2.187246
S	3.834575	-2.586395	-3.489992
C	1.711270	-0.756246	0.061642
N	0.792774	-0.112854	0.921140
H	0.445679	-0.728067	1.673851
H	1.166171	0.757739	1.331180

4-ATP - Stage IV

E= -4716.0881531

G= -4715.633925

N	-2.597062	1.416290	-0.731188
C	-3.653551	1.726546	-0.252896
S	-5.101977	2.125968	0.351263
Co	-0.997656	0.623070	-0.033321
C	-2.696170	-1.635953	0.901023
C	-3.255800	-2.908122	0.448880
C	-2.716243	-3.147690	-0.836890
C	-1.844641	-2.013307	-1.137104
N	-1.860048	-1.122869	-0.077325
C	-1.529098	2.083932	2.504806
C	-2.252908	1.954231	3.767700
C	-2.878090	0.683403	3.741581
C	-2.521204	0.073569	2.462917
N	-1.692950	0.930117	1.756334
C	0.609327	2.927981	-1.030852
C	1.019975	4.280128	-0.658245
C	0.499263	4.513013	0.638257
C	-0.222640	3.299649	1.016496
N	-0.133754	2.368838	-0.005073
C	-0.378838	-0.882116	-2.532729

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C     0.521311   -0.844385   -3.682834

C     1.140562    0.431433   -3.663255

C     0.602609    1.131467   -2.498944

N    -0.268519    0.298127   -1.817241

N    -1.142072   -1.929621   -2.257463

N    -2.981114   -1.109949    2.083345

N    -0.852687    3.176232    2.176828

N     0.964055    2.365059   -2.178191

C     0.720278    5.729402    1.304905

C     2.146598    0.768803   -4.579741

C     0.888575   -1.820277   -4.620206

C    -3.079005   -4.280749   -1.581349

C    -4.181571   -3.790249    1.027387

C    -3.674505    0.239661    4.810050

C    -2.404436    2.818491    4.864653

C     1.779291    5.255369   -1.325596

C     1.999442    6.473221   -0.659639

H     2.588386    7.262129   -1.152466

C     1.477390    6.706816    0.636500

C     2.534878   -0.216876   -5.503096

C     1.914573   -1.493508   -5.523094

H     2.248886   -2.240175   -6.259118

C    -4.003678   -5.167372   -1.002254
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C    -4.548353   -4.924758    0.282398

H    -5.275200   -5.637422    0.701850

C    -3.198707    2.373935    5.935313

H    -3.340102    3.024481    6.812199

C    -3.824872    1.103142    5.908417

H     2.184422    5.071748   -2.331723

H     0.316013    5.908456    2.312226

H     2.636369    1.753002   -4.552946

H     0.417367   -2.813863   -4.623852

H    -2.663603   -4.460720   -2.583850

H    -4.609033   -3.595554    2.021824

H     3.337201    0.000329   -6.224283

H     1.670524    7.672931    1.127953

H    -4.316238   -6.064783   -1.558251

H    -4.162316   -0.745979    4.785011

H    -4.441493    0.789425    6.764871

H    -1.920808    3.806330    4.882522

C     1.589892   -2.004207   -0.485688

C     2.458074   -2.403348   -1.496540

C     3.529904   -0.193069   -1.448303

C     2.662766    0.205855   -0.436454

C     3.428574   -1.496660   -2.035929

H     0.825453   -2.693102   -0.095837
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H   2.725324   1.217875   -0.009236

H   2.389928   -3.417999   -1.915419

H   4.291056   0.502617   -1.830791

S   4.420215   -1.948276   -3.367423

C   1.656116   -0.681528   0.012464

N   0.638593   -0.206867   0.882359

H   0.232987   -0.960392   1.459863

H   0.974077   0.547173   1.502116

S   -6.085848   -0.638320   -0.016780

C   -5.188694   -0.837529   -1.388484

N   -4.552155   -0.976949   -2.390074

4-ATP - Stage V

E= -4716.0880669

G= -4715.632595

N	-2.597095	1.418325	-0.729928
C	-3.656731	1.726106	-0.257717
S	-5.109624	2.123853	0.337813
Co	-0.997296	0.625995	-0.033135
C	-2.694209	-1.634500	0.901064
C	-3.252532	-2.907266	0.448941
C	-2.713212	-3.146023	-0.837074
C	-1.842918	-2.010658	-1.137445
N	-1.859114	-1.120303	-0.077633
C	-1.529202	2.085828	2.505542
C	-2.252419	1.955151	3.768662
C	-2.876875	0.683978	3.742227
C	-2.520059	0.074860	2.463192
N	-1.692697	0.932169	1.756647
C	0.608594	2.931990	-1.029988
C	1.018604	4.284196	-0.657013
C	0.497591	4.516550	0.639484
C	-0.223721	3.302764	1.017384
N	-0.134403	2.372317	-0.004430
C	-0.377620	-0.878375	-2.532584

C	0.523200	-0.840081	-3.682354
C	1.141487	0.436212	-3.662528
C	0.602869	1.135720	-2.498487
N	-0.268267	0.301738	-1.817105
N	-1.140446	-1.926307	-2.257796
N	-2.979154	-1.109015	2.083558
N	-0.853558	3.178611	2.177789
N	0.963814	2.369329	-2.177322
C	0.718078	5.732844	1.306509
C	2.147807	0.774443	-4.578646
C	0.891745	-1.815591	-4.619407
C	-3.074850	-4.279444	-1.581521
C	-4.176927	-3.790690	1.027750
C	-3.672532	0.239251	4.810852
C	-2.403996	2.818823	4.866084
C	1.777638	5.259943	-1.323983
C	1.997228	6.477678	-0.657658
H	2.585961	7.266942	-1.150168
C	1.474906	6.710718	0.638489
C	2.537270	-0.210747	-5.501715
C	1.918287	-1.488051	-5.521634
H	2.253457	-2.234508	-6.257474
C	-3.998162	-5.167289	-1.002157

C	-4.542583	-4.925546	0.282782
H	-5.268336	-5.639195	0.702452
C	-3.197525	2.373300	5.936884
H	-3.338922	3.023349	6.814139
C	-3.822929	1.102135	5.909683
H	2.183013	5.076757	-2.330093
H	0.313624	5.911448	2.313834
H	2.636531	1.759163	-4.551633
H	0.421592	-2.809671	-4.623239
H	-2.659642	-4.458747	-2.584220
H	-4.604173	-3.596689	2.022416
H	3.339956	0.006875	-6.222375
H	1.667620	7.676767	1.130238
H	-4.309844	-6.065012	-1.558147
H	-4.159740	-0.746682	4.785584
H	-4.438978	0.787647	6.766267
H	-1.920941	3.806939	4.884202
C	1.582451	-2.010342	-0.479019
C	2.447085	-2.417654	-1.489786
C	3.524899	-0.210257	-1.457389
C	2.660905	0.197038	-0.445990
C	3.418742	-1.516950	-2.036779
H	0.817452	-2.695143	-0.083140

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H      2.726885    1.211563   -0.025265

H      2.375091   -3.434547   -1.902551

H      4.286927    0.481185   -1.845777

S      4.406069   -1.979919   -3.367971

C      1.653256   -0.684952    0.010810

N      0.639018   -0.202500    0.881019

H      0.234149   -0.951716    1.464627

H      0.978614    0.554186    1.495369

S     -6.080493   -0.642488   -0.019733

C     -5.186280   -0.841443   -1.393556

N     -4.551794   -0.980686   -2.396397
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NH$_2$ - Stage I

E= -3761.570285

G= -3761.164004

N   -1.535294   0.738794   -0.570697

C   -1.781089   1.920766   -0.696749

S   -2.210747   3.458954   -0.892818

Co   0.066654   -0.071161   0.023395

C   -0.233485   1.231216   2.696366

C   -0.791097   1.001351   4.012640

C   -1.344106   -0.304356   3.997737

C   -1.094093   -0.835953   2.655714

N   -0.399694   0.090118   1.900100

C   1.490544   2.335825   -0.999756

C   1.796313   3.699936   -0.632531

C   1.381630   3.863640   0.714630

C   0.833742   2.571367   1.129089

N   0.940109   1.655137   0.097529

C   0.554496   -1.471830   -2.573746

C   1.121217   -1.247021   -3.887548

C   1.634479   0.074817   -3.889326

C   1.371859   0.612709   -2.552670

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N    0.748861   -0.340833   -1.769475

C   -1.255309   -2.543490    1.088217

C   -1.652052   -3.878370    0.690343

C   -1.234717   -4.042597   -0.655097

C   -0.585335   -2.784811   -1.033516

N   -0.598724   -1.903388    0.029719

N   -1.493362   -2.050077    2.294957

N    0.322758    2.379179    2.338955

N    1.706891    1.851544   -2.213786

N   -0.059601   -2.597469   -2.238648

C    2.251306    0.633265   -5.010196

C   -1.440454   -5.230471   -1.358937

C   -2.303249   -4.933757    1.361975

C   -1.966165   -0.862535    5.115996

C   -0.865236    1.786790    5.181562

C    1.521002    5.074263    1.394719

C    2.367373    4.783082   -1.333799

C    1.222624   -2.045563   -5.045516

C    1.833301   -1.503439   -6.176581

H    1.922586   -2.103790   -7.095815

C    2.356977   -0.165658   -6.185740

C   -2.097872   -6.302653   -0.688188

C   -2.522409   -6.126681    0.672923
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H   -3.030873   -6.966812   1.171913

C   -2.041805   -0.078073   6.303442

C   -1.486209   1.246846   6.308014

H   -1.560218   1.839356   7.233678

C   2.508299   6.002020   -0.672795

H   2.943867   6.867484   -1.196754

C   2.093893   6.174460   0.693259

H   0.827761   -3.072670   -5.063482

H   2.643131   1.661626   -5.000126

H   -1.108688   -5.348146   -2.401671

H   -2.633975   -4.824098   2.405958

H   -2.390962   -1.877509   5.092646

H   -0.446129   2.804037   5.209734

H   1.191312   5.191238   2.438113

H   2.689476   4.674873   -2.380499

N   -2.611836   -0.583582   7.437120

H   -2.810278   0.038320   8.222585

H   -3.139568   -1.456774   7.388519

N   -2.302340   -7.496657   -1.317490

H   -2.906368   -8.198893   -0.887717

H   -2.131120   -7.575658   -2.321163

N   2.970769   0.319854   -7.305198

H   3.199057   1.313778   -7.362554

H   2.889719   -0.191134   -8.185844

N   2.269567   7.378793   1.309070

H   1.854213   7.544662   2.227102

H   2.538676   8.195811   0.758704

NH$_2$ - Stage II

E= -3761.403312

G= -3760.995143

N -1.524220   0.733004   -0.564656

C -1.739587   1.913826   -0.755628

S -2.139174   3.443545   -1.037387

Co 0.071703 -0.072394   0.027401

C -0.238024   1.227194   2.700142

C -0.784449   0.998869   4.014948

C -1.329786 -0.309679   4.003253

C -1.088530 -0.841832   2.653219

N -0.402060   0.090089   1.898909

C   1.487358   2.338512   -0.993025

C   1.774552   3.704206   -0.635703

C   1.361750   3.866908   0.711475

C   0.827134   2.565854   1.134440

N   0.945140   1.649648   0.102744

C   0.536438 -1.459207   -2.578956

C   1.106012 -1.240844   -3.886412

C   1.641858   0.071481   -3.880550

C   1.377257   0.614367   -2.540010

N   0.739890 -0.335676   -1.765769

C -1.271788 -2.538069   1.080723

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C  -1.680835  -3.863173   0.683311

