

Electronic Supporting Information

Guanidine-Based Biomimetic Hydrides for Carbon Dioxide Reduction

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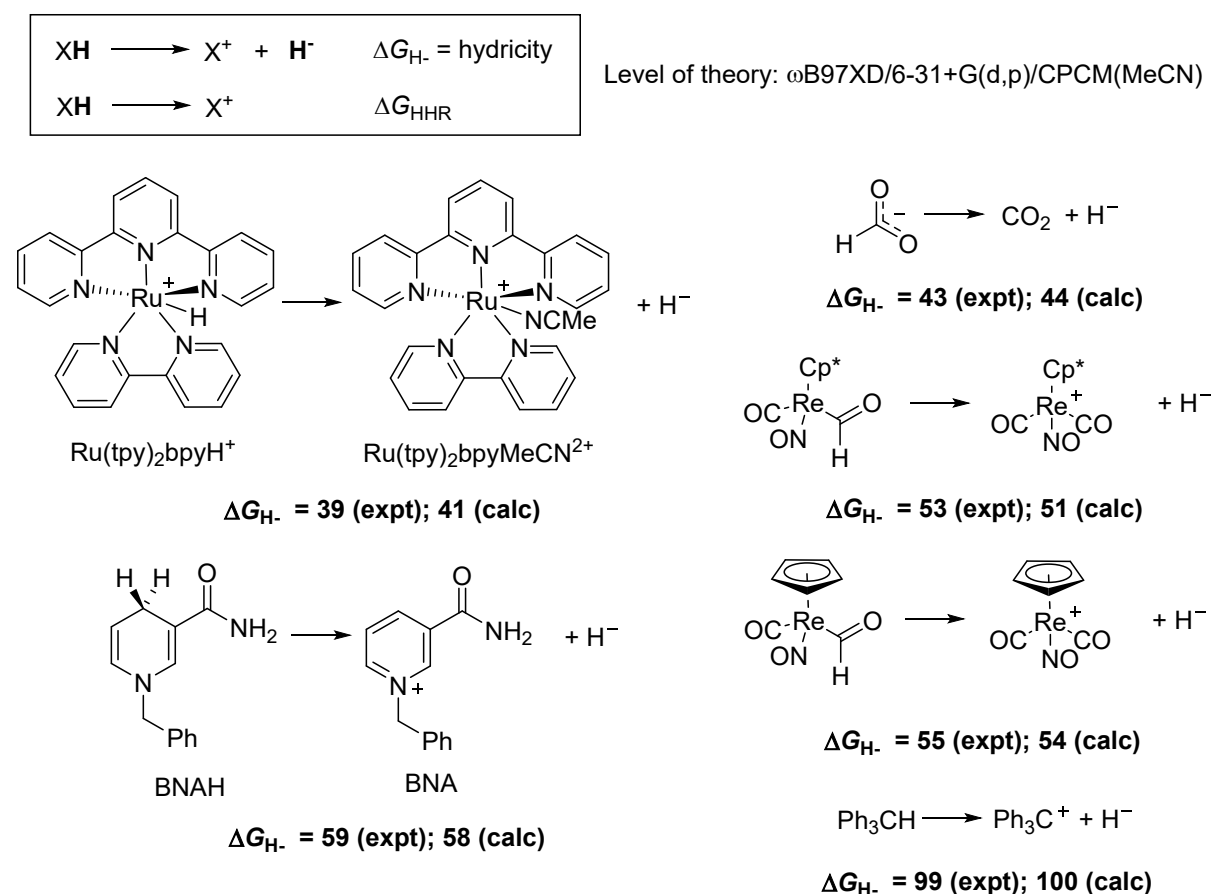
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Computational Methods and Discussion

Density functional theory (DFT) modelling was carried out with Gaussian 16 computational chemistry suite.¹ Geometries of minimum and transition state (TS) electronic structures were optimized with ω B97XD functional,^{2,3} Pople's basis-set 6-31+G(d,p),⁴ in CPCM model⁵ (acetonitrile parameters) at 298 K. Frequency calculations were carried out at that level to ensure convergence (all positive eigenvalues for minima and single negative for TS structures). This level of theory ω B97XD/6-31+G(d,p)/CPCM was benchmarked and found suitable for calculations of thermodynamic hydricities of organohydrides.⁶

Benchmarking studies and determination of ΔG_{H^-}

The thermodynamic hydricity, or the negative of hydride H^- affinity of hydride acceptor X^+ (see below Scheme S1),^{7,8} was determined by the direct approach extrapolating the calculated ΔG_{HHR} and experimental ΔG_{H^-} of the following hydride species ($\text{Ru}(\text{tpy})_2\text{bpyH}^+$, BNAH, HCOO^- , Ph_3CH , $\text{Cp}^*\text{Re}(\text{NO})(\text{CO})\text{CHO}$, and $\text{CpRe}(\text{NO})(\text{CO})\text{CHO}$)^{9–12} in Scheme S1 below and the ΔG_{H^-} was plotted against ΔG_{HHR} in Figure S1 at two different level of theories.⁹



Scheme S1. Gibbs energy hydricity calculations of known compounds and their experimental values in kcal/mol.

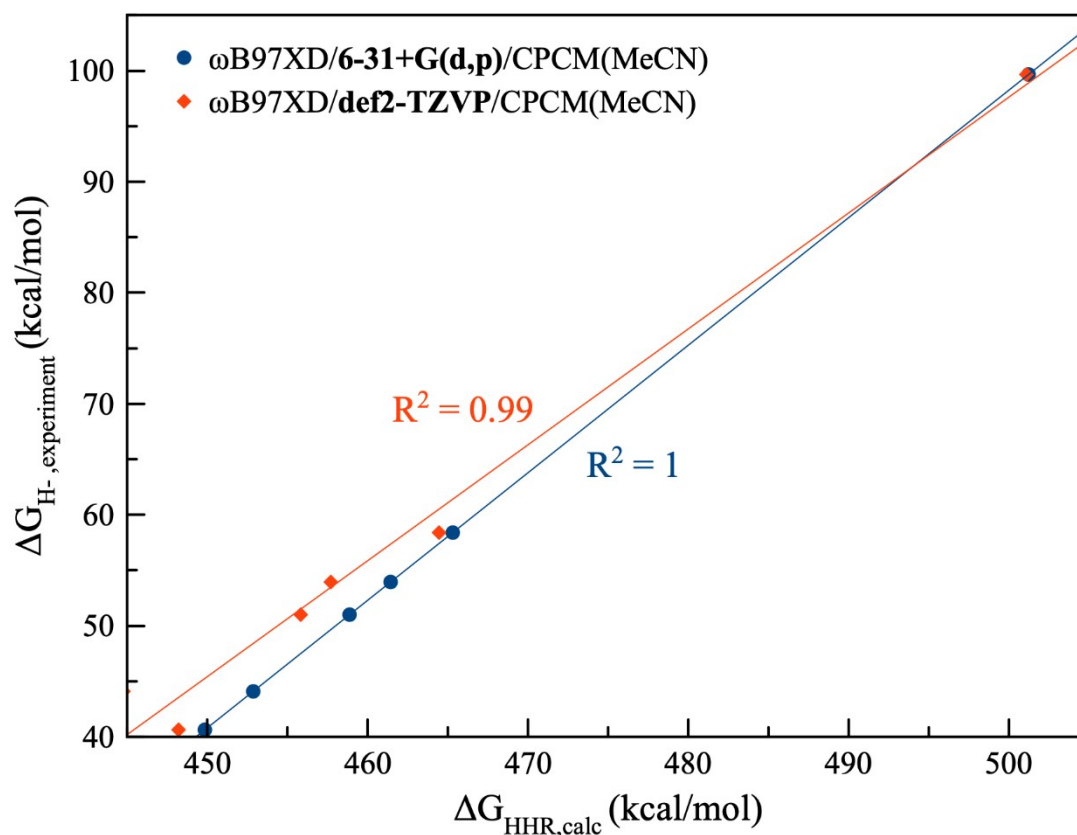


Figure S1. $\Delta G_{\text{H-}}$ (experimental) plotted against ΔG_{HHR} (calculated) for $\omega\text{B97XD/6-31+G(d,p)/CPCM(MeCN)}$ and $\omega\text{B97XD/def2-TZVP/CPCM(MeCN)}$ level of theories.

The level of theories assessed were $\omega\text{B97XD/6-31+G(d,p)/CPCM(MeCN)}$ and a single-point calculation of the optimized structures at higher level $\omega\text{B97XD/def2-TZVP/CPCM(MeCN)}$ employing Ahlrichs' triple-zeta basis set.¹³ Both level of theories have linear regression R^2 values close to 1 with $\omega\text{B97XD/6-31+G(d,p)/CPCM(MeCN)}$ having better agreement and based on the linear equation $y = 1.1489x - 476.22$, the calculated $\Delta G_{\text{H-}}$ for the tested species (Scheme S1) were determined to be within 2 kcal/mol of experimental values. As such all calculations were performed at this computationally efficient $\omega\text{B97XD/6-31+G(d,p)/CPCM(MeCN)}$ level of theory.

pK_a and reduction potential calculations

Reduction potential (E°)

Reduction potentials, E° , were calculated at $\omega\text{B97XD/6-31+G(d,p)/CPCM(MeCN)}$ level of theory with reference to the ferricenium/ferrocene (V vs. Fc^+/Fc) reduction potential, i.e. E°_{ref} , in acetonitrile (MeCN). The following equations were applied in calculating the reduction potential of an example electron transfer (ET) step involving $\text{R}^+ + \text{e}^- \rightarrow \text{R}^\bullet$:

$$E^{\circ} = -27.2114 \Delta G_{redox} - E_{ref}^{\circ}$$

$$\Delta G_{redox} = G_{R^{\bullet}} - G_{R^{+}}$$

where E_{ref}° is the absolute reduction potential of ferricenium in acetonitrile (4.988 V). Gibbs energies of the organohydride $G_{R^{\bullet}}$ and $G_{R^{+}}$ are in Hartrees.

pK_a calculations

The acidity calculation is calculated for the proton transfer (PT) step of the electrochemical reduction step. The pK_a values were calculated using the work from Thapa and Schlegel¹⁴:

$$pK_a = \frac{\Delta G}{2.303RT}$$

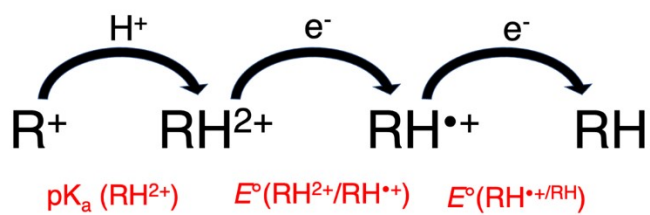
$$\Delta G = G_{R^{-}} - G_{RH} + G_{H^{+}}$$

Where $G_{H^{+}}$ is applied as the experimental proton solvation Gibbs energy in acetonitrile at -254.2 kcal/mol.¹⁵

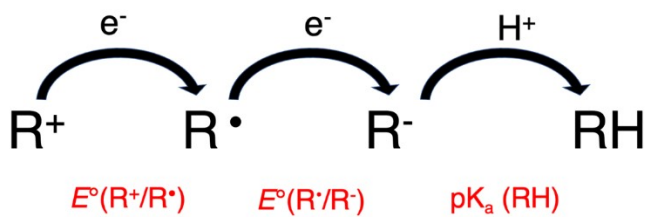
Hydride reduction pathways

To regenerate the hydride (RH) from its oxidized cationic form (R^{+}), $R^{+} + H^{+} + 2e^{-} \rightleftharpoons RH$, three possible stepwise pathways are envisaged in Scheme S2. Pathway 1 begins with the proton transfer (PT) step with an associated pK_a, while pathways 2 and 3 are initiated with electron transfer (ET) step. The reduction potential E° is calculated for the ET steps.

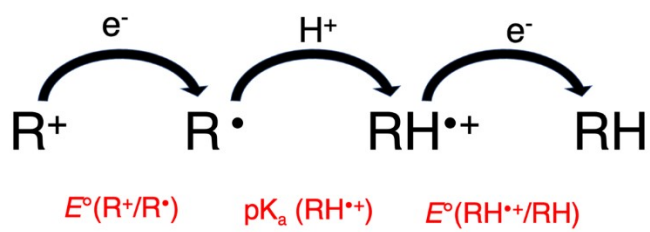
1) proton-electron-electron ($H \rightarrow e \rightarrow e$)



2) electron-electron-proton ($e \rightarrow e \rightarrow H$)



3) electron-proton-electron ($e \rightarrow H \rightarrow e$)



Scheme S2. Three different pathways for the hydride electrochemical reduction.

Pathways for selected molecules

Representative molecules							
	pK_a			E° (V vs. Fc^+/Fc)			
compound #	RH^{2+}	$RH^{+\bullet}$	RH	$R^+/R^\bullet$	$RH^{2+}/RH^{+\bullet}$	$R^\bullet/R^-$	$RH^{+\bullet}/RH$
1a	-33.7	27.3	70.5	-2.49	0.96	-3.0	-0.43
2	-34.8	14.1	108.4	-2.71	0.18	-5.1	0.48
7	-51.1	17.3	107.3	-3.18	0.65	-4.9	0.41
15	-46.9	23.5	76.3	-3.26	0.28	-3.4	-0.32

Table S1. Representative molecules with the pK_a and E° for all three pathways.

In Table S1, representative molecules from each group (**1a** – benzimidazole, **2** – monocyclic guanidine, **7** – bicyclic guanidine, **15** – pentandine) are shown to compare the pK_a and E° values of the three different pathways. For pathway 1 ($H \rightarrow e \rightarrow e$), the proton-transfer steps all indicate negative pK_a values and therefore are highly unlikely to occur. Pathway 2 ($e \rightarrow e \rightarrow H$) and 3 ($e \rightarrow H \rightarrow e$) have positive pK_a values, suggesting the first step to be an ET. The main difference is the 2nd step will be either be an ET or PT for pathway 2 and 3 correspondingly. When the 2nd step is another ET, $E^\circ_{R^\bullet/R^-}$ is still relatively negative, indicating an associated high electrochemical barrier. In contrast, when 2nd step is PT, the pK_a ($RH^{+\bullet}$) values become positive, meaning that the PT is preferred. Of the representative molecules considered, the trends are consistent and support that pathway 3 ($e \rightarrow H \rightarrow e$) as the most energetically preferred route for electrochemical reduction of R^+ . Hence, only calculations associated with pathway 3 were considered for the rest of the redox calculations.

Summary of reduction potential calculations

Table S2. Reduction potential calculation summary for hydrides **1 – 30**.