C  -1.265452  -4.026919  -0.662435

C  -0.604623  -2.768318  -1.041274

N  -0.612987  -1.894001   0.026114

N  -1.496919  -2.048640   2.296005

N   0.316144   2.380187   2.339612

N   1.714303   1.849474  -2.207286

N  -0.085890  -2.585020  -2.245143

C   2.270095   0.625383  -4.988825

C  -1.477870  -5.203662  -1.369379

C  -2.337470  -4.915546   1.357138

C  -1.941470  -0.871683   5.116701

C  -0.853381   1.786857   5.184022

C   1.480678   5.075210   1.386464

C   2.329363   4.791437  -1.345529

C   1.200546  -2.040855  -5.045479

C   1.824873  -1.508241  -6.171288

H   1.912148  -2.106657  -7.091355

C   2.366911  -0.177932  -6.172291

C  -2.146877  -6.276946  -0.694101

C  -2.566177  -6.104917   0.668823

H  -3.076688  -6.944089   1.166055

C  -2.013934  -0.079927   6.309824
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C   -1.463442    1.246879    6.314017

H   -1.534031    1.837032    7.240819

C    2.452888    6.015149   -0.693133

H    2.874680    6.884764   -1.220388

C    2.036319    6.186086    0.671981

H    0.790987   -3.061741   -5.065019

H    2.680396    1.646104   -4.975388

H   -1.148078   -5.324652   -2.412033

H   -2.661978   -4.804360    2.402505

H   -2.361615   -1.888329    5.098853

H   -0.436752    2.804812    5.207214

H    1.154467    5.193682    2.430473

H    2.652186    4.680282   -2.391290

N   -2.598702   -0.582805    7.423645

H   -2.664921   -0.024386    8.276799

H   -2.997111   -1.523626    7.424614

N   -2.379009   -7.444555   -1.340287

H   -2.853984   -8.217360   -0.869947

H   -2.082211   -7.572363   -2.309531

N    2.963801    0.318139   -7.282790

H    3.352769    1.262866   -7.288604

H    3.036215   -0.244225   -8.132804

N    2.163972    7.389897    1.278659
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H   1.869144   7.519594   2.248307

H   2.548046   8.191294   0.774484

NH$_2$ - Stage III-a

E= -3761.2150899

G= -3760.805434

N   -1.709173   0.813002   -0.648034

C   -1.905264   2.008374   -0.644702

S   -2.169606   3.600602   -0.633421

Co   0.008355   -0.055920   -0.002617

C   -0.237250   1.219438   2.686394

C   -0.732582   0.971378   4.011220

C   -1.280452   -0.339479   4.001411

C   -1.088788   -0.854654   2.633131

N   -0.432364   0.092241   1.870484

C   1.439553   2.365943   -1.011190

C   1.705684   3.733329   -0.670102

C   1.289676   3.897398   0.677892

C   0.767212   2.582869   1.107939

N   0.882358   1.680839   0.078557

C   0.565529   -1.469135   -2.571574

C   1.179918   -1.270052   -3.854576

C   1.716094   0.045693   -3.848779

C   1.399898   0.611925   -2.525304

N   0.733728   -0.332056   -1.764566

C   -1.324896   -2.529237   1.048036

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C  -1.746478  -3.842935   0.651192

C  -1.322155  -4.009404  -0.692842

C  -0.639335  -2.751921  -1.066422

N  -0.672142  -1.877707  -0.008552

N  -1.519877  -2.048970   2.276675

N   0.290730   2.385799   2.324696

N   1.707551   1.855023  -2.213289

N  -0.081631  -2.587953  -2.253499

C   2.366915   0.587394  -4.940713

C  -1.540209  -5.175449  -1.400599

C  -2.419272  -4.888180   1.324885

C  -1.857146  -0.911281   5.119295

C  -0.765117   1.755677   5.187302

C   1.399589   5.099720   1.347079

C   2.252339   4.821461  -1.389297

C   1.297043  -2.088984  -5.001517

C   1.950036  -1.573551  -6.114177

H   2.063622  -2.179966  -7.025568

C   2.493189  -0.240098  -6.113100

C  -2.233357  -6.244563  -0.723166

C  -2.659651  -6.072792   0.637246

H  -3.182716  -6.907135   1.128297

C  -1.886076  -0.123685   6.325422
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C   -1.335752   1.206629   6.328724

H   -1.377535   1.784155   7.264614

C   2.364828   6.049051   -0.747007

H   2.778128   6.920917   -1.276101

C   1.948113   6.217476   0.617721

H   0.882792   -3.107440   -5.014988

H   2.774057   1.609108   -4.935646

H   -1.205231   -5.305104   -2.440445

H   -2.746165   -4.770294   2.368388

H   -2.282896   -1.925390   5.108617

H   -0.348853   2.773326   5.200964

H   1.077811   5.224540   2.391650

H   2.576477   4.703335   -2.433563

N   -2.430106   -0.636631   7.443804

H   -2.461716   -0.090755   8.309669

H   -2.826656   -1.580546   7.447913

N   -2.470685   -7.397052   -1.377880

H   -2.959269   -8.170338   -0.918383

H   -2.167486   -7.520089   -2.347578

N   3.116709   0.239933   -7.204199

H   3.505622   1.186990   -7.211535

H   3.215020   -0.333694   -8.046664

N   2.060287   7.412849   1.226064

H   1.767986   7.534629   2.199419

H   2.441035   8.221393   0.726893

NH$_2$ - Stage III-b

E= -3761.2223459

G= -3760.810857

N   -1.495875   0.711305   -0.550857

C   -1.681211   1.876636   -0.850569

S   -2.057868   3.375083   -1.273844

Co   0.092422   -0.077906   0.038987

C   -0.234877   1.217986   2.710543

C   -0.763921   0.989221   4.025200

C   -1.294646   -0.325904   4.018844

C   -1.066645   -0.856839   2.658581

N   -0.394592   0.085765   1.904520

C   1.500247   2.338054   -0.975214

C   1.765100   3.705389   -0.629461

C   1.345773   3.869370   0.715496

C   0.824912   2.559498   1.147562

N   0.960571   1.642159   0.116378

C   0.536786   -1.448066   -2.577078

C   1.112779   -1.237812   -3.876028

C   1.676362   0.063132   -3.859946

C   1.406127   0.612658   -2.516333

N   0.748551   -0.333017   -1.754370

C   -1.272225   -2.538537   1.077806

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C   -1.699413   -3.850474    0.678659

C   -1.286525   -4.012897   -0.668465

C   -0.609726   -2.754678   -1.045834

N   -0.609858   -1.890599    0.029065

N   -1.481261   -2.055664    2.304382

N    0.311442    2.379759    2.345395

N    1.746821    1.841845   -2.188026

N   -0.097714   -2.573757   -2.246759

C    2.317053    0.610656   -4.955701

C   -1.513859   -5.175797   -1.380482

C   -2.371009   -4.896063    1.352072

C   -1.890630   -0.892282    5.130067

C   -0.830183    1.782204    5.193224

C    1.434555    5.078740    1.380647

C    2.302511    4.796613   -1.349482

C    1.195036   -2.037837   -5.038282

C    1.834821   -1.515656   -6.157802

H    1.915269   -2.109784   -7.080734

C    2.402496   -0.196535   -6.147268

C   -2.201053   -6.246828   -0.702479

C   -2.617332   -6.078124    0.661265

H   -3.138198   -6.913179    1.153578

C   -1.958705   -0.092541    6.328219
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C   -1.422910    1.239797    6.328667

H   -1.492804    1.828851    7.255684

C    2.398944    6.027250   -0.709343

H    2.804178    6.901362   -1.241184

C    1.971891    6.199150    0.651874

H    0.762755   -3.048834   -5.061506

H    2.747926    1.622673   -4.939079

H   -1.187985   -5.300033   -2.423869

H   -2.691744   -4.781787    2.397887

H   -2.303064   -1.912037    5.120079

H   -0.424662    2.804390    5.207431

H    1.104117    5.201786    2.422683

H    2.630012    4.680341   -2.392857

N   -2.526982   -0.606090    7.436961

H   -2.589120   -0.054875    8.297063

H   -2.912380   -1.553958    7.436662

N   -2.442860   -7.398607   -1.358574

H   -2.926470   -8.173447   -0.896960

H   -2.146488   -7.519158   -2.330462

N    3.014227    0.298551   -7.241325

H    3.419219    1.238160   -7.234705

H    3.085080   -0.256587   -8.098161

N    2.065038    7.401169    1.253413
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H   1.764086   7.525812   2.223310

H   2.437687   8.210823   0.750832

NH$_2$ - Stage IV

E= -4252.2857648

G= -4251.873891

-1.709604   0.813208   -0.850434

-1.983368   1.984474   -0.795318

-2.325224   3.566537   -0.692641

-0.034575   -0.078353   -0.127604

-0.462421   1.254621   2.517149

-1.100939   1.059127   3.790646

-1.664879   -0.240831   3.761802

-1.330388   -0.803545   2.436496

-0.597862   0.108267   1.716350

1.460291   2.318848   -1.091492

1.779956   3.673915   -0.722310

1.315105   3.847204   0.605941

0.713100   2.556644   1.001003

0.837471   1.650640   -0.027871

0.580589   -1.496765   -2.688916

1.190197   -1.287717   -3.977323

1.715630   0.029253   -3.962996

1.401817   0.581424   -2.629470

0.737560   -0.361640   -1.880117

-1.391998   -2.541015   0.902172

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-1.740177   -3.885376    0.521872

-1.257772   -4.065839   -0.799117

-0.613968   -2.790287   -1.178357

-0.710464   -1.893859   -0.142488

-1.689334   -2.030619    2.093438

 0.153820    2.387058    2.186312

 1.731608    1.818574   -2.295282

-0.041426   -2.626842   -2.361173

 2.368163    0.581445   -5.052035

-1.405795   -5.256880   -1.487556

-2.402088   -4.938861    1.189872

-2.384993   -0.762154    4.820869

-1.276052    1.889028    4.918642

 1.444923    5.043152    1.289598

 2.401096    4.742630   -1.404551

 1.321028   -2.094416   -5.128725

 1.971483   -1.565119   -6.240705

 2.088611   -2.166553   -7.155215

 2.502713   -0.231672   -6.231848

-2.081564   -6.336216   -0.815324

-2.568500   -6.149158    0.521537

-3.080376   -6.990843    1.012285

-2.562190    0.073348    5.979620
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-2.000552    1.394982    5.999531

-2.159600    2.015200    6.894875

 2.542440    5.960411   -0.743539

 3.018167    6.815401   -1.247580

 2.075210    6.138974    0.601563

 0.917994   -3.117688   -5.152170

 2.770013    1.605451   -5.035734

-1.027797   -5.393118   -2.511780

-2.778450   -4.810572    2.215553

-2.824810   -1.769990    4.791171

-0.856845    2.905432    4.943526

 1.077215    5.172240    2.318450

 2.763069    4.621830   -2.436298

-3.261174   -0.390483    7.037631

-3.406918    0.192763    7.865038

-3.669193   -1.328136    7.024712

-2.250306   -7.515457   -1.450811

-2.726850   -8.295016   -0.991226

-1.904212   -7.649684   -2.403566

 3.125133    0.267990   -7.321914

 3.504251    1.217557   -7.318649

 3.225436   -0.293796   -8.170471

 2.217514    7.327305    1.227639
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1.884106   7.456295   2.185539

2.653106   8.121073   0.752261

-3.519143   3.327314   2.066349

-3.773131   1.710168   1.872301

-3.976904   0.539907   1.729241

NH$_2$ - Stage V

E= -4252.2764835

G= -4251.867425

N -1.661220   0.646190 -0.504270

C -2.332940   1.344840   0.235970

S -3.273300   2.264440   1.153580

Co 0.068320 -0.033190 -0.001060

C -0.270230   1.288140   2.646970

C -0.895050   1.098400   3.926790

C -1.398690 -0.227350   3.934560

C -1.049820 -0.807090   2.623510

N -0.348720   0.115830   1.876940

C   1.454500   2.394040 -1.045740

C   1.859480   3.718220 -0.657710

C   1.471610   3.875750   0.696790

C   0.828750   2.605680   1.090050

N   0.859460   1.721150   0.033160

C   0.467870 -1.387980 -2.641050

C   0.952280 -1.146240 -3.974910

C   1.459140   0.177270 -3.982730

C   1.260850   0.699810 -2.615210

N   0.670510 -0.263720 -1.828810

C -1.138670 -2.544130   1.091810

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C   -1.481950   -3.892180    0.722000

C   -1.097810   -4.044420   -0.633880

C   -0.516130   -2.750110   -1.043900

N   -0.528880   -1.876680    0.020270

N   -1.402120   -2.037100    2.293900

N    0.307110    2.434680    2.289900

N    1.633340    1.921410   -2.278150

N   -0.077350   -2.546100   -2.273610

C    2.017950    0.753520   -5.109950

C   -1.279400   -5.227040   -1.330000

C   -2.076360   -4.966330    1.419970

C   -2.074900   -0.758710    5.018820

C   -1.072680    1.937740    5.049140

C    1.697010    5.043200    1.403610

C    2.504600    4.771870   -1.343050

C    1.003570   -1.936320   -5.144170

C    1.555520   -1.382260   -6.296240

H    1.607600   -1.969680   -7.225570

C    2.068380   -0.041900   -6.309630

C   -1.885180   -6.327630   -0.627020

C   -2.272250   -6.168830    0.745850

H   -2.734140   -7.025920    1.259140

C   -2.263940    0.090000    6.166170
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C -1.752660   1.432470   6.152710

H -1.914220   2.059900   7.042520

C   2.747030   5.958780 -0.657700

H   3.246160   6.800720 -1.160970

C   2.354890   6.122890   0.713530

H   0.616220 -2.965780 -5.149550

H   2.411500   1.780840 -5.109250

H -0.981260 -5.338830 -2.383100

H -2.379240 -4.859810   2.472070

H -2.463750 -1.787710   5.019680

H -0.687940   2.968090   5.051970

H   1.389620   5.162530   2.453170

H   2.808050   4.661210 -2.394520

N -2.921640 -0.382450   7.245670

H -3.073940   0.208970   8.066200

H -3.291870 -1.335790   7.256860

N -2.085530 -7.498980 -1.267930

H -2.520120 -8.290920 -0.788340

H -1.815010 -7.611390 -2.247700

N   2.597180   0.482460 -7.435760

H   2.964950   1.436680 -7.445410

H   2.639210 -0.065160 -8.298720

N   2.594170   7.280360   1.364040

H   2.315220   7.398120   2.341020

H   3.055210   8.061660   0.891290

S   -5.849190   2.453230   -0.527400

C   -5.111620   1.364060   -1.524310

N   -4.570570   0.573770   -2.243970

MeO - Stage I

E= -3998.0214922

G= -3997.557279

N   -1.424722   0.719990   -0.525876

C   -1.642696   1.904453   -0.693117

S   -2.061587   3.431933   -0.949921

Co   0.146707   -0.105066   0.061057

C   -0.119662   1.238995   2.710548

C   -0.680521   1.040456   4.037208

C   -1.261338   -0.252330   4.038920

C   -1.030973   -0.806754   2.705252

N   -0.318061   0.097783   1.934594

C   1.615049   2.251924   -0.998976

C   1.958158   3.618568   -0.648588

C   1.554730   3.804541   0.697813

C   0.977177   2.534720   1.130892

N   1.051530   1.604545   0.103355

C   0.557262   -1.533402   -2.526607

C   1.122023   -1.338126   -3.852686

C   1.680918   -0.035898   -3.865453

C   1.444794   0.522623   -2.535103

N   0.792892   -0.405943   -1.739890

C   -1.247329   -2.518370   1.153265

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C  -1.689516  -3.850256   0.770087

C  -1.284081  -4.036932  -0.575171

C  -0.601136  -2.805196  -0.970129

N  -0.581838  -1.913787   0.088698

N  -1.462559  -2.010947   2.357337

N   0.465998   2.367462   2.341687

N   1.817511   1.751336  -2.207418

N  -0.082033  -2.639566  -2.178790

C   2.309474   0.486572  -4.998593

C  -1.535299  -5.226801  -1.263035

C  -2.367123  -4.869689   1.458641

C  -1.895704  -0.774320   5.169137

C  -0.729898   1.846419   5.186348

C   1.719821   5.026356   1.355362

C   2.542789   4.672698  -1.370703

C   1.183729  -2.151712  -4.995870

C   1.808361  -1.644020  -6.144529

H   1.861675  -2.269661  -7.045644

C   2.368999  -0.334208  -6.149920

C  -2.218961  -6.252398  -0.567519

C  -2.631942  -6.070499   0.783755

H  -3.161770  -6.875395   1.310574

C  -1.944649   0.039481   6.325839
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C   -1.365118   1.341061   6.330172

H   -1.412271   1.962112   7.234782

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H   3.159633   6.742373   -1.284932

C   2.301720   6.088284   0.623871

H   0.753739   -3.164330   -4.999053

H   2.746296   1.495286   -5.019845

H   -1.221611   -5.384795   -2.304911

H   -2.684851   -4.738181   2.503712

H   -2.348489   -1.776102   5.182842

H   -0.283808   2.852009   5.197142

H   1.406207   5.183663   2.397246

H   2.857843   4.541287   -2.416477

O   2.431626   7.266013   1.295794

O   2.987309   0.214481   -7.233409

O   -2.442319   -7.395927   -1.274707

O   -2.573712   -0.506785   7.404445

C   2.988122   8.392953   0.610027

H   2.375752   8.671219   -0.274239

H   2.979773   9.225762   1.337121

H   4.033396   8.196218   0.289147

C   3.083209   -0.557178   -8.435240

H   2.078162   -0.811372   -8.834828

H   3.615408   0.080754   -9.164726

H   3.663070   -1.490783   -8.272001

C   -3.120376   -8.480947   -0.632920

H   -3.182230   -9.288711   -1.385306

H   -2.554872   -8.845582   0.251281

H   -4.146500   -8.190396   -0.321340

C   -2.664901   0.260647   8.609284

H   -3.231797   1.202477   8.447672

H   -3.208635   -0.373475   9.333576

H   -1.658455   0.499974   9.014480

MeO - Stage II

E= -3997.8400364

G= -3997.375693

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S   -1.970805   3.395841   -1.101123

Co   0.169751   -0.113483   0.075253

C   -0.106541   1.225404   2.723764

C   -0.652382   1.022422   4.052881

C   -1.223782   -0.272505   4.056300

C   -1.003385   -0.822944   2.713296

N   -0.302254   0.089070   1.941790

C   1.623303   2.250966   -0.980848

C   1.943557   3.622665   -0.639254

C   1.538717   3.807495   0.704924

C   0.978865   2.526308   1.145038

N   1.068439   1.594270   0.119794

C   0.571250   -1.528183   -2.516859

C   1.140048   -1.336175   -3.838523

C   1.711542   -0.041481   -3.844906

C   1.468752   0.520266   -2.511333

N   0.808198   -0.406353   -1.722506

C   -1.231094   -2.524300   1.156822

C -1.679718 -3.850595   0.772586

C -1.274405 -4.035671 -0.570955

C -0.585496 -2.800486 -0.964713

N -0.564457 -1.914078   0.096875

N -1.438947 -2.022714   2.367881

N   0.469976   2.361691   2.353279

N   1.837684   1.748228 -2.189236

N -0.071482 -2.636500 -2.172433

C   2.346518   0.480930 -4.966909

C -1.526314 -5.215994 -1.262631

C -2.360414 -4.867009   1.461184

C -1.845383 -0.802450   5.182335

C -0.695801   1.827398   5.202080

C   1.679207   5.028380   1.357471

C   2.509650   4.680453 -1.369113

C   1.197361 -2.149195 -4.981520

C   1.831928 -1.645336 -6.127426

H   1.882834 -2.269127 -7.029684

C   2.403265 -0.342742 -6.126615

C -2.217753 -6.246463 -0.564744

C -2.629844 -6.066802   0.784583

H -3.162193 -6.870568   1.310083

C -1.889591   0.013690   6.347985

C   -1.318207   1.316208   6.351372

H   -1.361479   1.934968   7.257482

C   2.656117   5.922952   -0.735618

H   3.089924   6.761718   -1.295683

C   2.245161   6.102525   0.615281

H   0.756665   -3.156837   -4.987743

H   2.791941   1.485670   -4.985233

H   -1.213435   -5.374220   -2.304479

H   -2.677144   -4.735054   2.506169

H   -2.293654   -1.805969   5.198182

H   -0.256249   2.835546   5.209573

H   1.364628   5.186471   2.398710

H   2.825932   4.547542   -2.413980

O   2.350152   7.273966   1.283178

O   3.027543   0.207013   -7.194001

O   -2.438431   -7.376087   -1.276666

O   -2.505087   -0.542019   7.417450

C   2.891209   8.416789   0.604485

H   2.275646   8.682630   -0.280424

H   2.863544   9.243650   1.336925

H   3.939932   8.233567   0.289493

C   -2.600655   0.211265   8.634677

H   -3.174944   1.148740   8.479122

H -3.137454 -0.437675   9.349989

H -1.593354   0.451891   9.034844

C -3.121818 -8.471439 -0.651123

H -4.147553 -8.178375 -0.343394

H -3.178005 -9.267930 -1.414982

H -2.557994 -8.841419   0.230974

C   3.128083 -0.550921 -8.407921

H   2.122397 -0.791946 -8.811886

H   3.668967   0.094774 -9.123095

H   3.700648 -1.488396 -8.246201

MeO - Stage III-a

E= -3997.6316317

G= -3997.169695

N -1.597871   0.791011   -0.604820

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S -2.128354   3.562259   -0.613082

Co 0.080236 -0.083819   0.034780

C -0.111095   1.226638   2.712243

C -0.608052   1.004291   4.048595

C -1.192343 -0.287500   4.050901

C -1.018247 -0.821979   2.689849

N -0.339941   0.097092   1.915757

C   1.566044   2.280036   -1.007647

C   1.871686   3.652407   -0.678873

C   1.461232   3.842275   0.663074

C   0.909262   2.549787   1.110973

N   0.989627   1.631348   0.088733

C   0.603326 -1.546932   -2.514401

C   1.214666 -1.374239   -3.810714

C   1.778073 -0.073383   -3.819860

C   1.484855   0.512462   -2.502086

N   0.806433 -0.407102   -1.726367

C -1.297050 -2.504946   1.122582

C   -1.749181   -3.824041   0.740898

C   -1.331681   -4.015653   -0.597778

C   -0.626217   -2.781020   -0.990014

N   -0.639077   -1.887357   0.055564

N   -1.479026   -2.010921   2.343551

N   0.439293   2.374639   2.334675

N   1.819412   1.754373   -2.202109

N   -0.066949   -2.643923   -2.180979

C   2.429844   0.440278   -4.927910

C   -1.579228   -5.191032   -1.285930

C   -2.440876   -4.834572   1.430643

C   -1.785704   -0.825577   5.179884

C   -0.612464   1.800670   5.208256

C   1.599980   5.057187   1.310890

C   2.439602   4.707334   -1.414527

C   1.299183   -2.204558   -4.943264

C   1.956192   -1.714267   -6.078626

H   2.033896   -2.348118   -6.971685

C   2.518312   -0.405568   -6.080268

C   -2.291208   -6.219873   -0.585156

C   -2.714216   -6.034962   0.758348

H   -3.256093   -6.833366   1.281788

C   -1.784096   -0.017973   6.363220

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C   -1.200935    1.281405    6.367712