Reduction potential summary			
	pK_a	E^0 (V vs. Fc^+/Fc)	
compound #	RH^{+*}	R^+/R^*	RH^{+*}/RH
1a	27.3	-2.65	-0.43
1b	26.6	-2.49	-0.44
1c	23.2	-2.29	-0.39
2	14.1	-2.71	0.48
3	32.7	-3.53	0.14
4	25.4	-3.31	0.45
5	13.0	-2.36	0.47
6	38.6	-4.23	0.36
7	17.3	-3.18	0.41
8	34.1	-4.24	0.26
9	16.6	-2.95	0.38
10	17.2	-3.08	0.32
11	36.8	-4.47	0.11
12	23.9	-3.57	-0.01
13	16.8	-3.34	0.28
14	13.1	-3.22	0.52
15	23.5	-3.26	-0.32
16	16.6	-2.97	0.00
17	17.2	-2.96	-0.06
18	21.4	-3.17	-0.12
19	19.6	-3.06	-0.42
20	14.1	-2.57	0.09
21	16.7	-2.72	-0.05
22	12.9	-2.50	0.17
23	14.3	-2.60	0.09

24	12.5	-2.68	0.27
25	15.5	-2.90	0.02
26	14.4	-2.80	0.05
27	13.2	-2.73	0.15
28	8.3	-2.06	0.51
29	6.6	-2.34	0.45
30	11.1	-2.58	0.28

Summary of Energies of Optimized Electronic Structures

Column 2 is the electronic energies of the optimized structures, followed by Gibbs energy and enthalpy corrections. Values are in Hartrees.

Molecules	E (wB97XD/6-31+G(d,p)/CPCM(MeCN))	G_{corr}	H_{corr}
MeCN	-132.722271	0.021656	0.050186
RutpybpyH	-1331.9425	0.350513	0.428367
RutpybpyMeCN	-1463.96181	0.38609	0.474552
CpMeReCHO	-826.269837	0.210827	0.281128
CpMeReCO	-825.532164	0.204418	0.270627
CpReCHO	-629.707218	0.08142	0.133629
CpReCO	-628.962782	0.072328	0.123808
formate	-189.257481	-0.003084	0.024648
CO2	-188.529861	-0.009021	0.015257
BNAH	-688.370489	0.206359	0.265297
BNA	-687.621346	0.198739	0.255781
Ph3CH	-733.468704	0.24879	0.309459
Ph3C	-732.661488	0.240356	0.298255
1a	-498.871865	0.190584	0.2388
1a_ox	-498.143764	0.180349	0.229971
TS1a	-687.369302	0.191298	0.251289
1a_rad	-498.22529	0.175881	0.226114
1a_H_rad	-498.703969	0.19021	0.240488
1b	-459.558349	0.164483	0.209391
1b_ox	-458.827147	0.155475	0.200473
TS1b	-648.054284	0.16477	0.221782
1b_rad	-458.9133	0.149672	0.196378
1b_H_rad	-459.3899	0.163323	0.210824
1c	-690.553471	0.23865	0.295531
1c_ox	-689.821803	0.230754	0.286807

TS1c	-879.048473	0.240239	0.307914
1c_rad	-689.9166	0.226229	0.283155
1c_H_rad	-690.3825	0.236597	0.296941
2	-593.504363	0.232925	0.287953
2_ox	-592.77424	0.222873	0.279003
TS2	-781.999652	0.235693	0.300484
2_rad	-592.854148	0.219207	0.274951
2_H_rad	-593.304374	0.233754	0.288788
3	-707.997811	0.262493	0.323432
3_ox	-707.270359	0.253256	0.314466
TS3	-896.493522	0.265312	0.335879
3_rad	-707.315611	0.244959	0.308177
3_H_rad	-707.811019	0.264161	0.324926
4	-692.718404	0.223806	0.280519
4_ox	-691.98753	0.214663	0.271655
TS4	-881.213165	0.225935	0.292935
4_rad	-692.040399	0.206009	0.265113
4_H_rad	-692.518655	0.223878	0.281334
5	-590.348051	0.195315	0.249778
5_ox	-589.609415	0.187293	0.24096
TS5	-589.700493	0.181749	0.236927
5_rad	-589.700493	0.181749	0.236927
5_H_rad	-590.145998	0.19396	0.249614
6	-401.814385	0.18585	0.231859
6_ox	-401.09095	0.176175	0.223331
TS6	-590.310507	0.186945	0.244326
6_rad	-401.115264	0.17248	0.219773
6_H_rad	-401.61545	0.183563	0.231302
7	-439.937738	0.199877	0.241648
7_ox	-439.217529	0.187337	0.232252

TS7	-628.426947	0.200501	0.254054
7_rad	-439.282865	0.186157	0.229154
7_H_rad	-439.739931	0.200442	0.243832
8	-479.224864	0.225215	0.270588
8_ox	-478.513597	0.213493	0.262034
TS8	-667.723977	0.228588	0.283382
8_rad	-478.537493	0.209812	0.259126
8_H_rad	-479.033568	0.22665	0.273957
9	-518.5277	0.252386	0.299877
9_ox	-517.804063	0.242046	0.291705
TS9	-707.017456	0.254482	0.312822
9_rad	-517.87504	0.238208	0.287304
9_H_rad	-518.331144	0.253221	0.30304
10	-556.637674	0.261496	0.307877
10_ox	-555.918833	0.250291	0.299201
TS10	-745.138196	0.264176	0.321008
10_rad	-555.987103	0.248303	0.295953
10_H_rad	-556.444552	0.263292	0.311584
11	-400.630248	0.170807	0.211153
11_ox	-399.928096	0.160066	0.201154
TS11	-589.129985	0.172626	0.223404
11_rad	-399.941821	0.1548	0.196789
11_H_rad	-400.440911	0.16876	0.210383
12	-439.927573	0.196814	0.239936
12_ox	-439.225718	0.186664	0.231099
TS12	-628.431066	0.201091	0.252795
12_rad	-439.273834	0.182816	0.22738
12_H_rad	-439.744509	0.196518	0.240583
13	-479.223151	0.223304	0.268992
13_ox	-478.516399	0.212385	0.261082

TS13	-667.72334	0.227026	0.28214
13_rad	-478.574915	0.210168	0.256962
13_H_rad	-479.027978	0.221701	0.268847
14	-517.322592	0.2327	0.277376
14_ox	-516.612115	0.222972	0.269423
TS14	-705.826284	0.235869	0.290475
14_rad	-516.673265	0.219232	0.265424
14_H_rad	-517.118613	0.231067	0.27694
15	-667.286106	0.280903	0.34111
15_ox	-666.585451	0.271392	0.332797
TS15	-855.79156	0.283276	0.353915
15_rad	-666.644935	0.267273	0.328397
15_H_rad	-667.116388	0.282573	0.343742
16	-626.786414	0.237071	0.289545
16_ox	-626.078628	0.227682	0.280913
TS16	-815.290167	0.23979	0.30232
16_rad	-626.148108	0.223118	0.274858
16_H_rad	-626.602012	0.235857	0.291243
17	-666.093697	0.265518	0.319793
17_ox	-665.385511	0.255033	0.311122
TS17	-854.598535	0.268086	0.33245
17_rad	-665.455422	0.250572	0.305919
17_H_rad	-665.911582	0.264341	0.321807
18	-705.40653	0.294251	0.350101
18_ox	-704.696654	0.281864	0.341806
TS18	-893.910525	0.295548	0.362888
18_rad	-704.761139	0.279431	0.337127
18_H_rad	-705.227961	0.294534	0.352949
19	-744.689553	0.321194	0.38031
19_ox	-743.991625	0.30985	0.371947

TS19	-933.19777	0.324318	0.393312
19_rad	-744.059958	0.307424	0.366829
19_H_rad	-744.522593	0.32228	0.382896
20	-1010.16004	0.334996	0.402922
20_ox	-1009.43835	0.324429	0.393576
TS20	-1198.65276	0.335759	0.415128
20_rad	-1009.52238	0.319662	0.389387
20_H_rad	-1009.97213	0.333764	0.404181
21	-1239.14774	0.393218	0.473677
21_ox	-1238.43147	0.382997	0.46426
TS21	-1427.64501	0.393975	0.485741
21_rad	-1238.50976	0.378102	0.460139
21_H_rad	-1238.96387	0.390825	0.474694
22	-1929.32107	0.311437	0.38612
22_ox	-1928.59606	0.300631	0.376664
TS22	-2117.81888	0.313442	0.398324
22_rad	-1928.68363	0.2968	0.372732
22_H_rad	-1929.12962	0.309695	0.38723
23	-1208.58772	0.315819	0.387826
23_ox	-1207.86595	0.304482	0.378344
TS23	-1397.08722	0.318387	0.400221
23_rad	-1207.94988	0.300706	0.374309
23_H_rad	-1208.39896	0.313506	0.388952
24	-1300.73796	0.235708	0.307089
24_ox	-1300.02006	0.227761	0.298406
TS24	-1489.2376	0.237939	0.319735
24_rad	-1300.09875	0.221775	0.293651
24_H_rad	-1300.5464	0.23724	0.308876
25	-1088.76621	0.385344	0.462902
25_ox	-1088.05741	0.376105	0.45424

TS25	-1277.2696	0.386356	0.475576
25_rad	-1088.12781	0.369798	0.449206
25_H_rad	-1088.58247	0.385709	0.464762
26	-1762.71156	0.381638	0.479071
26_ox	-1762.00061	0.372649	0.470469
TS26	-1951.21411	0.382968	0.491784
26_rad	-1762.07289	0.364406	0.465293
26_H_rad	-1762.52544	0.380574	0.480947
27	-2436.65123	0.377952	0.495183
27_ox	-2435.9411	0.373749	0.48695
TS27	-2625.15314	0.379715	0.507975
27_rad	-2436.01229	0.361821	0.48147
27_H_rad	-2436.46338	0.379059	0.49725
28	-1222.12734	0.183472	0.246759
28_ox	-1221.38423	0.17325	0.237385
TS28	-1410.61334	0.18538	0.259277
28_rad	-1221.48725	0.168516	0.233103
28_H_rad	-1221.92492	0.183076	0.248084
29	-1023.67632	0.202131	0.262617
29_ox	-1022.94927	0.191516	0.253542
TS29	-1212.17472	0.20356	0.27524
29_rad	-1023.0415	0.18653	0.248963
29_H_rad	-1023.47706	0.202641	0.264072
30	-825.227755	0.218409	0.276862
30_ox	-824.50757	0.209761	0.26819
TS30	-1013.72958	0.221884	0.289613
30_rad	-824.590409	0.203962	0.263337
30_H_rad	-825.034579	0.218985	0.278621

Naming and Abbreviation of Structures

MeCN = acetonitrile

RutpybpyH = ruthenium (tripyridine)(bipyridine) hydride complex

RutpybpyAcn = ruthenium (tripyridine)(bipyridine)(MeCN) complex

CpMeReCHO = pentamethyl cyclopentadienyl rhenium formyl complex

CpMeReCO = pentamethyl cyclopentadienyl rhenium carbonyl complex

CpReCHO = cyclopentadienyl rhenium formyl complex

CpReCO = cyclopentadienyl rhenium carbonyl complex

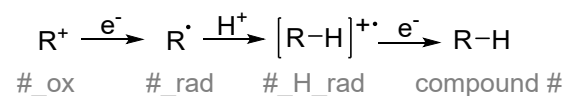
BNA = N-benzyl-nicotinamide

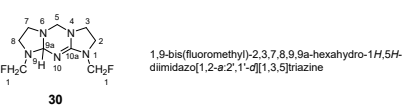
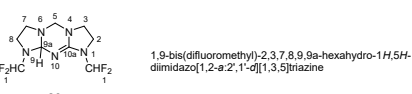
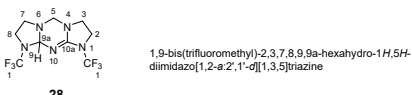
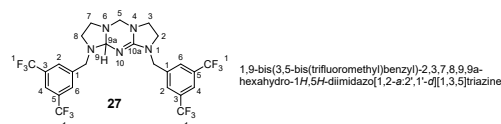
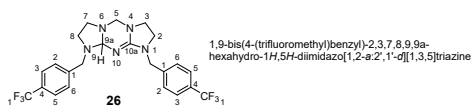
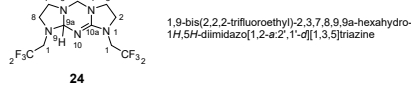
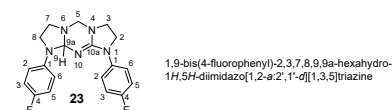
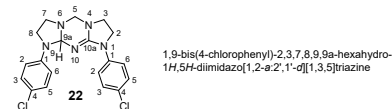
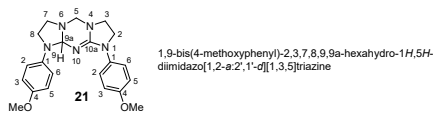
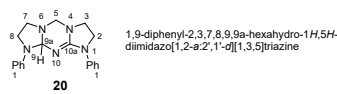
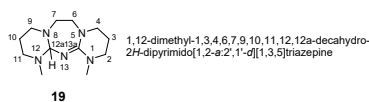
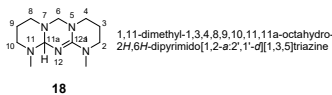
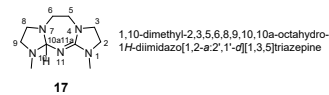
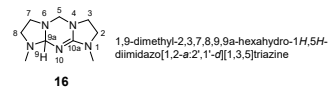
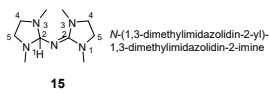
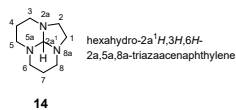
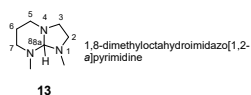
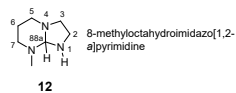
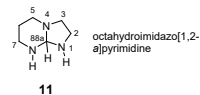
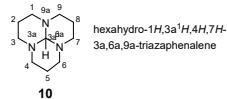
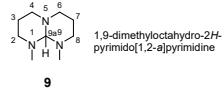
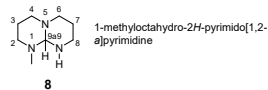
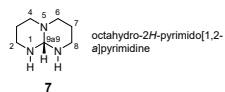
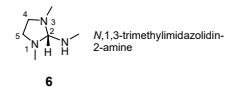
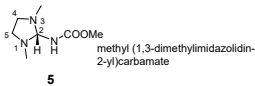
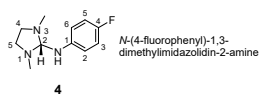
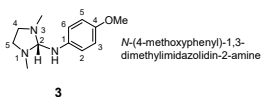
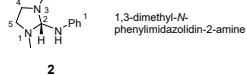
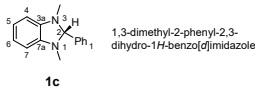
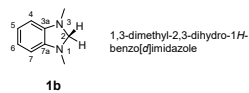
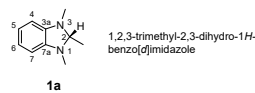
BNAH = N-benzyl-nicotinamide hydride

Ph₃CH = triphenyl methane

Ph₃C = trityl cation

For compounds **1-30**, “ox” refers to oxidized species prior to accepting an electron, “rad” refers to radical species after accepting one electron and “H_rad” refers to radical cation species after accepting one proton, as denoted in the following equation:





XYZ coordinates of Optimized Structures

Benchmarking

Ru(tpy)bpyH+

51
1 1
Ru 0.1386590336 1.8954330744 0.1344457524
H 1.0128779959 0.7351617019 -0.6142973384
C 2.4594348093 3.6652074512 0.1608239234
C 3.6287216485 3.0376144219 2.5678962927
N 1.8984275406 2.704678366 0.9461655916
C 3.6178993669 4.3324080005 0.5522131291
C 4.2115229688 4.0160320389 1.768263953
C 2.4753635258 2.4088431514 2.1195036893
H 4.0534731393 5.0935163104 -0.0837031351
H 5.1134114214 4.527693953 2.0850608523
H 1.9843704357 1.6399267659 2.7054965221
H 4.0548237091 2.7599166213 3.5246129725
C 1.7482303975 3.9401105047 -1.1072090478
C 0.1644597134 4.2327114539 -3.3536005082
C 2.108966987 4.8728834599 -2.0752312538
N 0.6416850834 3.1839274624 -1.2759442535
C -0.1554846024 3.3133676519 -2.3587607793
C 1.3090492278 5.0118314978 -3.2064248948
H 2.9943554868 5.4853154166 -1.9572026308
H 1.5749009023 5.7320970838 -3.9714967531
H -0.4620471648 4.3473964239 -4.2295301383
C -1.3323004252 2.4168870898 -2.331961715
C -3.4671119902 0.7015105938 -2.0970910981
C -2.2969481512 2.385107976 -3.336365719
N -1.4247495419 1.6106207787 -1.2385748134
C -2.4717611025 0.780145772 -1.1328624272
C -3.3766102181 1.5178487856 -3.220377221
H -2.2093929862 3.0316376952 -4.2010815323
H -2.496844768 0.1646199881 -0.240565978
H -4.1346089267 1.483035776 -3.9948363914
H -4.2920164842 0.0119531469 -1.9628189339
C -1.2899993617 1.1755125111 2.6681212664
C -0.5620793256 -1.4665798212 2.8839512385
N -0.4880765564 0.6304473935 1.7212495909
C -1.7515799628 0.4216808014 3.7477410869
C -1.3855878676 -0.9128547711 3.8593199155
C -0.1381632153 -0.6627357953 1.8365790926
H -2.3917500795 0.8664923735 4.4987701434
H -1.7384178152 -1.5081077846 4.6941043995
H 0.503267216 -1.0431700396 1.0513956724
H -0.2489081166 -2.5029230089 2.9265512207
C -1.6352541727 2.6059626296 2.4769684916
C -2.1666100987 5.2544300625 1.9589489588
C -2.4487072031 3.3248548826 3.3543434997
N -1.1068472138 3.1887293615 1.3813514175
C -1.3673304438 4.4776739806 1.1321103965
C -2.7167246502 4.6626592862 3.0920971438
H -2.8720068478 2.8557880241 4.2331404003
H -0.9145137783 4.8910023668 0.2363252733

H -3.3470354453 5.2332889667 3.7651334914
H -2.3494320933 6.2944081669 1.7162511837

Ru(tpy)bpyMeCN

56
2 1
Ru 0.0458482472 -0.0022017841 0.3402798348
C -1.5991500055 -2.3471764558 -0.2359092652
C 0.1331987575 -4.411349756 0.3092448328
N -0.3357846902 -2.0712207388 0.188333361
C -2.0311130544 -3.6582728301 -0.3977776536
C -1.1545466636 -4.7035935741 -0.1220104826
C 0.5022037151 -3.079140042 0.45191433
H -3.038007548 -3.8689182588 -0.7359382786
H -1.478183816 -5.7309302132 -0.2446607079
H 1.4942237121 -2.7977365131 0.7865175502
H 0.847513246 -5.1938567602 0.5342269728
C -2.4593327986 -1.1669588848 -0.50979937
C -3.767616428 1.2342734747 -0.9353499154
C -3.780766503 -1.1856571036 -0.9462231454
N -1.8446224865 0.0109740081 -0.3063441959
C -2.4464858892 1.1973015744 -0.4991714947
C -4.428816174 0.028834093 -1.1567326134
H -4.3030496966 -2.1178288353 -1.1200427283
H -5.4579688949 0.0359527378 -1.4966419838
H -4.279739242 2.1735834069 -1.1007600647
C -1.5735490254 2.365591475 -0.2146760118
C 0.1810507731 4.4058240326 0.349155549
C -1.9912505475 3.6827154287 -0.3646195954
N -0.313272376 2.0721126519 0.2069931179
C 0.535581519 3.0684501153 0.4796880725
C -1.1034187978 4.7159202121 -0.0793884576
H -2.9957715412 3.9073459821 -0.7008298668
H 1.5244792096 2.7732766702 0.8116584225
H -1.415889678 5.7477785042 -0.192682028
H 0.9037891341 5.178461547 0.5812334174
C 2.9480622453 -0.0156133985 -0.2044006901
C 3.9577923255 -0.0326650923 2.3510402415
N 2.0974507091 -0.0156724435 0.8482122177
C 4.3283245985 -0.0240478572 -0.0165445447
C 4.839324476 -0.0326765649 1.2753692554
C 2.5948837713 -0.0240102202 2.0937763528
H 5.0028586252 -0.023952986 -0.8627880895
H 5.9112784312 -0.0393036554 1.4367221384
H 1.8671001504 -0.0236180104 2.8962260956
H 4.3113700997 -0.0392178512 3.374848607
C 2.3024810137 -0.0060767196 -1.5363440405
C 0.9329286305 0.0121628134 -3.9212299774
C 3.012835712 -0.0045331875 -2.7341876974
N 0.9478601379 0.0012831277 -1.5291921459
C 0.2855397664 0.0101597076 -2.6952649827
C 2.322858581 0.0046742589 -3.9398188237
H 4.0949576805 -0.010427083 -2.7340119576
H -0.795980426 0.0157841447 -2.6350376782
H 2.865850257 0.0059520461 -4.878063674
H 0.3510357254 0.0194550505 -4.8346254031
N -0.6789741649 -0.0069599641 2.2832114099
C -1.1139195535 -0.0093968301 3.3519174297

C -1.6509165757 -0.0125718354 4.7029586724
H -2.2586280226 0.8812440942 4.8555910825
H -0.8282005591 -0.0200729926 5.4205734866
H -2.2679700926 -0.9012907151 4.8476761137

Formate

4
-1 1
C -0.0000052272 0.3340386332 0.
H -0.0000269002 1.4523814874 0.
O -1.1292196242 -0.2169078201 0.
O 1.1292267516 -0.2168673005 0.

CO2

3
O 1
C O. O. O.
O O. O. 1.164644
O O. O. -1.164644

Cp*ReCHO

33
O 1
C -1.396437791 1.0943279351 -0.6734781185
C -0.919968246 1.4622577953 0.631457035
C -1.1114842843 0.3305059952 1.5034185712
C -1.6780552184 -0.7301745007 0.734591723
C -1.8431119248 -0.2640475705 -0.6174266854
Re 0.4384880549 -0.2436255007 -0.1413783586
N 0.9917780572 -1.7575953253 -0.8675549713
O 1.2876668325 -2.8025752153 -1.3378703031
C 1.9103890117 -0.1076930486 1.0912117595
O 2.7561105359 -0.0208047158 1.874764555
C 1.5752505766 0.9836126915 -1.3965154222
O 1.589621192 2.2099098764 -1.4562367512
H 2.255425514 0.447923729 -2.0996594032
C -2.4998001999 -1.0270351087 -1.7280682646
H -3.5846756709 -0.8829881379 -1.6869166131
H -2.1491223466 -0.6888387842 -2.7048844991
H -2.299670445 -2.0978129618 -1.6505675997
C -2.1076395959 -2.0682211419 1.2547688555
H -3.1608643988 -2.0291749268 1.5532496095
H -2.0024304436 -2.8461333089 0.4955686717
H -1.5202561344 -2.3661001184 2.1253953304
C -0.8855323021 0.3168572049 2.9850803178
H -1.7994373581 0.6353537652 3.497161006
H -0.6258673894 -0.6814563962 3.3423600325
H -0.0835571652 0.9983232808 3.2753278082
C -0.4858752553 2.8386223751 1.0389648367
H -1.3616086843 3.4707642306 1.2216251069
H 0.1091206144 2.8139845526 1.9544960501
H 0.1198693309 3.2954187142 0.2541394557
C -1.5392414751 2.0240367292 -1.8361269093
H -2.4847425764 2.5700428651 -1.7492942225
H -0.7215917514 2.7463130562 -1.8572894099
H -1.5434330635 1.4834319652 -2.784749193

Cp*ReCO

32
1 1
C -1.4000181131 -0.7136747829 1.0827858258
C -1.2089815197 -1.415227793 -0.1571463168
C -1.3647176111 -0.4554194889 -1.2295694358
C -1.6152649652 0.8261173035 -0.6458066373
C -1.6237743071 0.6710469997 0.7906234514
Re 0.4868933271 0.1267547438 0.0079192063
C 1.5751254134 -0.6172554874 1.4651180615
O 2.1661157803 -1.0480045399 2.3432901489
N 1.3278112311 1.7112764565 -0.0192960009
O 1.8031095799 2.7652101696 -0.0425813233
C 1.646946226 -0.7227149038 -1.3286170746
O 2.2802113174 -1.2177458707 -2.1413400445
C -1.9420491576 2.0824300354 -1.3902729118
H -1.4608676061 2.1033948996 -2.3689970833
H -3.0252913134 2.1349960807 -1.5390029684
H -1.6334922858 2.9709585389 -0.8372322098
C -1.4199134187 -0.7750591162 -2.6912557399
H -2.4577547464 -0.9860764442 -2.9670683004
H -1.0677910336 0.0605672446 -3.2978350982
H -0.8214932041 -1.6535832854 -2.9371564196
C -1.0997560508 -2.9021511308 -0.3202532679
H -2.1033612262 -3.3349179557 -0.376188965
H -0.5650738363 -3.1675101582 -1.233642101
H -0.5768076803 -3.3603863685 0.5204449554
C -1.9695566434 1.7343537063 1.7857928789
H -1.6526297097 2.7211842754 1.4450180268
H -3.0549282958 1.7549973539 1.9275949339
H -1.5021284888 1.5419604011 2.7525298647
C -1.4714923548 -1.3390986791 2.4405473448
H -2.5146551259 -1.5952572705 2.6500000145
H -0.882490233 -2.2556221376 2.4964062619
H -1.1271089484 -0.6568017962 3.2191819237

CpReCHO

18
O 1
H 1.7464892066 -1.6418568147 1.6251567157
C 1.8353071809 -0.8955971827 0.8491148115
C 1.8381015465 0.5174771659 1.0486727272
H 1.9745270962 -2.1225346489 -1.0154789034
H 1.7842102855 1.0256564189 2.000341607
C 1.9688929696 1.1380645275 -0.2381572807
H 2.0210034724 2.2007041302 -0.4290666362
C 2.036941593 0.1114656683 -1.2158744385
H 2.1212333766 0.2576987641 -2.2838747647
C 1.9460640067 -1.1492161774 -0.5459816278
Re -0.0668405073 -0.0057470574 -0.1532848347
N -1.2283606478 -0.6406545774 -1.3225536679
O -1.9754367202 -1.0758820504 -2.1242928041
C -1.1015382461 1.5802855474 0.1810159748
O -1.6867198983 2.555173491 0.3794116267
C -1.0534112011 -0.8217673625 1.4976820098
O -0.6969970103 -0.7749017687 2.6685307312
H -2.0019627726 -1.3635798934 1.2808908139

CpReCO

17
 1 1
 H 1.9280265985 1.4328126817 -1.7993387479
 C 1.9180399913 0.7721600042 -0.943249009
 C 1.8899604819 -0.6568479874 -0.9884333605
 H 1.939006807 2.1990568052 0.7782411251
 H 1.9148333532 -1.2675441226 -1.8793465411
 C 1.9005505966 -1.1316041597 0.3672860921
 H 1.9113124899 -2.1670457076 0.6777972385
 C 1.9136503448 -0.002927546 1.2313496553
 H 1.9215615633 -0.0314206911 2.3120739222
 C 1.9207575449 1.1796368144 0.4195038915
 Re -0.0597726638 0.0271597014 0.0168488073
 C -1.0491334354 0.7706886656 -1.510095753
 O -1.5887915241 1.2274029517 -2.4054216034
 N -1.1889966178 0.7000741924 1.2357784141
 O -1.8621588041 1.1485575543 2.0555450382
 C -1.0373867626 -1.6652787173 -0.168262167
 O -1.5698019637 -2.6704144394 -0.2585110025

BNAH

30
 O 1
 C 2.6193867445 -1.2656202819 0.8506328318
 N 0.2360089862 -0.884533157 -0.7911164857
 C 2.372007454 -0.0735275995 -0.0568195774
 C 1.4306239241 -2.1953391723 0.8268439933
 C 0.3546740707 -1.9878458203 0.0624585041
 C 1.238378261 0.0406893911 -0.7889424434
 H 1.4563134909 -3.0797596644 1.4540040683
 H -0.4919432784 -2.665228564 0.0536455872
 H 1.0903106159 0.9077943015 -1.4242576952
 C 3.3602864813 1.0117133998 -0.1897855364
 O 3.1946496971 2.0054355267 -0.9175130384
 N 4.4970606685 0.8824021765 0.5436745321
 H 4.6920151355 0.0841182176 1.1247689124
 H 5.2032716864 1.597584269 0.4672961199
 C -1.03017571 -0.6271859012 -1.4534522138
 H -0.8459203648 0.0948577233 -2.2545315736
 H -1.3673402788 -1.5500359419 -1.9364538961
 C -2.1211045921 -0.1060209144 -0.533092887
 C -4.175734375 0.8967037705 1.0915647783
 C -1.8226774436 0.5265281399 0.6753284221
 C -3.4588347758 -0.2377113502 -0.9169471499
 C -4.4805966544 0.2626900747 -0.1133116745
 C -2.844702137 1.0248990297 1.4834824841
 H -0.7894215621 0.6271628868 0.9947368156
 H -3.7032011837 -0.7377248953 -1.8509094136
 H -5.5147903459 0.1519344996 -0.4243845079
 H -2.5979917601 1.5124037677 2.4216231216
 H -4.9706109804 1.2830510455 1.7217018241
 H 2.8090645033 -0.9413171428 1.8852473918
 H 3.5218448025 -1.8164156443 0.5424013068

BNA

29
 1 1
 H -3.336528126 -1.1645052753 -1.703150541

C -2.4854295203 -1.0416774923 -1.0428467755
 N -0.2845574438 -0.7251995176 0.5666563964
 C -2.4923075656 -0.0883839475 -0.0275835553
 C -1.3538932556 -1.8319950126 -1.2332615348
 C -0.2623910139 -1.6555648218 -0.4125161647
 C -1.3613558418 0.0500473189 0.7620152064
 H -1.3140683068 -2.5773657002 -2.0163368936
 H 0.6488888576 -2.2312865455 -0.5104821175
 H -1.3114431577 0.7871839414 1.5533115109
 C -3.6298748714 0.8612644069 0.2589761375
 O -3.3970314436 1.9423447662 0.7932599164
 N -4.8589359261 0.4610147841 -0.1085175434
 H -5.0687054819 -0.4794407051 -0.4030559381
 H -5.6377768514 1.0730645855 0.0863869347
 C 0.9243662746 -0.5590516816 1.4263094928
 H 0.6651120151 0.1758163829 2.188231269
 H 1.0979309275 -1.516202761 1.9197127197
 C 2.120155178 -0.1244656871 0.6159359151
 C 4.3291743086 0.6812536928 -0.8912547775
 C 3.2113393711 -0.979671151 0.4577610253
 C 2.1403969153 1.1398080171 0.018146676
 C 3.2392826578 1.5395681532 -0.7351247073
 C 4.3156266597 -0.5760842261 -0.2928960553
 H 3.2036860758 -1.9611295625 0.9237017536
 H 1.2968803479 1.8138784702 0.1408094786
 H 3.2485972768 2.5217228224 -1.1961589212
 H 5.1613388175 -1.2457020344 -0.4095663115
 H 5.1871175728 0.9952601698 -1.4768771957