H   -1.211414    1.886108    7.284038

C    2.582709    5.954308   -0.790110

H    3.017195    6.790572   -1.352874

C    2.170095    6.136252    0.557556

H    0.861448   -3.213159   -4.943538

H    2.865000    1.449111   -4.954873

H   -1.257179   -5.359437   -2.323326

H   -2.763189   -4.694559    2.472653

H   -2.246868   -1.822983    5.198935

H   -0.165489    2.805214    5.210522

H    1.287338    5.222852    2.351514

H    2.761134    4.565892   -2.456529

O    2.268024    7.296533    1.225334

O    3.155820    0.135206   -7.128320

O   -2.508410   -7.336617   -1.298908

O   -2.367328   -0.582009    7.430336

C    2.810820    8.451090    0.560796

H    2.197778    8.716221   -0.325168

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H    3.860802    8.267022    0.252967

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H   -2.996682    1.081778    8.553410
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H -2.950363 -0.530376 9.381145

H -1.405037 0.356224 9.048363

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H -2.662941 -8.813426 0.190979

C 3.293541 -0.620569 -8.345144

H 2.297207 -0.866762 -8.766155

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H 3.869860 -1.550956 -8.163729

MeO - Stage III-b

E= -3997.6431626

G= -3997.177490

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S -1.924620   3.368666   -1.184345

Co 0.182185 -0.117347   0.081404

C -0.101827   1.219062   2.729439

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C -1.192069 -0.284098   4.066679

C -0.987331 -0.831693   2.713516

N -0.300130   0.087175   1.940644

C   1.629441   2.251352   -0.971649

C   1.926729   3.625570   -0.642384

C   1.516016   3.813574   0.698743

C   0.972182   2.522755   1.148785

N   1.078413   1.588197   0.128491

C   0.579076 -1.524485   -2.514132

C   1.159529 -1.342608   -3.825415

C   1.747539 -0.056044   -3.826282

C   1.491955   0.514950   -2.492672

N   0.815166 -0.404652   -1.713520

C -1.232337 -2.523426   1.153420

C -1.697927 -3.836545   0.767369

C -1.295070 -4.021641 -0.576198

C -0.588681 -2.788661 -0.967825

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N -1.428625 -2.026206   2.372413

N   0.465391   2.362959   2.353999

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C   2.394002   0.459640 -4.937004

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C -2.392194 -4.845725   1.456147

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C   2.480483   4.684822 -1.381701

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H   1.913902 -2.291041 -7.010772

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C   -1.266948    1.305757    6.366210

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C    2.607170    5.934827   -0.759929

H    3.030137    6.775061   -1.325701

C    2.189267    6.117811    0.586813

H    0.758665   -3.160341   -4.974482

H    2.850862    1.459131   -4.955927

H   -1.249327   -5.352244   -2.313293

H   -2.705382   -4.710205    2.501498

H   -2.246943   -1.821824    5.212206

H   -0.225261    2.828900    5.211137

H    1.317349    5.198867    2.381901

H    2.801711    4.545382   -2.423975

O    2.270466    7.283490    1.248470

O    3.083763    0.174292   -7.153000

O   -2.498177   -7.331127   -1.288211

O   -2.435102   -0.559571    7.426569

C    2.798329    8.441189    0.577633

H    2.182829    8.693375   -0.310438

H    2.749362    9.262206    1.314550

H    3.851204    8.270288    0.271996

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H   -3.111867    1.113958    8.506444
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H   -3.065229   -0.483504   9.361892

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H   -4.219947   -8.127685   -0.378948

H   -3.253647   -9.214572   -1.460383

H   -2.638965   -8.814158   0.196826

C   3.191755   -0.570860   -8.378072

H   2.186039   -0.797440   -8.788280

H   3.744482   0.081085   -9.077303

H   3.754651   -1.513046   -8.214644

MeO - Stage IV

E= -4488.7161401

G= -4488.249618

N -1.469342   0.710951   -0.743116

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S -2.450877   3.341370   -0.938248

Co   0.047147   -0.096094   -0.079525

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C -1.615489   -0.157581   3.794307

C -1.267736   -0.757811   2.500665

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C   1.580724   2.240761   -1.092482

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C   1.690659   -0.048944   -3.959000

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N   0.778410   -0.419550   -1.843927

C -1.347275   -2.515516   0.996574

C -1.725513 -3.867170   0.631549

C -1.281220 -4.062957 -0.698130

C -0.630877 -2.810043 -1.102054

N -0.670561 -1.903125 -0.060792

N -1.627865 -1.988914   2.179336

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C   2.329956   0.477396 -5.076152

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H   1.868945 -2.263966 -7.152926

C   2.387574 -0.341320 -6.239988

C -2.130195 -6.311021 -0.663074

C -2.582603 -6.120089   0.671977

H -3.093065 -6.934164   1.203042

C -2.536158   0.227877   5.978695

C -1.982318   1.538811   5.981836

H -2.137790   2.201221   6.843583

C   2.755331   5.865013 -0.792657

H   3.252782   6.683522 -1.329246

C   2.281912   6.064759   0.534835

H   0.741887 -3.162060 -5.116111

H   2.775710   1.482011 -5.089536

H -1.124360 -5.433592 -2.400031

H -2.730085 -4.753688   2.360061

H -2.799202 -1.647605   4.878077

H -0.815015   3.017084   4.890751

H   1.267564   5.191430   2.268922

H   2.953060   4.480387 -2.460005

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O -3.263484 -0.284010   6.997314