Ph3CH

30
 O 1
 C 2.6193867445 -1.2656202819 0.8506328318
 N 0.2360089862 -0.884533157 -0.7911164857
 C 2.372007454 -0.0735275995 -0.0568195774
 C 1.4306239241 -2.1953391723 0.8268439933
 C 0.3546740707 -1.9878458203 0.0624585041
 C 1.238378261 0.0406893911 -0.7889424434
 H 1.4563134909 -3.0797596644 1.4540040683
 H -0.4919432784 -2.665228564 0.0536455872
 H 1.0903106159 0.9077943015 -1.4242576952
 C 3.3602864813 1.0117133998 -0.1897855364
 O 3.1946496971 2.0054355267 -0.9175130384
 N 4.4970606685 0.8824021765 0.5436745321
 H 4.6920151355 0.0841182176 1.1247689124
 H 5.2032716864 1.597584269 0.4672961199
 C -1.03017571 -0.6271859012 -1.4534522138
 H -0.8459203648 0.0948577233 -2.2545315736
 H -1.3673402788 -1.5500359419 -1.9364538961
 C -2.1211045921 -0.1060209144 -0.533092887
 C -4.175734375 0.8967037705 1.0915647783
 C -1.8226774436 0.5265281399 0.6753284221
 C -3.4588347758 -0.2377113502 -0.9169471499
 C -4.4805966544 0.2626900747 -0.1133116745
 C -2.844702137 1.0248990297 1.4834824841
 H -0.7894215621 0.6271628868 0.9947368156
 H -3.7032011837 -0.7377248953 -1.8509094136
 H -5.5147903459 0.1519344996 -0.4243845079

H -2.5979917601 1.5124037677 2.4216231216
H -4.9706109804 1.2830510455 1.7217018241
H 2.8090645033 -0.9413171428 1.8852473918
H 3.5218448025 -1.8164156443 0.5424013068

Ph3C+

34

1 1

C 0.0005105891 -0.0003948326 -0.0003476508
C 1.0139597156 1.0289286227 0.001562544
C 0.7960840187 2.2458650601 0.6862960974
C 2.2356705325 0.8319797396 -0.6809282097
C 1.7778705413 3.2233210122 0.6989473043
H -0.1211814194 2.391354375 1.2458402237
C 3.1973725519 1.8292428144 -0.6891314372
H 2.3973687819 -0.0811277936 -1.2427568704
C 2.9729249507 3.0193264915 0.006027726
H 1.6165569049 4.1434083471 1.2489392131
H 4.1210691644 1.6839815776 -1.2375798774
H 3.7339586569 3.7926308023 0.0077524061
C -1.3974817473 0.3629700656 -0.0017616405
C -1.8352046198 1.5201397459 -0.6848520574
C -2.3447629129 -0.4341319721 0.679764941
C -3.1794725316 1.8551108243 -0.6967486698
H -1.1228668178 2.1165979633 -1.2438490807
C -3.6820109704 -0.0720569268 0.688556931
H -2.0142841991 -1.3017105997 1.2398756633
C -4.1002814424 1.0655634878 -0.0048669026
H -3.5134540352 2.7282958966 -1.2455057548
H -4.4001250182 -0.6717932 1.2360459319
H -5.1503823102 1.3385267881 -0.0060921234
C 0.3847364586 -1.3927157673 -0.0005204912
C -0.3976842247 -2.35086326 -0.6839903077
C 1.5476510416 -1.8141573116 0.6830943787
C -0.0158687232 -3.682610019 -0.6940157009
H -1.2694948929 -2.0324234941 -1.2445421766
C 1.9023783346 -3.1533415846 0.6937408499
H 2.1330179903 -1.0939085639 1.2435981132
C 1.1271467421 -4.0848572525 0.0000322622
H -0.6044106912 -4.4089018099 -1.2428347159
H 2.7798634404 -3.4750778327 1.2429254843
H 1.4155121404 -5.1308153936 0.0003185972

CO₂ reduction calculations

1a

26

0 1

C -0.5119717323 0.7032438236 -0.1163882623
C -0.5119574971 -0.7032623271 -0.1163904333
C -1.6977977338 -1.416337888 -0.0710050411
C -2.9054039159 -0.6948323471 -0.0388030423
C -2.9054179735 0.6947652157 -0.038800877
C -1.6978263813 1.4162952701 -0.0710006774
H -1.7039133498 -2.5013121288 -0.0553371173
H -1.7039639375 2.5012693398 -0.0553293949
N 0.8138161967 -1.1464069111 -0.1931395306
N 0.8137930216 1.1464154446 -0.193135938
C 1.1522820644 -2.4229757896 0.4060782837
H 0.9902388401 -2.4235332351 1.4959846733
H 0.5448191287 -3.2124371507 -0.0405431005

H 2.198698632 -2.6598151178 0.2055735598
C 1.1522329803 2.4229891981 0.4060861467
H 0.5447539998 3.2124397171 -0.0405325774
H 0.9901897714 2.423539692 1.4959925416
H 2.1986447289 2.659850451 0.2055821895
C 1.6482954063 0.0000120684 0.1923634987
H 1.7869153639 0.0000116803 1.2990020904
H -3.8454730031 1.2362527587 -0.0013400833
H -3.845447994 -1.2363390171 -0.0013439162
C 3.0060785158 0.000026772 -0.4847109104
H 2.881874374 0.000027041 -1.5707323168
H 3.5831818 0.8802262503 -0.1891271472
H 3.5831996944 -0.880161811 -0.1891296176

1a_ox

25

1 1

C 0.5325269412 -0.6910988573 0.0010116269
C 0.5131757582 0.7019612049 0.0019896999
C 1.685198666 1.4552037514 0.000632925
C 2.876543224 0.7424650593 0.0019125617
C 2.8963332087 -0.6651730583 0.0038698782
C 1.7253997661 -1.4110671884 0.0031366416
H 1.6700149445 2.5387902311 -0.0029793099
H 1.7420158878 -2.4946683999 0.0042359405
N -0.8243624676 1.0774417784 0.0039815045
N -0.7948437904 -1.1090636849 -0.0020483095
C -1.2861321912 2.4597345713 -0.001611853
H -0.8163254423 2.9939778776 0.8248267084
H -1.0200007041 2.9293216554 -0.9496268054
H -2.3653502697 2.487242397 0.1269937988
C -1.1805473667 -2.5150456471 0.0005509003
H -0.7631068898 -2.9998493448 -0.8826314518
H -0.7952779896 -2.989016455 0.9040900643
H -2.2620853944 -2.6098709619 -0.018637105
C -1.5865606236 -0.0263111467 -0.0018545508
H 3.8507617356 -1.1798581507 0.0054610996
H 3.8161672521 1.2837463013 0.0009747782
C -3.0703544781 -0.0072217119 -0.0063396156
H -3.4334662056 0.5542221624 -0.8702051258
H -3.4828423182 -1.011663804 -0.0540749978
H -3.4400852532 0.4728344205 0.9030949969

TS1a

29

0 1

C 1.1308621291 -0.6877604019 -0.2711024866
C 1.0984085845 0.713310589 -0.3276484066
C 2.1786005188 1.4778067385 0.0859062848
C 3.3081129921 0.7976254112 0.5558647328
C 3.3412749226 -0.596782676 0.6096138546
C 2.2463535302 -1.3650757908 0.1972171153
H 2.1549400175 2.5613680399 0.0548000687
H 2.2750451043 -2.4475380235 0.252359759
N -0.1361579185 1.0803762032 -0.8625108365
N -0.08701214 -1.149839286 -0.7655112457
C -0.688353071 2.412309702 -0.7339920251
H -1.114123427 2.5678928545 0.2669051098
H 0.0998106807 3.1453954263 -0.9043642486
H -1.4627067089 2.5715968793 -1.4841983654
C -0.5758066687 -2.4997338318 -0.5818056941
H 0.2636623216 -3.192868067 -0.6239716544
H -1.0815026182 -2.606388206 0.38711439

H -1.2680443433 -2.7615758007 -1.3823204107
 C -2.2420801314 -0.0245312852 1.5028790892
 O -3.4145856531 0.2060451168 1.3305544775
 O -1.378967097 -0.255660361 2.3163620799
 C -0.958179706 -0.0577105386 -0.877335431
 H -1.6235200859 -0.0277632676 0.2543631648
 H 4.2271926804 -1.0983776109 0.9846260475
 H 4.1682301908 1.3683659543 0.8897487438
 C -2.1036899987 -0.1248630479 -1.8572297301
 H -1.7122595965 -0.1502607733 -2.8774273439
 H -2.7062856374 -1.015706981 -1.67579269
 H -2.7561658709 0.7408920344 -1.7390583492

1b

23

O 1

C	0.15761800	0.21026900	0.70422400
C	0.15761800	0.21026900	-0.70422400
C	0.03016900	1.38943300	-1.41750600
C	-0.08723600	2.59130900	-0.69486600
C	-0.08723600	2.59130900	0.69486600
C	0.03016900	1.38943300	1.41750600
H	0.01486000	1.39343200	-2.50256200
H	0.01486000	1.39343200	2.50256200
N	0.33060900	-1.10851400	-1.14438600
N	0.33060900	-1.10851400	1.14438600
C	-0.22046600	-1.51174700	-2.42236700
H	-1.31832300	-1.41991000	-2.44765200
H	0.20290500	-0.89795300	-3.21998200
H	0.05027900	-2.55162600	-2.61875600
C	-0.22046600	-1.51174700	2.42236700
H	0.20290500	-0.89795300	3.21998200
H	-1.31832300	-1.41991000	2.44765200
H	0.05027900	-2.55162600	2.61875600
C	-0.02178200	-1.94546800	0.00000000
H	-1.11244700	-2.17470800	0.00000000
H	-0.19100600	3.52668500	1.23574800
H	-0.19100600	3.52668500	-1.23574800
H	0.53617200	-2.88570500	0.00000000

1b_ox

22

1 1

C	-0.20386900	0.69855600	0.00000000
C	-0.20387500	-0.69855200	0.00000200
C	-1.38774600	-1.43514600	0.00000300
C	-2.56658600	-0.70476500	0.00000000
C	-2.56658600	0.70477500	-0.00000200
C	-1.38773300	1.43515900	-0.00000200
H	-1.38734300	-2.51873700	0.00000200
H	-1.38732800	2.51874900	-0.00000200
N	1.12872900	-1.09505000	0.00000500
N	1.12873900	1.09504300	0.00000100
C	1.60605600	-2.47296300	-0.00000600
H	1.24216800	-2.98043300	0.89376500
H	1.24223200	-2.98039700	-0.89382400
H	2.69435400	-2.46813300	0.00003300
C	1.60607300	2.47295400	-0.00000200
H	2.69437000	2.46812100	0.00002900
H	1.24224200	2.98039800	-0.89381200
H	1.24219400	2.98041700	0.89377700
C	1.88423300	-0.00000700	0.00000400
H	-3.51442500	1.23139600	-0.00000200

H	-3.51442700	-1.23138300	0.00000100
H	2.96388100	-0.00001200	0.00000700

TS1b

26

O 1

C	0.97638700	-0.64693400	-0.36365100
C	0.97218100	0.75520700	-0.28296300
C	2.00625100	1.44626900	0.32958000
C	3.06051700	0.69049100	0.85592100
C	3.06613100	-0.70356900	0.77119900
C	2.01660400	-1.39911100	0.15960100
H	2.00136300	2.52813500	0.40358400
H	2.01647000	-2.48223500	0.10705100
N	-0.18183800	1.20360400	-0.92376500
N	-0.18252500	-1.02344800	-1.03437500
C	-0.73984000	2.52866600	-0.76207400
H	-1.16964200	2.65564200	0.24023400
H	0.04085400	3.27431300	-0.91632600
H	-1.51916700	2.68311400	-1.50941200
C	-0.68760100	-2.37562600	-1.13746800
H	0.12309500	-3.04369900	-1.43211300
H	-1.10979000	-2.71109200	-0.18329000
H	-1.46005600	-2.41010300	-1.90677000
C	-0.99828400	0.09475600	-1.14582000
H	-1.86186100	0.04182700	-0.15294400
H	3.89436200	-1.26214600	1.19437700
H	3.88420600	1.20060700	1.34408800
H	-1.70727300	0.13829300	-1.97318300
C	-2.53982500	-0.15251700	1.04457000
O	-1.79965200	-0.78764200	1.75921600
O	-3.62249200	0.37520100	0.95057300

1c

33

O 1

C	-1.77396800	-0.70372600	0.06315500
C	-1.77396500	0.70372700	0.06315500
C	-2.95129000	1.41753700	0.20086600
C	-4.14948600	0.69478600	0.35223900
C	-4.14948800	-0.69478200	0.35224100
C	-2.95129300	-1.41753400	0.20086600
H	-2.95829800	2.50255300	0.18678300
H	-2.95830100	-2.50255000	0.18678300
N	-0.45091100	1.14185200	-0.05952800
N	-0.45091400	-1.14185400	-0.05952800
C	-0.17270000	2.42631900	-0.66835600
H	-0.49499300	2.46407000	-1.72116300
H	-0.68223700	3.21669700	-0.11385200
H	0.90136500	2.62043700	-0.62120700
C	-0.17271200	-2.42631800	-0.66836400
H	-0.68222900	-3.21670200	-0.11384800
H	-0.49503300	-2.46407000	-1.72116300
H	0.90135500	-2.62043000	-0.62124400
C	0.30414700	-0.00000100	-0.58239700
H	0.26053100	0.00000200	-1.69693200
H	-5.08463700	-1.23575900	0.45737400
H	-5.08463400	1.23576500	0.45737100
C	1.75575100	0.00000100	-0.15905700
C	4.44022500	-0.00000200	0.62333100
C	2.09351300	-0.00000400	1.19714600
C	2.76765100	0.00000600	-1.11689100
C	4.10898600	0.00000000	-0.72907200

C	3.42860700	-0.00000600	1.58746900
H	1.30190400	-0.00000700	1.94034600
H	2.50780700	0.00001000	-2.17252000
H	4.89014000	0.00000100	-1.48273900
H	3.68422600	-0.00001100	2.64257200
H	5.48194900	-0.00000400	0.92883800