C   3.021245   8.351120   0.559284

H   2.462178   8.641207 -0.354956

H   2.989983   9.178130   1.291298

H   4.076105   8.124837   0.297485

C   3.106576   -0.534490   -8.524749

H   2.099055   -0.771787   -8.926043

H   3.644610   0.117536   -9.236176

H   3.679754   -1.472990   -8.372354

C   -2.933436   -8.575022   -0.717969

H   -2.934583   -9.390019   -1.464047

H   -2.375082   -8.898008   0.185735

H   -3.978353   -8.321347   -0.441642

C   -3.502178   0.523834   8.158817

H   -4.066642   1.442897   7.895453

H   -4.106996   -0.100129   8.841226

H   -2.547884   0.800182   8.654376

MeO - Stage V

E= -4488.7174542

G= -4488.249072

N   -1.564061   0.706337   -0.915375

C   -1.644628   1.735115   -1.557903

S   -1.890986   3.047332   -2.440639

Co -0.066056   -0.036747   -0.088934

C   -0.607896   1.397701   2.471494

C   -1.251918   1.228134   3.762838

C   -1.795995   -0.076692   3.767639

C   -1.451681   -0.672652   2.467239

N   -0.709906   0.227579   1.721257

C   1.520717   2.271252   -1.053602

C   1.953509   3.599866   -0.671049

C   1.479049   3.812151   0.644450

C   0.750541   2.590477   1.023759

N   0.828839   1.661329   -0.016114

C   0.449990   -1.480670   -2.632647

C   0.992111   -1.270614   -3.960353

C   1.579155   0.016154   -3.954002

C   1.364854   0.559531   -2.602627

N   0.706999   -0.374110   -1.820948

C   -1.417020   -2.472612   1.014556

C   -1.719852   -3.851075   0.677378

C   -1.266279   -4.048267   -0.647165

C   -0.683051   -2.765577   -1.076115

N   -0.770453   -1.844228   -0.057542

N   -1.730473   -1.938048   2.180435

N   0.117950   2.482888   2.164523

N   1.766835   1.767619   -2.262550

N   -0.167451   -2.601915   -2.283870

C   2.206854   0.547957   -5.070409

C   -1.389644   -5.267764   -1.297141

C   -2.322869   -4.896989   1.392025

C   -2.482878   -0.587969   4.861507

C   -1.385880   2.064502   4.880847

C   1.693179   5.003641   1.322282

C   2.669788   4.599510   -1.347768

C   1.026189   -2.069241   -5.114032

C   1.650062   -1.555535   -6.261682

H   1.681525   -2.165955   -7.173767

C   2.236972   -0.261317   -6.247878

C   -1.997206   -6.335958   -0.568198

C   -2.458227   -6.144338   0.761744

H   -2.925431   -6.973255   1.309272

C   -2.630719   0.264459   5.992510

C   -2.081263   1.576740   5.997119

H   -2.200381   2.221483   6.877859

C   2.902507   5.814525   -0.685908

H   3.456692   6.609006   -1.202488

C   2.421790   6.022018   0.635869

H   0.576075   -3.072487   -5.127002

H   2.668661   1.545313   -5.078932

H   -1.041455   -5.435389   -2.326152

H   -2.680429   -4.752462   2.421932

H   -2.909739   -1.600505   4.876519

H   -0.966910   3.081084   4.885858

H   1.324106   5.186385   2.341394

H   3.035877   4.444478   -2.373032

S   -3.031848   2.789029   1.450664

C   -3.607999   1.255824   1.487636

N   -3.988227   0.119392   1.551295

O   2.601043   7.162678   1.332035

O   2.853361   0.298752   -7.307230

O   -2.086638   -7.503627   -1.236912

O   -3.316255   -0.268866   7.028647

C   3.312160   8.251493   0.721869

H   2.791348   8.599059   -0.194719

H   3.324342   9.061197   1.473244

H   4.352493   7.954762   0.473850

C   2.935609   -0.435522   -8.539270

H   1.922750   -0.657587   -8.934930

H   3.475986   0.220612   -9.244676

H   3.500193   -1.380704   -8.398321

C   -2.668801   -8.641375   -0.581488

H   -2.620557   -9.467560   -1.313199

H   -2.091901   -8.911649   0.327488

H   -3.726592   -8.442985   -0.309717

C   -3.523660   0.521777   8.207865

H   -4.098568   1.442159   7.973312

H   -4.106174   -0.113912   8.898761

H   -2.556417   0.794908   8.679467

H-Stage I

E= -3540.2264589

G= -3539.873673

N   -1.507806   0.696728   -0.541532

C   -1.747085   1.871232   -0.750173

S   -2.202725   3.376100   -1.062272

Co   0.085145   -0.084513   0.032251

C   -1.237031   -2.547276   1.090430

C   -1.638350   -3.893715   0.691455

C   -1.228767   -4.048218   -0.654712

C   -0.590640   -2.791364   -1.036077

N   -0.599489   -1.910192   0.035581

C   -0.227175   1.215292   2.692775

C   -0.783207   0.984095   4.022471

C   -1.314068   -0.327895   4.008783

C   -1.068628   -0.857669   2.670420

N   -0.388219   0.082367   1.906914

C   1.480901   2.323975   -0.993155

C   1.784080   3.701808   -0.625104

C   1.376795   3.854360   0.722279

C   0.836026   2.565826   1.137867

N   0.937149   1.649409   0.095441

C   0.521891   -1.457623   -2.572464

C   1.080458   -1.228763   -3.901993

C   1.610438   0.083552   -3.892032

C   1.362485   0.616303   -2.556168

N   0.730123   -0.340775   -1.772808

N   -0.081605   -2.589223   -2.242132

N   -1.461888   -2.068282   2.304669

N   0.325097   2.366645   2.342617

N   1.701644   1.848055   -2.208432

C   1.508558   5.083714   1.390580

C   2.225816   0.631881   -5.029787

C   1.150906   -2.035154   -5.050407

C   -1.449032   -5.247848   -1.351931

C   -2.281269   -4.934362   1.382528

C   -1.931913   -0.877427   5.144619

C   -0.854929   1.788717   5.171960

C   2.336323   4.774051   -1.346735

C   2.464384   6.003684   -0.680744

H   2.886318   6.868817   -1.215121

C   2.056397   6.156353   0.668700

C   2.294208   -0.172756   -6.179429

C   1.764937   -1.487383   -6.189257

H   1.836706   -2.088696   -7.108679

C   -2.094424   -6.288160   -0.662397

C -2.504660 -6.133583   0.685152

H -3.005940 -6.971482   1.193770

C -1.474518   1.240799   6.307736

H -1.550930   1.841925   7.226900

C -2.004792 -0.073359   6.294462

H   2.648328   4.654810 -2.394722

H   1.187544   5.200719   2.436116

H   2.635838   1.652553 -5.019571

H   0.739443 -3.055240 -5.056747

H -1.126478 -5.367094 -2.396827

H -2.595510 -4.814367   2.429869

H   2.766937   0.223379 -7.091390

H   2.169487   7.136956   1.156229

H -2.284649 -7.243199 -1.176084

H -2.342957 -1.897658   5.132044

H -2.482944 -0.469333   7.203671

H -0.442732   2.808503   5.180594

H-Stage II

E= -3540.0338265

G= -3539.682147

N   -1.507215   0.683923   -0.541065

C   -1.731603   1.863347   -0.747807

S   -2.164057   3.373240   -1.055790

Co   0.095156   -0.087133   0.035541

C   -1.252443   -2.533576   1.081394

C   -1.680608   -3.872810   0.674092

C   -1.271548   -4.027117   -0.669208

C   -0.606656   -2.777356   -1.040806

N   -0.603456   -1.900499   0.032739

C   -0.205182   1.205354   2.695535

C   -0.735615   0.963882   4.037528

C   -1.274280   -0.341703   4.020415

C   -1.055155   -0.859529   2.669207

N   -0.382407   0.082012   1.901958

C   1.471698   2.324060   -0.992882

C   1.741067   3.715539   -0.637149

C   1.335630   3.867400   0.707972

C   0.828804   2.565001   1.134616

N   0.944929   1.642952   0.099388

C   0.534644   -1.458564   -2.563278

C   1.120686   -1.241087   -3.886518

C   1.658330   0.064944   -3.873004

C   1.382595   0.607833   -2.543020

N   0.735186   -0.340827   -1.764007

N   -0.085034   -2.583772   -2.242936

N   -1.465887   -2.063092   2.300979

N   0.332907   2.363106   2.344675

N   1.707889   1.845618   -2.203740

C   1.435246   5.098779   1.368628

C   2.296763   0.606441   -4.995494

C   1.204250   -2.054611   -5.023378

C   -1.508560   -5.213009   -1.375184

C   -2.341697   -4.899119   1.360117

C   -1.875443   -0.900646   5.154954

C   -0.780276   1.759209   5.189173

C   2.260781   4.789827   -1.370990

C   2.357163   6.032599   -0.712263

H   2.752297   6.903417   -1.256943

C   1.952264   6.184195   0.632350

C   2.383379   -0.208869   -6.143494

C   1.847466   -1.514545   -6.156948

H   1.931776   -2.122389   -7.070479

C   -2.177902   -6.248800   -0.689828

C -2.586736 -6.094718   0.652133

H -3.104663 -6.924407   1.156566

C -1.385004   1.200938   6.335069

H -1.439734   1.794746   7.260006

C -1.921972 -0.104217   6.318461

H   2.572574   4.670662 -2.418644

H   1.116568   5.215237   2.414533

H   2.711617   1.624718 -4.983312

H   0.784770 -3.070978 -5.033279

H -1.185500 -5.332929 -2.419445

H -2.655326 -4.779637   2.407298

H   2.877082   0.180829 -7.046562

H   2.039083   7.170406   1.112922

H -2.383780 -7.196049 -1.210955

H -2.294733 -1.917056   5.139392

H -2.387093 -0.507673   7.230609

H -0.363036   2.776500   5.200160

H-Stage III-a

E= -3539.8087093

G= -3539.459079

N   -1.706225   0.790387   -0.622808

C   -1.888838   1.799036   -1.268893

S   -2.144694   3.135682   -2.124131

Co -0.020730   -0.032708   0.027811

C   -1.368037   -2.470127   1.063917

C   -1.941594   -3.736056   0.601754

C   -1.548900   -3.878188   -0.747728

C   -0.747625   -2.694022   -1.068634

N   -0.686754   -1.852314   0.032035

C   -0.168185   1.188970   2.727384

C   -0.471189   0.856104   4.121521

C   -0.984062   -0.461158   4.110939

C   -0.983034   -0.891717   2.712855

N   -0.451809   0.110994   1.909978

C   1.350639   2.379394   -0.994405

C   1.472720   3.806827   -0.689213

C   1.044710   3.961843   0.648322

C   0.674693   2.625814   1.117845

N   0.859095   1.695689   0.101427

C   0.571959   -1.451568   -2.509914

C   1.341351   -1.309363   -3.749313

C   1.911231   -0.016435   -3.717463

C   1.461270   0.599394   -2.469683

N   0.696739   -0.309719   -1.742431

N   -0.144794   -2.534511   -2.236132

N   -1.467240   -2.058862   2.322099

N   0.265107   2.384121   2.351334

N   1.710269   1.859776   -2.161705

C   1.032771   5.211306   1.272987

C   2.695771   0.465789   -4.769022

C   1.539948   -2.169439   -4.831583

C   -1.893782   -5.006119   -1.495450

C   -2.691807   -4.717711   1.254063

C   -1.394886   -1.097690   5.285788

C   -0.353561   1.585734   5.306458

C   1.906309   4.894433   -1.450692

C   1.879074   6.167517   -0.830090

H   2.197999   7.051497   -1.402141

C   1.451621   6.322512   0.500706

C   2.912376   -0.405379   -5.863578

C   2.347882   -1.693688   -5.893756

H   2.532425   -2.344279   -6.761533

C   -2.670789   -5.997902   -0.846449

C   -3.060442   -5.857195   0.497094

H   -3.658920   -6.648204   0.972916

C   -0.755334   0.941820   6.502870

H   -0.669089   1.481082   7.457921

C   -1.263293   -0.370155   6.493034

H   2.246718   4.771396   -2.488785

H   0.709100   5.329722   2.317058

H   3.125165   1.477673   -4.749350

H   1.087443   -3.170885   -4.861863

H   -1.575034   -5.123390   -2.541147

H   -2.982545   -4.613892   2.309262

H   3.531133   -0.065649   -6.707401

H   1.442595   7.325455   0.952718

H   -2.968808   -6.897655   -1.405093

H   -1.802343   -2.118720   5.274263

H   -1.567006   -0.840017   7.440280

H   0.033235   2.614752   5.313749

H-Stage III-b

E= -3539.822536

G= -3539.470784

N   -1.530341   0.636239   -0.542106

C   -1.769577   1.806623   -0.785109

S   -2.216115   3.300995   -1.135504

Co   0.101273   -0.078485   0.038387

C   -1.334784   -2.472257   1.049957

C   -1.950899   -3.713407   0.575308

C   -1.539534   -3.869325   -0.766459

C   -0.687215   -2.717505   -1.068879

N   -0.593332   -1.888338   0.036209

C   -0.100562   1.174234   2.717539

C   -0.433804   0.852206   4.106763

C   -0.970777   -0.453368   4.090299

C   -0.945635   -0.890719   2.692695

N   -0.365969   0.087992   1.898468

C   1.356257   2.366035   -1.028736

C   1.438750   3.795633   -0.734115

C   1.037171   3.946260   0.612249

C   0.720781   2.604679   1.098824

N   0.916122   1.667117   0.090355

C   0.634673   -1.486885   -2.512838

C 1.399611 -1.342002 -3.753518

C 1.929148 -0.033384 -3.742559

C 1.469413 0.583200 -2.496587

N 0.743351 -0.332621 -1.750219

N -0.073649 -2.568905 -2.233261

N -1.454301 -2.047073 2.298294

N 0.330845 2.366019 2.339304

N 1.688966 1.853871 -2.201282

C 0.996137 5.199538 1.229575

C 2.697994 0.455283 -4.801278

C 1.621815 -2.212981 -4.823047

C -1.915464 -4.981304 -1.523730

C -2.753131 -4.664188 1.210790

C -1.421286 -1.075312 5.257327

C -0.332202 1.587606 5.289857

C 1.813159 4.893244 -1.514354

C 1.754613 6.167646 -0.901844

H 2.025874 7.058756 -1.487245

C 1.355575 6.317330 0.439721

C 2.940041 -0.426885 -5.883344

C 2.414724 -1.730967 -5.893636

H 2.618336 -2.389669 -6.750908

C -2.744550 -5.941218 -0.892226

C -3.153873 -5.786239   0.443938

H -3.794084 -6.552212   0.906295

C -0.774195   0.958691   6.480231

H -0.702139   1.502678   7.433737

C -1.305332 -0.342945   6.464544

H   2.132145   4.774398 -2.559671

H   0.691909   5.314067   2.279780

H   3.097236   1.479620 -4.798565

H   1.198943 -3.227704 -4.836574

H -1.581914 -5.109497 -2.563515

H -3.059702 -4.550394   2.260463

H   3.548210 -0.081239 -6.732497

H   1.320852   7.323232   0.883829

H -3.069402 -6.826658 -1.458663

H -1.849448 -2.087806   5.241591

H -1.642438 -0.801752   7.405896

H   0.071731   2.610052   5.300042

H-Stage IV

E= -4030.9088875

G= -4030.555717

N   -1.505600   -0.042207   0.047512

C   -2.369201   0.781265   0.131479

S   -3.602735   1.841070   0.239110

Co   0.326068   -0.370820   0.003146

C   0.168673   -3.351919   -0.047476

C   0.040506   -4.474535   -0.972277

C   0.014310   -3.917592   -2.273957

C   0.136468   -2.471973   -2.105258

N   0.247354   -2.161960   -0.758194

C   0.403485   -0.429084   2.978916

C   0.313261   -1.351138   4.107565

C   0.235924   -2.651786   3.554116

C   0.267774   -2.484498   2.103313

N   0.388642   -1.139070   1.785780

C   0.796810   2.565952   0.046004

C   0.890626   3.691017   0.968412

C   0.765628   3.152401   2.270940

C   0.628809   1.708675   2.108819

N   0.667939   1.380685   0.759393

C   0.293043   -0.325801   -2.972905

C   0.325453   0.604496   -4.098968

C   0.531846   1.891966   -3.547327

C   0.613998   1.711464   -2.101446

N   0.473935   0.367858   -1.783840

N   0.136875   -1.631852   -3.130619

N   0.179292   -3.509551   1.267815

N   0.500081   0.882717   3.136665

N   0.798176   2.722576   -1.267567

C   0.740575   3.983189   3.403481

C   0.608732   3.033881   -4.361551

C   0.197247   0.418170   -5.485431

C   -0.109363   -4.730456   -3.412871

C   -0.057760   -5.861283   -0.769345

C   0.141792   -3.788973   4.373082

C   0.300468   -1.147095   5.497249

C   0.978387   5.075841   0.753741

C   0.945602   5.907981   1.886163

H   1.006428   6.999760   1.758557

C   0.831740   5.369267   3.191637

C   0.474749   2.848455   -5.747913

C   0.273697   1.559639   -6.301557

H   0.173185   1.453313   -7.392756

C   -0.208759   -6.117508   -3.210588

C   -0.183273   -6.674800   -1.908014

H   -0.264549   -7.766206   -1.788571

C   0.203136   -2.284069   6.317549

H   0.186210   -2.163380   7.411696

C   0.125298   -3.585677   5.763669

H   1.052633   5.490543   -0.262125

H   0.637877   3.564773   4.415574

H   0.759470   4.033210   -3.928188

H   0.039128   -0.582454   -5.914151

H   -0.129354   -4.296545   -4.423472

H   -0.038372   -6.291759   0.242726

H   0.525448   3.719634   -6.419147

H   0.806299   6.052426   4.054521

H   -0.308796   -6.786406   -4.079286

H   0.081538   -4.798991   3.941602

H   0.050068   -4.452971   6.437608

H   0.361570   -0.135642   5.925274

S   -2.374956   4.067116   0.627607

C   -2.057392   4.416578   -0.969953

N   -1.840016   4.697398   -2.105448

H-Stage V

E= -4030.9022574

G= -4030.547361

N	-1.408668	-0.005678	0.083377
C	-2.304819	0.758394	0.266965
S	-3.591752	1.746132	0.479787
Co	0.395107	-0.345646	0.015567
C	0.102395	-3.303107	-0.051869
C	-0.189973	-4.404873	-0.970247
C	-0.233667	-3.840810	-2.265705
C	0.029270	-2.412140	-2.101077
N	0.235567	-2.123590	-0.749272
C	0.518037	-0.430475	2.978880
C	0.533354	-1.366311	4.104006
C	0.483539	-2.662477	3.542450
C	0.399954	-2.480778	2.094011
N	0.474259	-1.119688	1.785435
C	0.826301	2.577751	0.073270
C	0.744671	3.710765	0.986191
C	0.608226	3.169960	2.284590
C	0.627572	1.720020	2.130289
N	0.749213	1.392268	0.774630
C	0.357974	-0.282036	-2.948377