1c_ox

32

C	-1.83407300	-0.69223600	0.08451000
C	-1.83405700	0.69222300	-0.08455000
C	-3.01773500	1.42320900	-0.17349500
C	-4.19777300	0.69922000	-0.08514700
C	-4.19779200	-0.69914800	0.08519600
C	-3.01777600	-1.42317900	0.17349100
H	-3.01842400	2.49933000	-0.30078200
H	-3.01850500	-2.49930200	0.30076100
N	-0.50353800	1.08669600	-0.13914800
N	-0.50356100	-1.08674000	0.13907300
C	-0.06152800	2.45847100	-0.36421700
H	-0.63026700	2.87575800	-1.19545500
H	-0.22659300	3.05129600	0.53651900
H	0.99622500	2.45839600	-0.61835400
C	-0.06157900	-2.45851100	0.36422700
H	0.99626800	-2.45844900	0.61797500
H	-0.63004500	-2.87561000	1.19574700
H	-0.22698400	-3.05148200	-0.53635000
C	0.27103500	-0.00002800	-0.00002800
H	-5.14518300	-1.22283300	0.14823000
H	-5.14514900	1.22293500	-0.14814000
C	1.74057800	-0.00001600	-0.00000500
C	4.51976400	0.00002600	0.00002400
C	2.43470200	-0.72647300	-0.97315200
C	2.43466000	0.72645500	0.97316100
C	3.82577300	0.72244000	0.96995100
C	3.82581300	-0.72241400	-0.96991600
H	1.89048400	-1.28121300	-1.73074800
H	1.89041200	1.28117300	1.73075000
H	4.36631800	1.28114800	1.72600700
H	4.36639000	-1.28111200	-1.72595700
H	5.60468000	0.00004400	0.00003100

TS1c

36

0 1

C	-1.78260200	-0.45252800	-0.74810300
C	-1.78205400	-0.63108700	0.64314800
C	-2.95231600	-0.89227900	1.33965100
C	-4.13440900	-0.98488700	0.59644900
C	-4.13321000	-0.81479600	-0.79020900
C	-2.95199500	-0.54055700	-1.48830700
H	-2.95576100	-1.01800200	2.41669900
H	-2.95705100	-0.39311200	-2.56251400
N	-0.46416100	-0.51601300	1.07632100
N	-0.47002800	-0.21059000	-1.13040400
C	-0.09862000	-0.28247600	2.45806600
H	-0.40685600	0.71959300	2.78215300
H	-0.57787700	-1.03086400	3.09052300
H	0.98223800	-0.37837300	2.56564800
C	-0.05054300	0.19799100	-2.45382700
H	-0.61312900	-0.36908400	-3.19651500
H	-0.21946100	1.26958000	-2.60547500
H	1.00980300	-0.02408300	-2.58088100

C	0.30080100	-0.01123300	0.01625100
H	0.33444100	1.30932400	0.18924700
H	-5.06647900	-0.88584800	-1.33885900
H	-5.06823300	-1.18605400	1.11070200
C	1.76716700	-0.35100900	-0.02856800
C	4.45372700	-1.08059500	-0.17788600
C	2.14310700	-1.68180800	0.17816500
C	2.73552900	0.61058800	-0.30835900
C	4.07843600	0.24453200	-0.38608600
C	3.48428700	-2.04368500	0.10555000
H	1.38274900	-2.42565800	0.39591900
H	2.44745300	1.64570600	-0.46092100
H	4.82886300	0.99689500	-0.60476300
H	3.77288800	-3.07681400	0.26894900
H	5.49977300	-1.36400100	-0.23415700
C	-0.02945300	2.63836900	0.31297500
O	0.70227000	3.16348000	1.12007600
O	-0.96991500	2.80524200	-0.42890500

2

31

0 1

C	-1.8837218409	0.8113491039	1.1675428424
N	-1.6941793616	1.0536195431	-0.2541505037
N	-1.7392634241	-0.6311661422	1.271659113
C	-1.3745177421	2.4258395398	-0.5859044487
C	-0.750858204	0.046759939	-0.7502458294
C	-1.6139048589	-1.1147483505	2.6311379177
C	-0.5964136511	-0.9358779133	0.4213536896
H	0.2186620337	0.4926565181	-1.009873792
H	-1.1485097208	-0.4387133869	-1.6482087692
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H	-0.6071675418	-1.984216812	0.1119588815
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H	-0.715250198	-0.7166664088	3.1380858886
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C	-0.1904132307	0.8908238402	-1.9408689189

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H 2.3704092326 0.3800364966 3.0996348691
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TS2

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3

35

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3_ox

34

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TS3

38

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4

31

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4_ox

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5
27
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5_ox

26
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TS5

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6

24

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H -0.4131826362 -2.640604185 1.1332620365
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23

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25

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7_ox

24

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TS7

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8

28

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8_ox

27

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TS8

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9_ox

30

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TS9

34

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H 1.5054564158 1.3358904141 2.1079053776
H 4.1730423202 0.6409352822 1.8950122904
H 4.3805723766 -1.0977113711 1.6508231357
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H 2.8922287278 0.9571465342 -0.0786820365
H 1.4313947472 0.0729084593 -1.7996062433
H 1.0870605554 -1.3903077638 -0.8598716395
H 0.3167640679 1.483541758 -0.1164468712

H -0.7841474654 0.1689059118 -0.5535995041
H 1.6368008847 1.3600585819 4.6056963479
H -0.0219703387 1.2877029908 3.989973432
H 0.4679346528 0.2075988805 5.2966867204
H -1.9658298825 -0.1781650777 1.3142794932
H -1.2176500981 -0.3485340234 2.9059886823
H -1.3377872867 1.2634049437 2.1393010566

10

32

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C 0.3660012453 2.6763305845 0.8954407018
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H 3.0407795421 -2.2593190958 -0.6446800578
H 2.1244947585 -1.2521420581 -1.7807976993
C 2.4196697431 -0.3596308591 0.1557197258
H 2.6259031246 -0.6992432101 1.1904835795
H 3.289767364 0.2155917114 -0.1743857512
H 0.15317777 -0.5164116021 1.6001955718
C 0.9140378596 -2.2537792063 -0.3096744317
H 1.0461396634 -2.685978641 0.7024430612
H 0.6702190194 -3.080074579 -0.9840003445
C -0.8983063369 1.9433854286 1.3015128983
H -0.8322477215 1.6621935466 2.3716367779
H -1.7762916291 2.586620381 1.1906431216
C -2.3549523644 0.1115348301 0.8497571218
H -3.15569914 0.8519120961 0.7625214659
H -2.322182067 -0.2111210799 1.9096809387
C -2.6289301899 -1.0906759388 -0.0333595427
H -3.5283809318 -1.6107794347 0.3099644594
H -2.794749877 -0.7662316548 -1.0659694842
C -1.4335689726 -2.0219451749 0.0311610717
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10_ox

31

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H 2.7745954826 0.1102404686 1.1951163636
C 2.4611092993 -1.2877711555 -0.4236396633
H 3.414159985 -1.7749808762 -0.2089450037
H 2.3279744135 -1.258161104 -1.5092960474
C -0.1152191831 2.7756992184 -0.4234924832
H -0.0741282522 2.6463211286 -1.50922933
H -0.1698086736 3.8445515202 -0.2081502614
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H 2.0236584895 2.5743552972 -0.2527715597
H 1.1639064327 2.4176761581 1.285442527

C 1.3284802165 -2.0596741609 0.2152875835
H 1.2175801085 -3.0397877696 -0.2514415327
H 1.5119280248 -2.2153205185 1.2858692864
C -1.3315829648 2.0773727165 0.1416258537
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H -1.4847021167 2.3482485674 1.1938723751
C -2.4481793286 -0.120923645 0.2131780192
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C -2.345443651 -1.486813327 -0.427662297
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H -2.2526530282 -1.384628511 -1.5131158943
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TS10

35

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H -1.4539788297 1.9533522993 0.5979440399
C -0.0870112945 -0.0285892831 2.3391357173
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H 1.1332404286 2.2457514053 0.8670564564
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C -0.7580999614 -2.2827443317 -0.5137370672
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C 1.6305653642 -2.0128371823 -0.2652906366
H 1.6881518336 -3.0228950722 -0.6774054564
H 1.6061878357 -2.1046603611 0.8350014867
C 2.8219537586 -1.18290712 -0.6978837595
H 3.7414264937 -1.5991072397 -0.2779013734
H 2.9063693479 -1.198045527 -1.7891232044
C 2.6303632942 0.2370532512 -0.2054286862
H 2.7136788307 0.2709208011 0.8909958875
H 3.3980335194 0.8962951102 -0.6189097058

11

22

O 1

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C 2.474788438 -0.091827877 -0.0035590318
C 1.587528999 1.1798324839 0.0733855337
N 0.2718185257 0.6714387868 -0.2914538901

C -0.8814530673 1.4530636909 0.1242205192
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H -0.8814032809 1.6043787108 1.221558184
H 1.5930293287 1.5884174119 1.0989896537
H 1.9062365255 1.970892818 -0.6109305426
H 3.0970037345 -0.1806912027 0.8909683714
H 3.1323579796 -0.085962551 -0.8751186181
H 0.2381490533 -0.5783877081 1.3985744867
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H -2.2132648225 -0.7229953702 1.3160072342
H -2.9670702481 -1.3017258918 -0.1812025062
C -2.1448721392 0.7019782416 -0.2989287127
H -2.2129645655 0.6987824264 -1.392857728
H -3.030924002 1.2120805886 0.0922779574
H -0.8565391944 -2.3426840622 0.2010419086
H 1.4484050278 -1.5021741447 -1.0741995379

11_ox

21

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N 1.5185318047 -1.1650493269 0.0661101662
C 2.4726531413 -0.0798151395 -0.1955655875
C 1.636960424 1.1585901672 0.1583909149
H 1.7793720231 1.4669655667 1.2007588534
H 1.8331053008 2.004842314 -0.500782925
H 3.3570972273 -0.1819770796 0.4320211343
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N -0.8503456951 -1.3850348221 0.0186295425
C -2.1581978114 -0.7427878759 0.1864168461
H -2.4153690674 -0.7218246228 1.2507654117
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H -2.0503483614 0.6240470041 -1.4775770492
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TS11

25

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H 0.8231695507 -1.2198471408 -1.7650307188
H -0.1187739233 -2.7129511862 -1.508971285
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H -2.4956493054 1.7552642979 1.5150756104
H -2.2272432812 -0.9636037924 -1.8127344763
H -1.1046423166 0.4126580757 -1.8187618465
C 1.679934801 1.4138276854 -0.3911970352

O 2.5258123001 1.2308471176 0.4460397796
O 1.3599716052 1.9920671463 -1.3946911025
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H -3.2812034346 -0.1978764533 0.2576755824
H -0.3764773114 0.8788235072 2.2230694221
H 1.6935891573 -0.6741210408 1.552583616

12

25

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C -0.163310458 0.1961970362 0.0862397674
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C -1.1423833259 -1.8723575737 0.0498141646
N 0.1051170019 -1.1884491151 -0.2469373875
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H 1.4775284261 -2.7196698969 0.0926582139
H 1.2321417826 -1.6436622163 1.4870243346
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12_ox

24

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N -1.4994521711 0.1621493108 -0.0253565568
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C -0.8916296685 -2.0737359635 0.1610642737
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H -0.8165650897 -2.9735814141 -0.450404851
H -2.9466395387 -1.3271742658 0.3810333812
H -2.3315287913 -1.3092542553 -1.2949339212
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H 1.7681253154 -1.6812837618 1.2897186587
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TS12

28

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H -0.1804205356 1.4308194707 -2.5276395913
H 1.7491479029 -2.5426172656 1.2386580441
H 1.3332632421 -0.921328986 1.8345595739
C -0.8404102542 1.4561151262 1.3225623171
O -0.0921525974 1.6843037054 2.2350792368
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C 2.6884795412 -0.923755423 0.1350298539
H 3.5521578157 -0.7845036121 0.7910125931
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13

28

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C -2.9219991006 -0.6635498776 -0.1143762328
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13_ox

27

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TS13

31

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N -0.9260860282 -1.4991231707 -0.5813335836
C -1.2085282685 -1.2636168037 -1.9920192955
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H -0.3466760311 -0.8331079565 -2.5001495117
H -1.4418388515 -2.2191058567 -2.4669435768
C -2.074791105 -2.0396761195 0.1821109045
C -2.3009732843 -1.0274662875 1.303395678
H -3.0109063783 -0.2414964208 1.0096029656
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H -2.9475641787 -2.1436105823 -0.4659198181
H -1.8165828897 -3.0236505345 0.5858425062
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C 1.7261216867 -0.3042450257 -1.077751968
H 1.4395187469 0.4692529915 -1.8040940301
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C -1.4801309391 1.8112911457 -0.9403340153
O -0.6686749233 2.2854785753 -1.6931188462

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H 1.2816574263 0.0750012258 2.9300410771

14

29

O 1

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N -0.1458189365 -1.3991543246 -0.3779195401
N -0.8726016036 0.860057149 0.022541567
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H -0.5490476507 2.2279659745 1.6228178212
C 2.3022656834 -1.7093999258 -0.4717817276
H 3.1055799255 -2.384980651 -0.1627157459
H 2.3555973765 -1.5996944558 -1.5599472687
C 2.4973078764 -0.3374148781 0.1802420788
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H 0.166208602 -0.3478132835 1.406794174
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H -2.7120286102 -0.7268307112 -1.1883502175
C -1.4370984451 -1.9111292229 0.088120539
H -1.3814367091 -2.1756511642 1.1627574046
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14_ox

28

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H -3.3639225515 -1.5815657244 -0.1206133215
C -2.4257038036 0.343058226 0.1076884776
H -3.1523366676 0.938429387 -0.4486340676
H -2.6789649882 0.3995754651 1.174746069
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H 1.2905081532 2.943023515 0.6270469157
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H -1.4421025828 -2.0668229629 1.3015040193
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H 1.4594038379 -1.9640238179 1.3536278933
H 1.1791329942 -2.8635494719 -0.1481310786
C 2.3948867272 -1.0927236103 -0.4088916061
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32

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H -2.194054 2.158109 -0.906363
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H 1.217721 2.270286 0.889527
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15

36

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15_ox

35

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H 0.1347556565 2.3568057161 1.1618150022
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H 2.7018943347 -2.7947710863 -0.6043531353
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H -4.3245835861 -0.4617609588 -0.1519749199
H -3.6278041788 0.5437971473 1.1440649584
C -2.3482965296 -1.9395022885 1.3088216753
H -2.4009670082 -1.5332004493 2.3261075299
H -3.2272491577 -2.5600407669 1.1252299273
H -1.4507563561 -2.5492404045 1.2104395462
H -0.4829143882 0.8743039877 -2.577941179
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TS15

39

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C 3.8471237485 0.5778705249 0.1878815761
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16

31

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H 1.5092825607 -2.148562768 2.5056863091
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16_ox

30

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C 2.5221371649 1.5606045674 0.0194479975
C 3.3339037328 0.272873287 -0.1774487574
N 2.3459181901 -0.7650325424 0.1211276301
C 2.6715489323 -2.1752277178 0.0666023213
H 1.7922022914 -2.7531135594 0.3477695218
H 2.9855331313 -2.4572279794 -0.9439823484
H 3.4821384258 -2.3840967329 0.7671622773
H 4.1860184222 0.2018274376 0.4992692178
H 3.6834456825 0.1642217934 -1.2105699439
H 2.6289950414 1.9551150851 1.0373367976
H 2.7775063856 2.3384812847 -0.6998669083
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H -2.6289725719 1.9551096377 1.0373985274
H -3.6834691122 0.1642171437 -1.2104877512
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H -1.7921923553 -2.7531170062 0.3478176072
H -3.4821261951 -2.3841025705 0.7672207037
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TS16

34

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17

34

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H 2.0996887026 -1.2873405287 3.6476715935
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17_ox

33

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 H -2.446137347 2.5446659234 -1.4482320513
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TS17