C   0.526133   0.631223   -4.080146

C   0.829309   1.897208   -3.529224

C   0.802077   1.731292   -2.079051

N   0.551843   0.388222   -1.762618

N   0.080159   -1.573626   -3.116421

N   0.222501   -3.487022   1.260126

N   0.542421   0.887432   3.150175

N   0.937947   2.736381   -1.242265

C   0.395487   3.993363   3.399666

C   1.046081   3.018586   -4.341987

C   0.441421   0.439109   -5.465030

C   -0.490704   -4.626295   -3.397553

C   -0.395426   -5.774484   -0.761411

C   0.482380   -3.809395   4.347771

C   0.592657   -1.171036   5.489350

C   0.637458   5.087524   0.750098

C   0.404955   5.917800   1.871568

H   0.304719   7.003857   1.725269

C   0.295361   5.381054   3.171477

C   0.961213   2.829762   -5.735283

C   0.665508   1.562864   -6.286502

H   0.604420   1.452544   -7.379875

C   -0.707481   -6.003533   -3.191292

C   -0.659863   -6.567265   -1.897190

H   -0.835053   -7.646751   -1.773206

C   0.596723   -2.322890   6.303213

H   0.639407   -2.210486   7.397193

C   0.542449   -3.617961   5.742975

H   0.719171   5.503522   -0.264463

H   0.286199   3.571562   4.409392

H   1.271361   4.003603   -3.908658

H   0.204147   -0.545199   -5.894038

H   -0.522814   -4.186078   -4.404743

H   -0.356854   -6.212695   0.246371

H   1.127298   3.684492   -6.408349

H   0.113371   6.056893   4.020391

H   -0.916474   -6.653034   -4.054801

H   0.437597   -4.816936   3.909486

H   0.546747   -4.494042   6.409026

H   0.629356   -0.162042   5.924969

S   -2.377909   3.979934   0.450702

C   -2.075338   4.005801   -1.189406

N   -1.860396   4.034376   -2.358084

F-Stage I

E= -5126.6841716

G= -5126.480070

N -1.502020   0.674337 -0.550070

C -1.736923   1.850993 -0.758776

S -2.186357   3.355701 -1.071528

Co 0.098381 -0.088127   0.036660

C -1.233904 -2.542787   1.092513

C -1.637868 -3.886381   0.694223

C -1.215201 -4.047170 -0.650868

C -0.569110 -2.795577 -1.029030

N -0.587405 -1.915639   0.040499

C -0.230093   1.220594   2.688746

C -0.786906   0.990741   4.015990

C -1.319486 -0.324444   4.002398

C -1.070797 -0.854568   2.666859

N -0.389464   0.086044   1.908682

C   1.473582   2.325331 -0.996217

C   1.753210   3.708540 -0.638009

C   1.341729   3.863458   0.711673

C   0.820480   2.571504   1.133927

N   0.935600   1.655451   0.095609

C   0.554168   -1.470434   -2.556978

C   1.123434   -1.247207   -3.880584

C   1.650163   0.070421   -3.872729

C   1.385942   0.609132   -2.544543

N   0.752419   -0.348274   -1.766169

N   -0.049601   -2.600781   -2.229847

N   -1.465504   -2.063412   2.303300

N   0.313571   2.374062   2.338823

N   1.709901   1.845428   -2.205046

C   1.452982   5.100249   1.361515

C   2.271527   0.604868   -5.008954

C   1.212851   -2.050172   -5.025193

C   -1.435694   -5.249335   -1.335444

C   -2.287555   -4.925208   1.373141

C   -1.936116   -0.863006   5.139279

C   -0.865987   1.787327   5.165621

C   2.282569   4.788846   -1.357318

C   2.388611   6.030938   -0.706766

F   2.880406   7.089404   -1.357674

C   1.980426   6.184560   0.638249

C   2.359242   -0.200504   -6.158713

C   1.834887   -1.512793   -6.166730

F   1.939402   -2.244290   -7.280686

C -2.090669 -6.291697 -0.654528

C -2.511986 -6.131392   0.684563

F -3.129220 -7.147445   1.295684

C -1.487284   1.247353   6.306256

F -1.586032   1.974001   7.423909

C -2.016816 -0.062758   6.293245

F   2.678319   4.690590 -2.629902

F   1.075865   5.291565   2.629041

F   2.780008   1.840357 -5.046859

F   0.733689 -3.296743 -5.078643

F -1.051642 -5.446971 -2.600407

F -2.698189 -4.820458   2.640854

F   2.941650   0.271221 -7.265386

F   2.100065   7.383004   1.217298

F -2.320317 -7.455255 -1.271243

F -2.448737 -2.096901   5.173727

F -2.598180 -0.537372   7.399234

F -0.380014   3.031081   5.223322

F-Stage II

E= -5126.4855978

G= -5126.281643

N   -1.503394   0.621866   -0.548126

C   -1.905882   1.768452   -0.460723

S   -2.574660   3.220661   -0.416859

Co   0.124646   -0.091130   0.029207

C   -1.215038   -2.535203   1.081060

C   -1.649937   -3.868086   0.675076

C   -1.231061   -4.029852   -0.668814

C   -0.553521   -2.790464   -1.037629

N   -0.554666   -1.915541   0.034694

C   -0.209019   1.225431   2.670151

C   -0.751564   0.991903   4.003792

C   -1.279163   -0.322958   3.993366

C   -1.038585   -0.851647   2.654529

N   -0.364727   0.090244   1.890708

C   1.458293   2.331385   -1.022499

C   1.724142   3.722124   -0.673640

C   1.312233   3.881413   0.672971

C   0.803806   2.584826   1.102992

N   0.918661   1.665166   0.069633

C   0.590727   -1.479848   -2.557606

C   1.182820   -1.268186   -3.874837

C   1.709234   0.047329   -3.868123

C   1.415365   0.598405   -2.549635

N   0.774545   -0.352264   -1.772246

N -0.024216   -2.605476   -2.236073

N -1.440275   -2.058710   2.294294

N   0.316237   2.386300   2.315757

N   1.718859   1.843717   -2.222795

C   1.416899   5.117066   1.319127

C   2.345056   0.576372   -4.994889

C   1.284757   -2.078606   -5.009257

C -1.485111   -5.214625   -1.365563

C -2.329416   -4.888747   1.345929

C -1.890849   -0.863810   5.128020

C -0.828191   1.790269   5.148535

C   2.252179   4.795883   -1.397160

C   2.356007   6.048772   -0.748651

F   2.847232   7.095754   -1.407391

C   1.947698   6.206428   0.589802

C   2.450191   -0.240087   -6.145247

C   1.925612   -1.546490   -6.153014

F   2.040306   -2.288377   -7.252506

C -2.176969   -6.248838   -0.691972

C   -2.593015   -6.088068   0.642960

F   -3.240191   -7.080986   1.249295

C   -1.446388   1.246932   6.299044

F   -1.538398   1.977479   7.408191

C   -1.970661   -0.059609   6.288972

F   2.650570   4.697313   -2.661468

F   1.041121   5.314725   2.578601

F   2.852527   1.804495   -5.036503

F   0.807359   -3.318104   -5.065081

F   -1.109745   -5.414584   -2.625192

F   -2.737578   -4.786221   2.607035

F   3.048472   0.229752   -7.237595

F   2.062185   7.398726   1.170177

F   -2.438028   -7.390912   -1.324392

F   -2.400408   -2.091078   5.166749

F   -2.546060   -0.540438   7.388696

F   -0.351017   3.029759   5.206120

F-Stage III-a

E= -5126.2573789

G= -5126.054116

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N   -1.707837   0.725872   -0.570545
C   -2.517040   1.391283    0.038587
S   -3.602336   2.279167    0.823280
Co   0.037538  -0.038503   -0.035017
C   -1.106598  -2.541871    1.091201
C   -1.338479  -3.944018    0.758372
C   -0.913990  -4.109723   -0.583817
C   -0.437646  -2.805008   -1.027575
N   -0.536923  -1.893294    0.011536
C   -0.316257   1.299855    2.584729
C   -1.043357   1.148048    3.841304
C   -1.576222  -0.164170    3.835683
C   -1.157514  -0.771234    2.575616
N   -0.415130   0.139105    1.840846
C    1.567410   2.307081   -1.028012
C    2.071930   3.607800   -0.598825
C    1.676214   3.762603    0.753097
C    0.938431   2.555305    1.104734
N    0.930228   1.681627    0.027522
C    0.460028  -1.407044   -2.633274
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C   0.902205   -1.142401   -3.999330

C   1.413442   0.177998   -4.002509

C   1.267825   0.676028   -2.637208

N   0.664823   -0.288455   -1.847990

N   -0.018011   -2.586179   -2.262505

N   -1.448837   -2.022680   2.260247

N   0.342111   2.407644   2.276230

N   1.704577   1.870510   -2.270989

C   1.972585   4.927471   1.464304

C   1.939224   0.744361   -5.164430

C   0.911890   -1.922109   -5.156677

C   -1.014724   -5.345794   -1.226480

C   -1.874973   -5.011413   1.480737

C   -2.331229   -0.638075   4.909415

C   -1.257516   2.010280   4.917661

C   2.774941   4.614207   -1.262953

C   3.086564   5.801112   -0.542689

F   3.754539   6.773652   -1.146585

C   2.692208   5.955557   0.795509

C   1.939283   -0.039168   -6.353235

C   1.435262   -1.347643   -6.349051

F   1.443222   -2.059731   -7.467564

C   -1.558658   -6.438305   -0.496097

C   -1.977223   -6.274717   0.833724

F   -2.478348   -7.307926   1.495569

C   -2.036928   1.538609   6.011337

F   -2.269165   2.340220   7.041641

C   -2.563933   0.239115   6.006575

F   3.161769   4.523633   -2.523831

F   1.617522   5.122753   2.722358

F   2.433977   1.969087   -5.219123

F   0.456668   -3.162327   -5.204581

F   -0.635462   -5.549926   -2.476082

F   -2.288953   -4.910009   2.732207

F   2.421395   0.477027   -7.475217

F   2.991897   7.071870   1.444753

F   -1.670063   -7.623650   -1.079069

F   -2.844265   -1.855373   4.959703

F   -3.289992   -0.180775   7.033350

F   -0.782102   3.242639   4.969434

F-Stage III-b

E= -5126.2705556

G= -5126.064448

N   -1.511160   0.576584   -0.559265

C   -1.919810   1.724705   -0.577432

S   -2.613202   3.161517   -0.665841

Co   0.131257   -0.091820   0.036836

C   -1.212499   -2.530374   1.085736

C   -1.662378   -3.856334   0.674243

C   -1.244041   -4.017719   -0.668066

C   -0.551334   -2.785289   -1.030452

N   -0.542450   -1.914479   0.044705

C   -0.201880   1.223421   2.675032

C   -0.727438   0.983265   4.014394

C   -1.255800   -0.329415   4.003505

C   -1.030341   -0.851575   2.659907

N   -0.367803   0.094417   1.891026

C   1.444264   2.336706   -1.018987

C   1.702722   3.729333   -0.672375

C   1.296989   3.886387   0.674654

C   0.796270   2.587567   1.106676

N   0.906788   1.668132   0.072514

C   0.598407   -1.477981   -2.545542

C   1.198860   -1.269409   -3.858997

C   1.724242   0.044755   -3.851874

C   1.417017   0.600336   -2.538675

N   0.774787   -0.348587   -1.761452

N   -0.019338   -2.603261   -2.228256

N   -1.435710   -2.057614   2.301297

N   0.319407   2.387302   2.323222

N   1.711918   1.849338   -2.217613

C   1.402460   5.118993   1.322869

C   2.361115   0.574982   -4.975062

C   1.302415   -2.080785   -4.990459

C   -1.508159   -5.195054   -1.370085

C   -2.351907   -4.869853   1.341737

C   -1.861593   -0.874315   5.137208

C   -0.795717   1.778453   5.159425

C   2.226160   4.801834   -1.397660

C   2.333071   6.062294   -0.745823

F   2.819885   7.101016   -1.410090

C   1.932843   6.217218   0.590209

C   2.472392   -0.245852   -6.132184

C   1.949353   -1.547626   -6.140843

F   2.062714   -2.294143   -7.230829

C   -2.215365   -6.231945   -0.698578

C -2.629264 -6.072117   0.631834

F -3.285158 -7.051033   1.239651

C -1.410631   1.230311   6.319821

F -1.489667   1.961308   7.423228

C -1.934403 -0.071098   6.309367

F   2.618870   4.708730 -2.656302

F   1.035926   5.316617   2.577184

F   2.864390   1.796515 -5.019320

F   0.827436 -3.312831 -5.050052

F -1.136518 -5.396518 -2.622395

F -2.759205 -4.771277   2.595301

F   3.073342   0.229541 -7.213965

F   2.046717   7.400204   1.177540

F -2.482607 -7.360784 -1.340712

F -2.372080 -2.092924   5.176530

F -2.502124 -0.560947   7.402581

F -0.322436   3.011177   5.220956

F-Stage IV

E= -5617.3640493

G= -5617.158814

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N   -1.548071    0.689871   -0.319154
C   -2.160706    1.241574   -1.169231
S   -3.026903    2.010527   -2.369774
Co   0.174541   -0.088994    0.301803
C   -1.045239   -2.590712    1.353558
C   -1.521211   -3.902543    0.918196
C   -1.219248   -3.995030   -0.463382
C   -0.568249   -2.737608   -0.825057
N   -0.485333   -1.914722    0.283930
C    0.107918    1.085092    3.032107
C   -0.280496    0.774600    4.405740
C   -0.796938   -0.545016    4.383565
C   -0.711910   -0.993471    2.994834
N   -0.146513   -0.000629    2.213283
C    1.452051    2.381598   -0.733031
C    1.810104    3.739178   -0.327171
C    1.515504    3.829895    1.056123
C    0.984454    2.526406    1.448343
N    0.960343    1.679533    0.353284
C    0.459922   -1.358426   -2.373792
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C   0.930731   -1.080331   -3.728108

C   1.431008   0.245590   -3.710978

C   1.271952   0.726087   -2.339591

N   0.707853   -0.267775   -1.558080

N   -0.133268   -2.497257   -2.052582

N   -1.148651   -2.182628   2.609236

N   0.608451   2.262662   2.689830

N   1.612588   1.952027   -1.975593

C   1.744948   5.011977   1.765104

C   1.877347   0.861611   -4.884657

C   0.873744   -1.812355   -4.916242

C   -1.535630   -5.142959   -1.194200

C   -2.144875   -4.957069   1.590329

C   -1.262109   -1.154452   5.552018

C   -0.227126   1.507327   5.594355

C   2.334164   4.831214   -1.023899

C   2.563414   6.031615   -0.310963

F   3.058659   7.093588   -0.944830

C   2.272338   6.121108   1.062820

C   1.817431   0.124467   -6.090240

C   1.327619   -1.194736   -6.104488

F   1.279750   -1.861238   -7.256611

C   -2.169662   -6.211702   -0.518251

C   -2.469767   -6.120156   0.853409

F   -3.067587   -7.144151   1.461038

C   -0.697711   0.894333   6.779107

F   -0.660302   1.563210   7.930688

C   -1.206710   -0.417396   6.758547

F   2.624328   4.797351   -2.322298

F   1.486414   5.144840   3.063643

F   2.344830   2.107178   -4.920781

F   0.394988   -3.050905   -4.985305

F   -1.270372   -5.278019   -2.491267

F   -2.446688   -4.919059   2.885943

F   2.231908   0.679724   -7.227767

F   2.495571   7.266975   1.704798

F   -2.487843   -7.320967   -1.184292

F   -1.753563   -2.390779   5.583864

F   -1.641540   -0.967180   7.891458

F   0.243882   2.749986   5.664361

S   -1.494195   2.087477   -3.994180

C   -1.754780   0.567203   -4.679625

N   -1.915558   -0.487558   -5.189894

F-Stage V

E= -5617.3563697

G= -5617.157999

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N   -1.552341    0.693026   -0.321271
C   -2.165298    1.248608   -1.168039
S   -3.031071    2.024213   -2.366134
Co   0.173597   -0.089061    0.301213
C   -1.037528   -2.594867    1.355547
C   -1.500635   -3.912264    0.922849
C   -1.202265   -4.002628   -0.459551
C   -0.563554   -2.739690   -0.823920
N   -0.484417   -1.915157    0.283511
C    0.098318    1.088946    3.029588
C   -0.301504    0.782905    4.400947
C   -0.817876   -0.536697    4.378873
C   -0.720409   -0.990175    2.992551
N   -0.150791    0.000191    2.211818
C    1.459193    2.378959   -0.732740
C    1.830079    3.732012   -0.323534
C    1.531988    3.823747    1.058882
C    0.988101    2.524434    1.447998
N    0.960174    1.678857    0.352874
C    0.452624   -1.356380   -2.376623
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C   0.913699   -1.074543   -3.733380