37

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TS18

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TS19

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TS20

48

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21

53

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45

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44

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23

45

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TS23

48

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24

37

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24_ox

36

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25

51
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25_ox

50

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54

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26

57

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26_ox

56
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 H 3.615966 -1.9113 -1.664178
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TS26

60
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 H -2.963042 3.3898 -2.080916
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27

63

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TS27

66

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31

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28_ox

30
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TS28

34
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31
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 C 3.1109403768 0.9403335051 -0.927657294
 C 2.4032999909 2.1794178835 -0.377127121
 N 1.0279916085 1.7189204836 -0.3727579781
 C 0.0521300329 2.5225737474 0.3244755744
 H -0.1350476847 3.4405441488 -0.242241184
 H 0.3800501572 2.7993392693 1.3418428109
 H 2.7630868023 2.4249453147 0.6370323714
 H 2.5271493552 3.0566136956 -1.0156574349
 H 4.1347202925 0.852226678 -0.5559019142
 H 3.142663304 0.9531374918 -2.0190446552
 H 1.2114035559 0.3889203171 1.2686314996
 N -1.1772975927 1.7418681872 0.4034767816
 C -2.4894041349 2.3408426821 0.189598251
 C -3.4023413119 1.1116301454 0.2065055338
 H -4.2549782085 1.2131501682 -0.4642691965

H -3.7552898275 0.8918670266 1.2192793289
H -2.5250854587 2.8570056903 -0.7786528376
H -2.7357494075 3.0486799833 0.9823620325
C 2.9757641182 -1.1168314921 0.3386921233
F 3.9682830891 -1.6933616984 -0.412265562
F 2.1388157642 -2.1214797627 0.730837198
C -2.8475783956 -1.2799770736 -0.3259646743
F -3.3672382883 -1.736328948 0.8730155721
F -3.8654668632 -1.4519370777 -1.2263683615
H 3.4506033214 -0.7152390125 1.2442465364
H -1.9989103966 -1.905885001 -0.5957683906

29_ox

30

1 1

C -0.0000001422 2.7167996577 -0.1707957214
N 1.1622161317 1.8881939129 0.0903948495
C 1.1052695466 0.5608528864 -0.0621353084
N -0.00000066 -0.172207124 -0.1556912058
C -1.1052705791 0.5608532802 -0.0621351291
N -1.1622166915 1.8881943112 0.0903948339
C -2.5370171472 2.3755026214 -0.0416430003
C -3.3534467467 1.0902415227 0.177876646
N -2.352299647 0.044320226 -0.0963068376
H -4.1935003828 1.0061870846 -0.5092383574
H -3.704732506 1.0015876851 1.2082134293
H -2.6860462296 2.7919997536 -1.0429497676
H -2.7492570776 3.1379291047 0.7071039811
N 2.3522983613 0.0443194481 -0.0963073496
C 3.3534461383 1.0902403909 0.1778747569
C 2.5370166701 2.3755018332 -0.0416436797
H 2.7492573256 3.1379278664 0.7071035556
H 2.6860451712 2.791999477 -1.0429503187
H 3.7047333659 1.0015863416 1.2082110088
H 4.1934987799 1.0061857164 -0.5092414505
H -0.0000000188 3.5716122655 0.5076665732
H -0.000000063 3.0740284642 -1.2108258904
C -2.6147681556 -1.3410840301 -0.0213130317
F -3.1379302727 -1.6633310775 1.1999388153
F -3.5728762149 -1.6692094145 -0.9303364394
C 2.6147667557 -1.3410849512 -0.0213163135
F 3.1379325281 -1.6633337615 1.1999334627
F 3.5728719202 -1.6692095627 -0.9303431231
H 1.712037428 -1.9237351455 -0.1974715178
H -1.712039528 -1.9237347228 -0.1974701704

TS29

34

0 1

N 2.578043 0.244974 -0.380644
C 1.271942 -0.176533 -0.385436
C 3.480595 -0.896743 -0.170632
N 0.240721 0.625933 -0.380742
N 1.250807 -1.523915 -0.405464
H 3.775516 -0.955088 0.880621
H 4.367018 -0.809563 -0.797175
C 2.590028 -2.08108 -0.573612
C -0.937378 -0.09473 -0.415849
H 2.73778 -2.946851 0.072721
H 2.744723 -2.376008 -1.617344
N -0.979787 -1.326718 -1.084484
N -2.130292 0.553987 -0.745369
C 0.033001 -2.273873 -0.669999

C -2.377293 -1.758254 -1.120733
C -3.139451 -0.421085 -1.188622
H -2.636112 -2.31478 -0.210803
H -2.561062 -2.386946 -1.992399
H -4.010842 -0.420451 -0.531361
H -3.454002 -0.179463 -2.205524
H 0.210006 -2.990685 -1.477015
H -0.268157 -2.827618 0.233694
C -1.06258 -0.825076 2.167523
H -1.085046 -0.435516 0.883041
O -2.010946 -1.556624 2.351508
O -0.098602 -0.312122 2.686499
C -2.454247 1.784035 -0.176612
F -3.230465 1.644688 0.963219
F -3.234458 2.502662 -1.037841
C 2.91991 1.565643 -0.055971
F 3.367882 1.662962 1.241333
F 3.972693 1.973063 -0.824738
H -1.5622 2.35113 0.087039
H 2.074281 2.237797 -0.190738

30

31

0 1

C 2.6874620031 -0.9894797224 -0.7581432671
N 2.4414154541 0.3626765397 -0.4986228744
C 1.178183803 0.9227149802 -0.5105125547
N 0.0782035198 0.2611623051 -0.626750473
C -1.052138891 1.1537118437 -0.5954315265
N -2.2999559564 0.5484975925 -0.1692747087
C -2.9154526036 -0.4233515973 -0.9424028695
H -2.4001217284 -0.5677928718 -1.8942424104
H -3.9832421246 -0.2401867569 -1.0862051132
C -3.0520045948 1.4839857704 0.6712776236
C -2.2017902764 2.759473159 0.6095446928
N -0.8751452347 2.2022431177 0.3996073507
C 0.1825680147 3.1023708794 0.0087061473
H 0.4679003124 3.7252541141 0.8632901613
H -0.1133488847 3.7665260893 -0.8229454453
H -2.517306481 3.3984703016 -0.2334711626
H -2.243814568 3.3467494198 1.5292840533
H -4.0621332639 1.6459081649 0.2813452298
H -3.132437853 1.1150447537 1.6994416467
H -1.1789677463 1.5991137317 -1.6091538294
N 1.3216193703 2.2862058157 -0.3992620173
C 2.6806833571 2.6219684683 0.0117266182
C 3.4732134504 1.3967825318 -0.4593342979
H 4.2722985604 1.132108579 0.234420234
H 3.8991354791 1.5517360624 -1.4573262813
H 2.7338614201 2.7398296823 1.1024614698
H 3.0214434431 3.5441706688 -0.4618578923
H 1.8261516984 -1.4467534327 -1.2443915913
H 3.6046303718 -1.1194874558 -1.3343023802
F -2.8748117049 -1.725680611 -0.3097666554
F 2.8922107041 -1.7167535631 0.4501530628

30_ox

30

1 1

C -0.000009327 2.9561659524 0.5711935529
N -1.1615503833 2.3067539644 -0.0034875359
C -1.1080148746 1.013386321 -0.3634171085
N -0.0000022409 0.3010656207 -0.5506151246

C 1.1080055266 1.0133965119 -0.3634272567
 N 1.1615324138 2.3067647723 -0.0034984184
 C 2.5308954425 2.694539352 0.3395459119
 C 3.3560814148 1.5715620259 -0.3151828355
 N 2.348065676 0.5271164501 -0.5441074286
 C 2.6385399302 -0.7815711656 -1.003024485
 H 1.7614660675 -1.2090387137 -1.4864431905
 H 3.5044646257 -0.7644781881 -1.6647602631
 H 4.1483310095 1.2056029825 0.3372628435
 H 3.7840111575 1.8824446126 -1.2718027888
 H 2.6490698723 2.7104356752 1.4282135051
 H 2.7666112957 3.6787052964 -0.0649576577
 N -2.3480721818 0.5270949378 -0.5440862918
 C -3.3560954933 1.5715311302 -0.3151521873
 C -2.5309138705 2.6945161697 0.3395688775
 H -2.7666422998 3.6786798352 -0.0649329259
 H -2.6490787652 2.7104117989 1.4282375077
 H -3.7840371327 1.8824097784 -1.2717680912
 H -4.1483355468 1.2055646664 0.3373009188
 C -2.6385386002 -0.7815953719 -1.003000552
 H -3.5044694512 -0.7645104375 -1.6647284862
 H -1.7614652027 -1.2090549417 -1.4864271582
 H -0.0000155188 4.0138520952 0.3008456187
 H -0.000003759 2.8616409875 1.6680569631
 F 2.9706595667 -1.6091681558 0.0798488447
 F -2.9706408364 -1.6091952725 0.0798759019

TS30

34

O 1

C 2.938951 1.29964 1.095629
 N 2.543751 0.171059 0.355081
 C 1.251374 -0.017472 -0.065109
 C 3.461139 -0.597566 -0.492842
 N 0.226363 0.648531 0.393013
 N 1.241993 -0.990054 -1.010619
 H 4.269057 -1.02337 0.102632
 H 3.881382 0.038467 -1.278826
 C 2.530138 -1.666807 -1.07968
 C -0.972771 0.118093 -0.071945
 H 2.519654 -2.578954 -0.470595
 H 2.78297 -1.922697 -2.109399
 N -0.990936 -0.514483 -1.334752
 N -2.1573 0.865432 0.007435
 C -0.005766 -1.561321 -1.479122
 C -2.390115 -0.768512 -1.65159
 C -2.229771 2.102435 0.655062
 C -3.050072 0.501232 -1.099293
 H -2.761235 -1.667199 -1.135899
 H -2.532701 -0.888234 -2.725961
 H -4.065869 0.321413 -0.742249
 H -3.065196 1.294278 -1.854319
 H 3.881442 1.105493 1.606594
 H 2.146951 1.587883 1.785301
 H 0.087752 -1.830691 -2.533651
 H -0.263751 -2.467616 -0.902388
 H -3.263257 2.348074 0.900001
 H -1.586386 2.114009 1.533459
 C -1.28323 -1.807117 1.75792
 H -1.183165 -0.855731 0.769725
 O -2.453494 -1.899708 2.034033
 O -0.161735 -2.190635 1.985458
 F 3.16992 2.414452 0.25003

F -1.77794 3.170948 -0.181768

Reduction potential calculations

1a_rad

25

O 2

C	0.49979200	0.70494800	-0.06201500
C	0.49975700	-0.70495200	-0.06191600
C	1.68749300	-1.42330200	-0.04925900
C	2.89092000	-0.69613900	-0.06080500
C	2.89095600	0.69600700	-0.06090200
C	1.68756800	1.42323200	-0.04946200
H	1.69278700	-2.50790500	-0.02776700
H	1.69292500	2.50783800	-0.02813600
N	-0.81855700	-1.12076600	-0.05141200
N	-0.81851600	1.12084100	-0.05159000
C	-1.19377800	-2.47239900	0.30068200
H	-0.62236600	-3.18009100	-0.30381600
H	-1.00765100	-2.67856700	1.36336600
H	-2.25159300	-2.62953300	0.09009300
C	-1.19358700	2.47243600	0.30087600
H	-1.00700100	2.67842100	1.36351400
H	-0.62244800	3.18023400	-0.30375600
H	-2.25149600	2.62960100	0.09078500
C	-1.65735300	0.00005300	0.17524900
H	3.83366100	1.23412400	-0.05630000
H	3.83359700	-1.23430400	-0.05612600
C	-3.04371600	0.00003700	-0.39681400
H	-3.60351100	-0.87638300	-0.06229700
H	-3.60326300	0.87681800	-0.06283600
H	-3.03244600	-0.00029800	-1.49950600

1a_H_rad

1 2

C	0.4924110808	-0.7156105817	0.2074795301
C	0.4924109354	0.7156106275	0.2074793165
C	1.687428902	1.4392783955	0.0565957438
C	2.8497980365	0.7105313854	-0.0860486041
C	2.8497982038	-0.7105307645	-0.0860483876
C	1.6874292659	-1.4392780515	0.0565961584
H	1.6924137927	2.5222781191	0.0466511728
H	1.6924145398	-2.522277774	0.0466519041
N	-0.7738434289	1.1330142282	0.3726720863
N	-0.7738432367	-1.1330143326	0.3726724269
C	-1.2378342891	2.506110818	0.3955316686
H	-0.4844218182	3.1354731422	0.8697351981
H	-1.4295940479	2.8676474977	-0.6187378529
H	-2.1560432188	2.5615491533	0.9807753844
C	-1.2378343473	-2.5061108239	0.3955319402
H	-1.4295987378	-2.8676458874	-0.6187372867
H	-0.4844198701	-3.1354740563	0.8697309993
H	-2.1560406633	-2.5615498603	0.9807797359
C	-1.6881244292	-0.0000001131	0.4266394252
H	-2.2119915999	-0.0000000269	1.3929307084
H	3.7922364483	-1.2327697193	-0.2065994229
H	3.7922361521	1.2327705346	-0.2065998053
C	-2.6960232583	-0.0000004201	-0.7210859428
H	-2.1743130686	-0.0000007383	-1.6806386829
H	-3.3338992096	-0.8833120958	-0.6512509213
H	-3.3338991335	0.883311349	-0.6512514925

1b_rad

22

0 2

C -0.173352484 0.7067773014 0.1088071081
C -0.1733597479 -0.7067769557 0.1087883963
C -1.3611421578 -1.4257309747 0.0745485818
C -2.5634907497 -0.6962821157 0.0597449029
C -2.5634837602 0.6963066884 0.0597548542
C -1.361127845 1.42574336 0.0745703574
H -1.3647649775 -2.510451647 0.0566677773
H -1.3647394749 2.5104642909 0.0567019846
N 1.1426729633 -1.1175932358 0.1279030289
N 1.142684301 1.1175845346 0.127950811
C 1.5717940674 -2.4733999827 -0.1212220889
H 1.0142284435 -3.1621532834 0.5178499552
H 1.4209299505 -2.7581862913 -1.170601046
H 2.6322693227 -2.5614193242 0.1199427433
C 1.5718052779 2.4733844836 -0.1212105668
H 2.6322195474 2.561474231 0.1201962709
H 1.4211698947 2.7580740401 -1.1706496867
H 1.0140613097 3.1621667996 0.5176730248
C 1.9795307135 -0.0000052204 -0.0586449387
H -3.506515575 1.2333491805 0.0363590205
H -3.5065279487 -1.233314885 0.0363429794
H 2.9504919289 -0.0000209945 0.4385035306

1b_H_rad

23

1 2

C -0.0699949335 0.219123381 0.7154131537
C -0.0699949335 0.2191234007 -0.7154131476
C -0.0413629532 1.4219409839 -1.4399001847
C -0.0078453833 2.5926746389 -0.7104205818
C -0.0078453833 2.5926746193 0.7104206533
C -0.0413629532 1.4219409442 1.4399002239
H -0.0504541108 1.4263235776 -2.5229610697
H -0.0504541108 1.426323508 2.522961109
N -0.0995858239 -1.0586659292 -1.1338506789
N -0.0995858239 -1.0586659605 1.1338506497
C -0.1826731667 -1.5227409149 -2.5049342145
H -1.215154661 -1.4783544899 -2.862690557
H 0.4525051881 -0.9023466729 -3.1384857871
H 0.1731220847 -2.5516651447 -2.5517916056
C -0.1826731667 -1.522740984 2.5049341726
H 0.4525051881 -0.9023467594 3.1384857623
H -1.215154661 -1.4783545688 2.8626905163
H 0.1731220847 -2.551665215 2.5517915352
C -0.1682722812 -1.9565208494 -0.000000027
H -1.1099207361 -2.523294476 -0.0000000348
H 0.0145121289 3.5426929525 1.232376849
H 0.0145121289 3.5426929865 -1.2323767513
H 0.6728172778 -2.6612744281 -0.0000000367

1c_rad

32

0 2

C -1.8295446621 -0.7022205694 -0.0621441303
C -1.8317321619 0.6959552056 0.0664891221
C -3.0181541245 1.4135540369 0.1250826178
C -4.2170836691 0.6877038013 0.0612860203
C -4.2148928929 -0.7019290469 -0.0514969882
C -3.0136985229 -1.4237771304 -0.1180233263
H -3.0231957268 2.4929667393 0.2312618365

H -3.0153823767 -2.5032016083 -0.2241887827
N -0.5108581333 1.1163481992 0.1020764209
N -0.5073629067 -1.1182075734 -0.1007438213
C -0.1257813982 2.4785249273 -0.222422025
H -0.9135566311 2.9368925763 -0.8250910433
H 0.0272001159 3.0827679954 0.6761846702
H 0.7945024555 2.4694517299 -0.8076559891
C -0.117035752 -2.4791103834 0.2228009426
H 0.8045253686 -2.4670165656 0.805964068
H -0.9019222595 -2.9401147755 0.8272283179
H 0.0359105446 -3.0827990876 -0.6761846394
C 0.3233403808 0.000453428 -0.0002583793
H -5.1569863379 -1.2388289099 -0.0941879007
H -5.1608636016 1.2214570194 0.106126337
C 1.7356206286 0.0028062269 -0.0019020544
C 4.5884847199 0.0075320934 -0.0051824495
C 2.4884095693 -1.0155630592 -0.6697628336
C 2.4865670841 1.0236493177 0.6642558653
C 3.8702808885 1.0167763959 0.6533435082
C 3.8721167198 -1.0040987466 -0.6620391905
H 1.9710916926 -1.7892048677 -1.2270096282
H 1.96796876 1.7955398829 1.2227397126
H 4.4039870052 1.8023444759 1.1815630253
H 4.4072075364 -1.7879092084 -1.191467719
H 5.6733776873 0.0093314812 -0.0064325638

1c_H_rad

33

1 2

C -1.7115589342 -0.7156758634 -0.1464306257
C -1.7115574947 0.7156794349 -0.146429126
C -2.8283451294 1.4405223546 0.3017754909
C -3.9121159103 0.7109692214 0.7437614018
C -3.9121172823 -0.7109632171 0.7437599944
C -2.8283479101 -1.4405175529 0.3017726038
H -2.8362466078 2.5235345324 0.2940096404
H -2.8362514201 -2.5235297049 0.2940045605
N -0.5258559522 1.1342041115 -0.6186764563
N -0.5258583554 -1.1342019537 -0.6186790759
C -0.1290750257 2.5072802013 -0.8607841969
H -0.5545732968 2.868360557 -1.8012700097
H -0.4692806555 3.1356162239 -0.0367796227
H 0.9589059655 2.5553892501 -0.9113524269
C -0.1290799393 -2.5072785349 -0.860788247
H -0.4692830875 -3.1356141315 -0.0367822871
H -0.5545822242 -2.8683584778 -1.801272389
H 0.9589007873 -2.5553887407 -0.911360705
C 0.3054078665 0.0000005847 -1.008645991
H 0.4297870572 0.0000018456 -2.1023240858
H -4.794384096 -1.2324292611 1.0973775932
H -4.7943817267 1.2324362702 1.097380008
C 1.665703025 -0.0000014882 -0.340629169
C 4.1627701562 -0.0000041682 0.8888980149
C 1.7548601085 -0.000007537 1.0538900831
C 2.8215625772 0.0000031711 -1.1172508962
C 4.0730897068 0.0000018745 -0.5002775759
C 3.0022871333 -0.0000089219 1.66671902
H 0.8514392838 -0.0000113867 1.6577459976
H 2.7483976242 0.0000077925 -2.2010546178
H 4.9728400213 0.0000054726 -1.1063489554
H 3.0722347045 -0.0000137111 2.7493533174
H 5.135777031 -0.0000052471 1.3693627334

2_rad

30

O 2

C 1.2798297936 -0.1783554786 -0.7952772615
N 1.8385825208 -0.6614571952 0.4189173008
N 1.6491996409 1.1804658372 -0.9231480282
C 2.1360465784 -2.0782591871 0.4816353348
C 2.9324047186 0.2381238718 0.757802007
C 0.7557501416 2.1518965338 -1.5118121346
C 2.4023964936 1.5780630731 0.2578770863
H 3.8568940129 -0.0368011288 0.2208980788
H 3.1355257177 0.2286466819 1.8314102962
H 3.1951395852 2.2890433687 0.0107828588
H 1.7410523037 2.0430014315 1.0094725631
H 1.2466421493 -2.6489565786 0.202473593
H 2.4102295167 -2.3474696102 1.5051771032
H 2.9619030242 -2.3600026121 -0.1929899454
H 1.3300005897 3.0299810808 -1.8200147839
H 0.2760776618 1.7225182114 -2.3929804877
H -0.0305158315 2.4782359232 -0.8119416773
N -0.0058662858 -0.6062482006 -1.175260034
C -1.1649798194 -0.4635002027 -0.4112450566
C -1.2061143886 0.3436199657 0.7360169093
C -2.3390015013 -1.1241025231 -0.8113020322
C -2.3927053331 0.4854054128 1.4518598415
H -0.3085293955 0.8488221117 1.0725345568
C -3.517282234 -0.9735568443 -0.0883877237
H -2.321794519 -1.7553092103 -1.6962887632
C -3.5577217544 -0.1668002367 1.0503876697
H -4.4781370428 -0.0514420376 1.6132471883
H -2.4005213894 1.1151311529 2.3369098862
H -4.4117820147 -1.4932497751 -0.4194484743
H -0.0509329392 -1.2964918354 -1.9088508711

2_H_rad

31

1 2

C -1.2419105638 0.2097809259 -0.7165045083
N -1.4176385945 1.2458622826 0.2666106634
N -1.5928497658 -1.0110113486 -0.0329516808
C -1.6506993602 2.5725694289 -0.2783023213
C -2.3983013652 0.7643728701 1.2547991028
C -1.7926647687 -2.1569994957 -0.9042118879
C -2.7543330982 -0.644445374 0.7746002143
H -3.2811109926 1.4109344828 1.2809697026
H -1.9515925931 0.7550551986 2.2546277617
H -3.6735992255 -0.62865191 0.1655611099
H -2.8923032088 -1.3593511351 1.5886155023
H -1.6590803063 3.2984440488 0.5372428915
H -2.6044173207 2.6457178282 -0.8259028907
H -0.8356761201 2.8412566296 -0.9560776939
H -2.029153337 -3.0293850025 -0.2918220714
H -2.6129312356 -1.9979964346 -1.6236818491
H -0.8742935071 -2.369358636 -1.4576924646
H -1.8441316038 0.3788989516 -1.6313476945
N 0.1470112301 0.1581689438 -1.2192787409
C 1.2612940379 -0.0018301756 -0.5053259212
C 1.2447910398 -0.1729662319 0.9193995418
C 2.5149621859 -0.0046756432 -1.2064300048
C 2.4342986728 -0.3404374212 1.5851283906
H 0.3006360259 -0.1733442743 1.4422723449
C 3.6848408268 -0.1728365249 -0.5124852207
H 2.518594737 0.1270981059 -2.2833141018

C 3.6562300877 -0.3418824533 0.8862771286
H 4.5852860929 -0.4736543196 1.4294475394
H 2.4317374491 -0.4719674668 2.660777005
H 4.632071672 -0.1758538943 -1.0385171178
H 0.2562709092 0.2709180448 -2.221622729

3_rad

34

O 2

C -1.9602728748 -0.2007599994 0.0334896575
N -3.1786864684 -0.520120162 -0.4567141922
N -1.930425919 1.0799337217 0.4297862908
C -3.6334384602 -1.8747852736 -0.6996459443
C -4.1187892247 0.5581861814 -0.153058939
C -0.8045987463 1.8490700954 0.9267641247
C -3.1701376817 1.7428863053 0.0214486531
H -4.6707133131 0.3358523836 0.7687890205
H -4.8236641563 0.6936551544 -0.9735310442
H -3.4973732698 2.4402418048 0.7931643777
H -3.0160417355 2.2883340521 -0.9173609027
H -2.9157313804 -2.4117593425 -1.3243715751
H -4.5727168249 -1.822435479 -1.2502635163
H -3.8000063839 -2.4257751711 0.23351073
H -1.1983716637 2.6119670659 1.6010847787
H -0.1227746229 1.2018506835 1.4772885189
H -0.2583821703 2.3263714928 0.1073827613
N -0.9727997314 -1.0906510482 0.1237422831
C 0.4407162484 -0.789511513 0.1204460592
C 0.9649607788 -0.0851841792 -0.9662961127
C 1.212994594 -1.2356690068 1.1795077215
C 2.3749812326 0.2722823695 -0.935594347
H 0.3210631414 0.2474616065 -1.7742346665
C 2.641611249 -1.0030087617 1.1460537738
H 0.7490391357 -1.7636533657 2.0073205323
C 3.1623911582 -0.2092418268 0.1032883091
H 2.7917856967 0.8611108859 -1.7433932603
H 3.2895289018 -1.3225011395 1.955202446
H -1.2278437932 -2.0546805632 -0.0361032039
O 4.5123799271 0.0446662009 0.2011644438
C 5.1295930751 0.7984830631 -0.8220298693
H 6.1849158622 0.8679654161 -0.5556642819
H 5.0336398782 0.3058132519 -1.7972530662
H 4.7063895413 1.8082470968 -0.8885465545

3_H_rad

1 2

C 2.2256420349 0.4583500766 0.6230252128
N 2.4889041127 1.3063601778 -0.5136899104
N 2.4585926377 -0.8797759158 0.1647619841
C 1.8224006078 2.5897786079 -0.5928848311
C 2.4958439891 0.4795463953 -1.7131499951
C 3.0799733048 -1.7787743702 1.1191149883
C 3.0647905477 -0.8192080577 -1.1643296883
H 3.1296372103 0.931830861 -2.4797066579
H 1.4892154601 0.3388869661 -2.1401702099
H 4.1632520254 -0.7670612028 -1.1083462458
H 2.784494701 -1.6971059134 -1.7531906435
H 1.9586322481 3.1411229548 0.3415768354
H 0.7426313741 2.5046068255 -0.7965231936
H 2.2770056022 3.1708155776 -1.3985226798
H 3.0880919323 -2.7896106928 0.7051389876
H 4.1160485791 -1.4873135081 1.3561837231
H 2.4977491911 -1.7976820732 2.0439026308

H 2.8568540736 0.7524030646 1.4735132589
 N 0.8443281304 0.6135041143 1.1928482076
 C -0.3481877031 0.229790308 0.7159451027
 C -0.515640451 -0.6859517971 -0.3721610743
 C -1.5193212304 0.7658815271 1.343364634
 C -1.769131665 -1.0055443613 -0.8056355502
 H 0.3554232672 -1.1462413327 -0.8141050461
 C -2.7742589113 0.4406173575 0.9052737242
 H -1.402739272 1.4555942501 2.1729781329
 C -2.9196737746 -0.4493899411 -0.1860390621
 H -1.9126093102 -1.7021927066 -1.6234891014
 H -3.6381696431 0.8715349927 1.3943173414
 H 0.8057611031 1.2472598941 1.9837856763
 O -4.0813182722 -0.8294115047 -0.6920376826
 C -5.3051973688 -0.3361180202 -0.1306254612
 H -6.0957893197 -0.7966505576 -0.7178564063
 H -5.3925088698 -0.6389126897 0.915275834
 H -5.3553683417 0.7509936938 -0.2246748344

4_rad

30

O 2

C -1.55837676 -0.2254905269 0.0690293719
 N -2.7647966111 -0.6748958438 -0.3392002789
 N -1.611797656 1.0833414797 0.3541885563
 C -3.1202495725 -2.0736901788 -0.467036207
 C -3.7734073674 0.3541142114 -0.0892069257
 C -0.5338156139 1.9546531824 0.7805149617
 C -2.9124980468 1.6169614371 -0.0530926658
 H -4.2759316489 0.172425883 0.8690093904
 H -4.5133458006 0.365980404 -0.8897671105
 H -3.2640651124 2.3501130374 0.6732418401
 H -2.8367063368 2.0913974204 -1.0386427849
 H -2.3646351555 -2.6048073125 -1.0504313932
 H -4.0624026802 -2.135745626 -1.0119672572
 H -3.2431927468 -2.5568758074 0.5094283336
 H -0.974010121 2.7564776363 1.3760443138
 H 0.1735800638 1.4010368871 1.3983596544
 H -0.0013271627 2.3803873545 -0.0754543955
 N -0.4990494202 -1.0262725327 0.1866739743
 C 0.8811817986 -0.6268685707 0.081119247
 C 1.2879792881 0.0427712477 -1.0560883024
 C 1.7429344601 -0.9651209089 1.1384170429
 C 2.6653142424 0.4726772669 -1.1685286716
 H 0.5756655749 0.2524551866 -1.8486742194
 C 3.151194935 -0.632252754 0.9842773483
 H 1.3671427724 -1.4584002347 2.0275839793
 C 3.5206765301 0.0709924953 -0.1363902858
 H 3.0420653919 0.993961071 -2.03988299
 H 3.8863689301 -0.8930712546 1.7375502569
 H -0.6823534423 -2.0201267866 0.2058044577
 F 4.8500532678 0.4137321366 -0.2665982404

4_H_rad

31

1 2

C 1.6606761837 0.2592815927 0.654184068
 N 1.7330219713 1.2237065659 -0.4116711158
 N 1.9413169971 -1.0071753848 0.0234020252
 C 2.011844288 2.585081346 0.0130994306
 C 2.6134922083 0.6724529158 -1.4563391529
 C 2.2292833514 -2.0924587822 0.9464503109
 C 3.0151623582 -0.7038039333 -0.9204978914