C   1.412361   0.251925   -3.716640

C   1.263683   0.728449   -2.342449

N   0.704249   -0.266233   -1.559905

N   -0.134760   -2.497102   -2.053576

N   -1.148126   -2.183782   2.609064

N   0.604704   2.263755   2.688266

N   1.612390   1.952030   -1.976629

C   1.770245   5.002628   1.769969

C   1.850629   0.870677   -4.891851

C   0.850193   -1.804487   -4.922531

C   -1.509269   -5.153964   -1.188834

C   -2.111554   -4.972740   1.597370

C   -1.290441   -1.143109   5.545928

C   -0.256331   1.519022   5.587793

C   2.366641   4.820016   -1.017308

C   2.605531   6.016995   -0.302137

F   3.114050   7.074786   -0.932709

C   2.310803   6.107398   1.070831

C   1.784105   0.135634   -6.098540

C   1.295979   -1.184160   -6.112428

F   1.241799   -1.848508   -7.265561

C   -2.129730   -6.229059   -0.510304

C   -2.426413   -6.139727   0.862194

F   -3.011611   -7.169471   1.472427

C   -0.734815   0.909319   6.770956

F   -0.705409   1.581416   7.920958

C   -1.243409   -0.402599   6.750618

F   2.660750   4.784702   -2.314853

F   1.508645   5.136753   3.067905

F   2.316328   2.116962   -4.928800

F   0.372846   -3.043589   -4.990644

F   -1.247065   -5.286905   -2.486779

F   -2.409610   -4.937332   2.893954

F   2.190604   0.693796   -7.237479

F   2.543137   7.250121   1.715235

F   -2.438156   -7.342010   -1.174760

F   -1.781680   -2.379612   5.578074

F   -1.686111   -0.949087   7.882141

F   0.214459   2.761872   5.657505

S   -1.501554   2.093815   -3.987814

C   -1.770744   0.575260   -4.674735

N   -1.937424   -0.478290   -5.185383

NO$_2$-Stage I

E= -4357.7479384

G= -4357.404352

N -1.481128   0.692726 -0.548522

C -1.701718   1.873804 -0.749677

S -2.133959   3.384626 -1.053894

Co 0.112051 -0.089138   0.038203

C -0.217781   1.207847   2.696036

C -0.783379   0.977843   4.021047

C -1.327406 -0.329004   3.996254

C -1.079007 -0.857239   2.656900

N -0.387451   0.081422   1.905052

C   1.523081   2.315057 -0.971848

C   1.826055   3.691560 -0.601534

C   1.410435   3.840717   0.744035

C   0.864312   2.552402   1.156193

N   0.966208   1.642939   0.110101

C   0.553590 -1.454150 -2.566292

C   1.120528 -1.226349 -3.891439

C   1.659354   0.082701 -3.872424

C   1.406687   0.615134 -2.536401

N   0.761651 -0.340428 -1.764463

C -1.245896 -2.538392   1.074766

C   -1.651416   -3.881550   0.671784

C   -1.223385   -4.037288   -0.668904

C   -0.574178   -2.783309   -1.044281

N   -0.592840   -1.906294   0.028258

N   -1.479614   -2.061689   2.287635

N   0.347251   2.355446   2.356143

N   1.751958   1.841892   -2.186188

N   -0.055299   -2.584579   -2.244006

C   2.282810   0.636499   -4.995061

C   -1.433680   -5.227295   -1.372600

C   -2.310976   -4.915538   1.357965

C   -1.958070   -0.882425   5.115037

C   -0.852273   1.781920   5.171577

C   1.525046   5.062326   1.416428

C   2.377192   4.764120   -1.324546

C   1.188585   -2.032852   -5.040451

C   1.808697   -1.495297   -6.174841

H   1.892420   -2.073698   -7.104332

C   2.338394   -0.184487   -6.131694

C   -2.093576   -6.246680   -0.669095

C   -2.532650   -6.114096   0.668686

H   -3.041186   -6.960028   1.149416

C   -2.016397   -0.063135   6.252827

C -1.481184   1.245162   6.301578

H -1.568730   1.822712   7.231242

C   2.495700   5.995056 -0.669304

H   2.910339   6.873490 -1.180980

C   2.071154   6.120060   0.674749

H   0.770294 -3.049118 -5.053817

H   2.705140   1.649518 -5.002948

H -1.105719 -5.371473 -2.410025

H -2.640571 -4.794238   2.399486

H -2.385802 -1.893195   5.118559

H -0.430388   2.796658   5.188709

H   1.202715   5.201521   2.456246

H   2.695650   4.647567 -2.369973

N -2.671780 -0.597911   7.462166

O -2.717881   0.122535   8.466976

O -3.142624 -1.741247   7.411259

N -2.335098 -7.526616 -1.362714

O -2.908566 -8.428558 -0.739260

O -1.950488 -7.635185 -2.533994

N   2.983831   0.351179 -7.345828

O   3.446355   1.498178 -7.300908

O   3.030931 -0.372369 -8.348394

N   2.201823   7.435682   1.331244

O   1.826518   7.539494   2.505853

O   2.678912   8.369455   0.674664

NO$_2$-Stage II

E= -4357.5391735

G= -4357.197810

N   -1.479280   0.682391   -0.538256

C   -1.917536   1.770596   -0.205541

S   -2.605898   3.168228   0.148305

Co   0.134969   -0.089530   0.019368

C   -0.167264   1.205100   2.673097

C   -0.726979   0.974520   4.007113

C   -1.291424   -0.319893   3.977650

C   -1.056479   -0.845048   2.631423

N   -0.353592   0.085207   1.878032

C   1.510102   2.318925   -1.010640

C   1.794295   3.709888   -0.651024

C   1.401068   3.856400   0.697812

C   0.883640   2.555736   1.121670

N   0.977738   1.643637   0.079497

C   0.583874   -1.463402   -2.578112

C   1.180115   -1.250294   -3.900229

C   1.713061   0.057795   -3.885115

C   1.425690   0.604969   -2.558201

N   0.772338   -0.341849   -1.785760

C   -1.247345   -2.517575   1.047266

C   -1.679506   -3.857520   0.639186

C   -1.245674   -4.019559   -0.695389

C   -0.568357   -2.774409   -1.063755

N   -0.577677   -1.896309   0.007113

N   -1.477848   -2.041894   2.260290

N   0.395047   2.353082   2.333723

N   1.748573   1.842552   -2.220368

N   -0.034095   -2.588759   -2.259855

C   2.356757   0.603804   -4.996294

C   -1.472301   -5.199650   -1.404749

C   -2.362747   -4.871309   1.321217

C   -1.928967   -0.870043   5.090538

C   -0.777517   1.776545   5.153329

C   1.505708   5.076549   1.367607

C   2.313803   4.780720   -1.388609

C   1.270088   -2.070433   -5.031176

C   1.916254   -1.540664   -6.163335

H   2.020187   -2.131085   -7.083374

C   2.439087   -0.234041   -6.123612

C   -2.160908   -6.207512   -0.704731

C   -2.605303   -6.069086   0.623760

H   -3.135622   -6.903813   1.100847

C   -1.969630   -0.051554   6.234087

C   -1.415027   1.241401   6.287725

H   -1.489842   1.817981   7.219272

C   2.422423   6.021753   -0.735193

H   2.813080   6.904323   -1.258864

C   2.021924   6.142922   0.609320

H   0.854037   -3.087394   -5.042689

H   2.774805   1.618621   -5.007803

H   -1.139545   -5.348907   -2.439969

H   -2.697414   -4.745479   2.360335

H   -2.375445   -1.872729   5.090128

H   -0.341130   2.784818   5.173355

H   1.200637   5.213225   2.412997

H   2.617406   4.666432   -2.438493

N   -2.634991   -0.582896   7.446492

O   -2.664581   0.133687   8.451653

O   -3.123509   -1.715891   7.383689

N   -2.425420   -7.485195   -1.405932

O   -3.020184   -8.373151   -0.787196

O   -2.033907   -7.591980   -2.572913

N   3.111534   0.292404   -7.333976

O   3.566627   1.440013   -7.284987

O   3.180732   -0.442481   -8.323921

N   2.142962   7.467229   1.262606

O   1.785265   7.561031   2.441410

O   2.592691   8.403244   0.594585

NO$_2$-Stage III-a

E= -4357.3001181

G= -4356.961330

N   -1.545346   0.707144   -0.586101

C   -1.978354   1.846682   -0.629373

S   -2.683385   3.268654   -0.744553

Co   0.032887   -0.050884   -0.000173

C   -0.221009   1.217705   2.671824

C   -0.755943   0.974373   4.012633

C   -1.292380   -0.333153   3.994256

C   -1.088420   -0.849468   2.642898

N   -0.397878   0.103547   1.881749

C   1.484407   2.328638   -0.991205

C   1.788096   3.715953   -0.626456

C   1.379299   3.869128   0.716972

C   0.828085   2.583039   1.133343

N   0.912314   1.671261   0.074433

C   0.565895   -1.455940   -2.560315

C   1.159859   -1.237958   -3.881138

C   1.724857   0.057365   -3.854009

C   1.443032   0.607137   -2.531800

N   0.774793   -0.352326   -1.759532

C   -1.308060   -2.497417   1.035712

C -1.720964 -3.847493 0.635714

C -1.267340 -4.019782 -0.690761

C -0.609821 -2.770484 -1.069071

N -0.656563 -1.873756 -0.000117

N -1.521797 -2.030704 2.262429

N 0.330270 2.377974 2.333912

N 1.755811 1.839921 -2.195826

N -0.062118 -2.583919 -2.251891

C 2.373715 0.603366 -4.963381

C -1.460147 -5.213481 -1.387483

C -2.387647 -4.863530 1.325449

C -1.888659 -0.901374 5.121467

C -0.788692 1.771477 5.161174

C 1.502004 5.085013 1.391858

C 2.346782 4.770872 -1.353114

C 1.226442 -2.049357 -5.018266

C 1.879084 -1.518689 -6.149041

H 1.962859 -2.100481 -7.076808

C 2.429658 -0.224821 -6.098816

C -2.136614 -6.225769 -0.680210

C -2.597582 -6.078245 0.638860

H -3.116341 -6.916642 1.122548

C -1.911341 -0.087040 6.268559

C   -1.383205   1.216024   6.311660

H   -1.442624   1.787392   7.247716

C   2.472369   6.011681   -0.693412

H   2.890679   6.885286   -1.211043

C   2.053934   6.140899   0.641933

H   0.787221   -3.056197   -5.039282

H   2.813774   1.609016   -4.966151

H   -1.110853   -5.370126   -2.416294

H   -2.735710   -4.732446   2.359384

H   -2.312046   -1.914135   5.130202

H   -0.372462   2.788175   5.174224

H   1.187077   5.226321   2.433885

H   2.666008   4.651923   -2.397725

N   -2.526052   -0.639516   7.501967

O   -2.556799   0.081584   8.502106

O   -2.969813   -1.789944   7.451809

N   -2.365618   -7.520898   -1.367461

O   -2.942518   -8.412363   -0.739580

O   -1.962705   -7.629737   -2.529224

N   3.106390   0.301396   -7.311345

O   3.597441   1.431634   -7.245112

O   3.137049   -0.419648   -8.311506

N   2.194273   7.463694   1.300632

O   1.822235   7.559187   2.473688

O   2.671778   8.388656   0.639017

NO$_2$-Stage III-b

E= -4357.3126105

G= -4356.971812

N   -1.497737   0.625729   -0.570286

C   -1.849430   1.783433   -0.713644

S   -2.487635   3.227341   -0.958102

Co   0.116335   -0.080414   0.038121

C   -0.211787   1.218476   2.682775

C   -0.708959   0.959785   4.040293

C   -1.243487   -0.345605   4.019160

C   -1.055373   -0.847543   2.656411

N   -0.406819   0.105997   1.883781

C   1.495471   2.324764   -0.982833

C   1.757003   3.725091   -0.632027

C   1.325657   3.883345   0.702445

C   0.816512   2.579729   1.129816

N   0.945747   1.654117   0.101100

C   0.580036   -1.457506   -2.547029

C   1.203808   -1.253841   -3.860499

C   1.752413   0.045681   -3.837635

C   1.438819   0.602434   -2.519337

N   0.764541   -0.335633   -1.754314

C   -1.263049   -2.508979   1.065789

C -1.728171 -3.837376 0.643278

C -1.305873 -3.992092 -0.693894

C -0.599751 -2.758059 -1.047909

N -0.585567 -1.890750 0.030835

N -1.472712 -2.047396 2.287224

N 0.318150 2.379085 2.337557

N 1.758119 1.841607 -2.183963

N -0.056437 -2.575025 -2.241274

C 2.417673 0.584941 -4.935982

C -1.555667 -5.156414 -1.416769

C -2.422730 -4.840961 1.319674

C -1.814523 -0.927782 5.149317

C -0.724412 1.746473 5.192486

C 1.399923 5.109575 1.361618

C 2.285568 4.786708 -1.369374

C 1.298745 -2.077090 -4.984046

C 1.973305 -1.553803 -6.111605

H 2.082557 -2.147978 -7.028789

C 2.508676 -0.259095 -6.063963

C -2.262605 -6.161911 -0.721906

C -2.694326 -6.031421 0.604886

H -3.237998 -6.860143 1.077870

C -1.817568 -0.123770 6.309132

C   -1.295498   1.176546   6.354089

H   -1.335945   1.740306   7.295782

C   2.362215   6.042427   -0.725641

H   2.757368   6.921780   -1.251724

C   1.925591   6.174832   0.600896

H   0.867617   -3.087580   -5.002951

H   2.845494   1.595916   -4.943788

H   -1.229169   -5.300988   -2.454874

H   -2.746384   -4.723661   2.363191

H   -2.238535   -1.940410   5.155239

H   -0.313585   2.765431   5.207662

H   1.068431   5.255602   2.397895

H   2.621608   4.663141   -2.408196

N   -2.408865   -0.691367   7.547473

O   -2.419418   0.016413   8.556918

O   -2.853915   -1.840858   7.489464

N   -2.555731   -7.428786   -1.439987

O   -3.157549   -8.312338   -0.825952

O   -2.175693   -7.519357   -2.610505

N   3.208425   0.261840   -7.266859

O   3.678294   1.401010   -7.201791

O   3.277739   -0.471903   -8.255024

N   2.013418   7.511726   1.242972

O   1.619187   7.609655   2.408181

O   2.472025   8.441290   0.575582

NO$_2$-Stage IV

E= -4848.4187541

G= -4848.074943

N   -1.909194   0.536502   -0.491500

C   -2.705232   0.494122   -1.364939

S   -3.827655   0.435569   -2.605262

Co -0.097795   0.048455   0.213689

C   -0.398959   1.255209   2.914349

C   -0.888677   0.950941   4.263166

C   -1.300967   -0.400351   4.234775

C   -1.057134   -0.877031   2.870428

N   -0.510821   0.138396   2.104202

C   1.127532   2.570190   -0.771105

C   1.486685   3.924151   -0.335579

C   1.108815   4.011824   1.023104

C   0.534047   2.710461   1.376465

N   0.564728   1.865633   0.279602

C   0.335925   -1.199772   -2.447162

C   0.777382   -0.877966   -3.808286

C   1.236489   0.457628   -3.767813

C   1.041818   0.919439   -2.391026

N   0.511718   -0.102780   -1.620710

C   -1.125002   -2.536341   1.258466

C   -1.457795   -3.899363   0.830139

C   -1.111149   -3.975883   -0.537578

C   -0.573434   -2.661795   -0.901661

N   -0.584177   -1.824249   0.200300

N   -1.348028   -2.112913   2.492973

N   0.077319   2.448200   2.591300

N   1.338903   2.151599   -2.009936

N   -0.159022   -2.385626   -2.128632

C   1.695532   1.110666   -4.911564

C   -1.306040   -5.139715   -1.281258

C   -2.013238   -4.988769   1.511766

C   -1.822981   -1.033092   5.363274

C   -0.983205   1.726556   5.424660

C   1.309438   5.174120   1.767932

C   2.081883   4.999091   -1.006312

C   0.745745   -1.612278   -5.000935

C   1.193890   -0.968426   -6.168328

H   1.187182   -1.484583   -7.137313

C   1.657580   0.359003   -6.100371

C -1.867065   -6.224607   -0.581114

C -2.218802   -6.173495   0.780991

H -2.652917   -7.063154   1.256058

C -1.912620   -0.238540   6.521919

C -1.509982   1.109456   6.574225

H -1.613164   1.662980   7.516915

C   2.293214   6.182020   -0.274359

H   2.756215   7.061293   -0.741412

C   1.908478   6.245292   1.078297

H   0.377354   -2.647121   -5.032551

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