H 3.4893062962 1.310563198 -1.6106052087
 H 2.071813983 0.6004765583 -2.4053666192
 H 3.9911827891 -0.6540358124 -0.4098228878
 H 3.0695099965 -1.4725582399 -1.6942419873
 H 1.9402199547 3.2508846037 -0.8492215341
 H 3.0129957609 2.6935940561 0.4610298594
 H 1.2639575287 2.9040903463 0.744412177
 H 2.4039873018 -3.0057738404 0.374320432
 H 3.1178302352 -1.8890874491 1.5666831156
 H 1.3717261706 -2.2613764473 1.6029288971
 H 2.3517778755 0.4882244953 1.4899511733
 N 0.3303864263 0.2517954423 1.2965699321
 C -0.8489152906 0.0591579755 0.7050260021
 C -0.9673818376 -0.2118972048 -0.6992845062
 C -2.0316517161 0.1263726764 1.5162393749
 C -2.2081138106 -0.4049152892 -1.2488326704
 H -0.0763986621 -0.2693577904 -1.3052884493
 C -3.2651768014 -0.0667859411 0.9564322792
 H -1.938113635 0.3333722586 2.5767154409
 C -3.3363998392 -0.3294880579 -0.4202289226
 H -2.3313976752 -0.613264199 -2.3044995782
 H -4.1725146909 -0.0209641503 1.5457230583
 H 0.3226689203 0.4281234031 2.2952334913
 F -4.5331136381 -0.5165969118 -0.9640815441

5_rad

26

O 2

C -0.6357090841 0.234273427 0.155176986
 N -1.5478269553 -0.7557925135 0.5791799744
 N -1.3586567095 1.2494934047 -0.5093788582
 C -1.161446649 -2.1503106421 0.5423727852
 C -2.8663976222 -0.415616899 0.0479497992
 C -0.822812386 2.5978038577 -0.4341082406
 C -2.754784835 1.094761217 -0.1130683185
 H -3.6638417153 -0.7198799239 0.7297771677
 H -3.0300766663 -0.8998973363 -0.9289830428
 H -2.9536561436 1.6043560735 0.8441892706
 H -3.4263457595 1.4998042639 -0.8732240074
 H -1.0662861194 -2.5324472725 -0.4863505533
 H -1.9185239641 -2.74103078 1.0637721832
 H -0.2075503987 -2.2875908546 1.0560421072
 H -0.8985484162 3.0141657656 0.582933841
 H 0.2279589918 2.5901256063 -0.7326832653
 H -1.3725472786 3.2442232683 -1.122930249
 N 0.5826637357 -0.1352637328 -0.465097671
 H 0.6151886689 -0.2405313902 -1.4745301404
 C 1.7512432552 -0.289843777 0.2099465709
 O 1.8997925382 -0.1879132386 1.4183197038
 O 2.7464823418 -0.5896779709 -0.6453757236
 C 4.0352974592 -0.7995815637 -0.0603018877
 H 4.3781084539 0.1039905839 0.4474705758
 H 4.0045049742 -1.6307274408 0.646897057
 H 4.694905284 -1.0370491321 -0.8928990643

5_H_rad

27

1 2

C -0.824726271 0.1827922711 -0.8579367058
 N -1.2475116079 1.2463225883 0.0231760631
 N -1.3269109083 -1.0152739545 -0.1688730389
 C -1.288054415 2.5538028587 -0.6148820329
 C -2.5016972825 0.811825264 0.6279347873

C -1.0116468657 -2.3575427057 -0.5557776214
 C -2.2296501641 -0.6644247911 0.8990571933
 H -3.359004741 0.923697146 -0.0542336984
 H -2.7021127374 1.3688733111 1.5433999791
 H -3.1037093166 -1.3190667202 0.8842865885
 H -1.6862871946 -0.822024726 1.8407425096
 H -0.302273843 2.7931388242 -1.0194767524
 H -1.5386175201 3.3038837973 0.1371270595
 H -2.0318474642 2.6005787247 -1.4263057098
 H -0.6668080359 -2.9038220947 0.3270891613
 H -1.9271935099 -2.8355137163 -0.9226240854
 H -0.2458590854 -2.3509705699 -1.3287911711
 H -1.3246568607 0.1967389296 -1.8464907025
 N 0.575396874 0.1128185216 -1.0979046062
 H 0.9353310134 0.3875553208 -1.9996872576
 C 1.4523945168 -0.1661743408 -0.0810101655
 O 1.1053560777 -0.587792706 1.0089866512
 O 2.7072009175 0.0486975926 -0.4643532212
 C 3.7270996078 -0.291037857 0.4896384322
 H 3.6718054536 -1.3519896673 0.7378052349
 H 4.6677926108 -0.0637891764 -0.0064429282
 H 3.6147577517 0.3121988758 1.3914290373

6_rad

23

O 2

C 0.108115249 -0.2947714107 -0.0449086357
 N -1.2282289464 -0.4484233674 -0.1860696642
 N 0.4206549788 1.0057278175 0.1834867817
 C -1.9287152633 -1.7127958751 -0.0484099439
 C -1.9006270569 0.7914510719 0.1980021199
 C 1.6864121732 1.6437655999 -0.1638113709
 C -0.7917985746 1.8166412441 0.0077763114
 H -2.2284672063 0.7332762202 1.2435978614
 H -2.7666802001 0.9740155463 -0.4392852365
 H -0.8208656847 2.6237297467 0.7403231626
 H -0.8068147569 2.2443584964 -1.0026729811
 H -1.5270909425 -2.4534289118 -0.7462416764
 H -2.9810198685 -1.5381432013 -0.2833415205
 H -1.8396715807 -2.1150010775 0.9693383596
 H 1.5818989102 2.7048940895 0.0632102712
 H 2.5088387301 1.256656354 0.4333030913
 H 1.9138197374 1.5340112761 -1.2295971054
 N 0.9498865259 -1.3088629154 -0.1165789331
 C 2.3691514437 -1.3089665682 0.1842024525
 H 2.5683959917 -0.8868975832 1.1718111341
 H 2.6679384873 -2.3647072272 0.1903096864
 H 2.9574545888 -0.7865851424 -0.5724973784
 H 0.559829265 -2.2701041824 -0.3063657862

6_H_rad

24

I 2

C 0.1847855874 -0.1913466044 -0.6492589264
 N 0.7970856306 0.873828273 0.1235942535
 N -1.2258584571 -0.0919883287 -0.1836508281
 C 2.0934334987 1.2858444645 -0.3902798634
 C -0.192321272 1.9375237702 0.2253203674
 C -2.21794342 -1.0855816733 -0.4489806969
 C -1.4732088031 1.1525890373 0.4936379739
 H -0.2879009308 2.5137921698 -0.7093092332
 H 0.0502253108 2.6216721053 1.0389929849
 H -2.3972080462 1.6071312589 0.1265667101

H -1.6054485537 0.9239385785 1.5611359911
 H 2.7674907067 0.4264232156 -0.4164688467
 H 2.5201092487 2.0341867571 0.2801715805
 H 2.0247235496 1.7139941588 -1.4034155815
 H -2.8563097167 -1.2025784859 0.4298311718
 H -2.8425017043 -0.7342514133 -1.2817352655
 H -1.7211284841 -2.0171435009 -0.7169491537
 H 0.1368155453 0.0311622091 -1.7353217816
 N 0.6932045815 -1.4976828041 -0.4890563218
 C 1.1209617625 -1.9051302304 0.8455322233
 H 1.3860580036 -2.96263673 0.8086663928
 H 1.97475583 -1.3328930756 1.2252886311
 H 0.2915264943 -1.7889348698 1.5487214698
 H 1.3356016381 -1.7542892818 -1.2247292515

7_rad

24

O 2

C -0.0000132017 -0.6853643941 -0.0495893732
 N -1.1828166023 -1.3806882745 0.3170201022
 N 0.0000071478 0.6924267402 0.3056728463
 N 1.1827667631 -1.3807175347 0.3170422928
 C -2.4628106289 0.6756148812 0.3404476933
 H -2.5217813904 0.6899996641 1.434284351
 H -3.3466244078 1.1856301327 -0.0540858471
 C -2.4235194283 -0.7639906338 -0.1515531261
 H -3.2634948709 -1.3388361451 0.2461653366
 H -2.4924018336 -0.7753033187 -1.2519269091
 C -1.2062954915 1.4028261585 -0.1180711526
 H -1.1663295216 2.4104164399 0.306606598
 H -1.2238713343 1.5073219997 -1.2191527752
 C 1.2063290644 1.4027859804 -0.1180878725
 H 1.223893164 1.5072757086 -1.2191698863
 H 1.1664000926 2.4103791873 0.3065863628
 C 2.4628284039 0.6755393446 0.3404199453
 H 3.3466513497 1.1855222869 -0.0541351678
 H 2.5218175106 0.6899381464 1.4342553876
 C 2.4234859755 -0.7640733424 -0.1515569986
 H 2.4923554527 -0.7754091675 -1.2519310415
 H 3.2634463239 -1.3389389037 0.2461643477
 H -1.1278801697 -2.3474998674 0.0167010015
 H 1.1277986327 -2.3475410886 0.0167698849

7_H_rad

25

I 2

C 0.0152936393 -0.7070969595 0.1416520284
 N -1.1663825549 -1.3493903834 -0.1646618833
 N -0.0039757175 0.7433599686 -0.2921071911
 N 1.1764323773 -1.4039562426 -0.158174475
 C -2.4745388294 0.6987300786 -0.2838099664
 H -3.3587393299 1.209986195 0.102812784
 H -2.5336189181 0.7155737278 -1.3773650508
 C -2.4384708226 -0.7366556955 0.2208359056
 H -2.5630373239 -0.7559537 1.3117018712
 H -3.2416412895 -1.3227401394 -0.2270011223
 H -0.0133650593 0.763184804 -1.320997296
 C -1.2402613733 1.4492847637 0.1841135244
 H -1.1780736428 1.4770297557 1.2746883395
 H -1.1989801234 2.4674676167 -0.2046281043
 C 2.424377378 -0.7496758962 0.2315318999
 H 3.254214247 -1.3392573022 -0.1603223712
 H 2.4923489627 -0.7610746852 1.3244784508

C 2.4818693072 0.6882253425 -0.2806364533
H 3.3599530464 1.2055205206 0.1147501643
H 2.558144787 0.6980163125 -1.3739227798
C 1.2431319035 1.4493855957 0.164420888
H 1.1810848748 1.5043009936 1.253973468
H 1.2037680593 2.4584910724 -0.2477549642
H -1.1084339927 -2.3441671158 0.0139255647
H 1.1979003948 -1.7905886276 -1.1005032309

8_rad

27

O 2

C -0.0008290515 0.4167458113 -0.044140007
N -0.3189903928 -0.8906097865 0.016755572
N 1.2818355046 0.8216204887 0.0384971841
N -0.9604758793 1.3396081237 -0.1682582841
C -1.7097091197 -1.3488853507 -0.0538235279
H -1.9390420381 -1.6454725932 -1.0845892975
H -1.7862688854 -2.2386277574 0.5761607118
C -2.6692549639 -0.2742748517 0.4275318749
H -2.5554735602 -0.1347385539 1.5074905004
H -3.6969803769 -0.5895676937 0.2335916231
C 2.0191270665 -1.46754827 -0.4149401152
H 1.94391945 -1.3688688964 -1.5025882728
H 2.7983585823 -2.1993059501 -0.193100671
C 0.6943407113 -1.9365769155 0.1521665488
H 0.3332066032 -2.8110052131 -0.3946389353
H 0.7928110953 -2.2155426809 1.2084551349
H -0.7372895651 2.3276336352 -0.4216647184
C -2.3704241334 1.0214719663 -0.2989006302
H -2.6386210897 0.9382719118 -1.3603075176
H -2.9276555438 1.8710303568 0.1122439806
C 2.3819293075 -0.1295730356 0.1987953748
H 3.2571158917 0.2908966486 -0.3002958377
H 2.6200132913 -0.2401904915 1.2644541527
C 1.5945541249 2.2410466352 0.1523625676
H 1.4090480985 2.7720089328 -0.7887252628
H 0.9934977782 2.719163306 0.9347798967
H 2.6489580944 2.3375622242 0.4126039549

8_H_rad

28

1 2

C 0.1045627737 0.4279778581 0.8650532995
N -0.3915465726 -0.9703598145 0.6572541492
N 0.9993769875 0.6700189799 -0.2583468318
N -0.9632086888 1.3502495416 0.9307106008
C -1.7578210013 -1.1536631439 0.2326301289
H -2.3874765439 -1.0773105021 1.1320168396
H -1.8664305043 -2.1610581307 -0.1693230902
C -2.1277166399 -0.0655123576 -0.7800379416
H -1.5096420592 -0.2034090491 -1.6699756774
H -3.1695922467 -0.2165688169 -1.0691357807
C 1.6175066428 -1.7162533727 -0.4014467719
H 2.443697124 -2.4227449207 -0.2970200712
H 1.1547137868 -1.8654523955 -1.3805214699
C 0.5838569742 -2.0245988806 0.7026000475
H 1.073004869 -1.985908532 1.6835129804
H 0.0972393089 -2.9899241913 0.5705888133
H 0.6272737967 0.4137519462 1.8376744837
C 2.1135794929 -0.2845108541 -0.2612203884
H 2.717986757 -0.1833398427 0.6585186394
H 2.7589707779 -0.040587144 -1.1076294835

C -1.9197712545 1.3397730796 -0.1836274224
H -2.8593207729 1.7330477413 0.2077011142
H -1.5791143774 2.0235350173 -0.965973585
H -1.4081912819 1.3328350112 1.8381374047
C 1.4824519895 2.0507049522 -0.2793471112
H 0.6446846107 2.7440057237 -0.3378358905
H 2.1076785587 2.1791779689 -1.1649363284
H 2.0793444931 2.2955071281 0.6140383431

9_rad

30

O 2

C -0.0508031868 0.2843715398 -0.2607564716
N 1.1080541837 1.1051821698 -0.1751166702
N 0.0788962003 -1.0205782343 0.308373494
N -1.2535463868 0.9745724807 0.0213662102
C 2.5239193845 -0.9220136454 -0.0675514809
H 2.7966662907 -0.7917861855 0.985372701
H 3.3490074343 -1.4485256025 -0.5579034258
C 2.2839503505 0.4354740757 -0.7265936632
H 3.1490331214 1.0950981193 -0.6079943905
H 2.1195329557 0.2935004323 -1.8019952828
C 1.2527488727 -1.752114148 -0.1765825781
H 1.3382643222 -2.6698805325 0.4135976811
H 1.099865482 -2.0505270483 -1.2306599768
C -1.1118367711 -1.8596666685 0.2470644428
H -1.3071964196 -2.1836329749 -0.7927132023
H -0.9204001483 -2.759697375 0.8395179146
C -2.3152942844 -1.1030095598 0.7761659446
H -3.2164575441 -1.7153933857 0.6797377582
H -2.1738152689 -0.8703563182 1.8373100336
C -2.4752890392 0.1784722917 -0.0208939329
H -2.7378398104 -0.0698282745 -1.0667050736
H -3.2881807335 0.7895291579 0.3827895831
C -1.4199381996 2.2261336276 -0.7065309679
H -2.2803523859 2.7592998407 -0.2935072573
H -0.5341946501 2.8512462848 -0.6035061705
H -1.5986505197 2.0529717067 -1.7813031733
C 1.3458830537 1.6926119296 1.1494144984
H 0.4723943491 2.2744860136 1.4512346817
H 1.538280997 0.9408104029 1.9297121892
H 2.2063973507 2.3651568799 1.0909975849

9_H_rad

31

1 2

C -0.0320150143 0.2892024895 -0.2767386458
N -1.281315865 0.847712482 -0.0655637117
N 0.1147155741 -1.1229440249 0.2659434762
N 1.0762824364 1.0965039178 -0.0227689637
C -2.3203826118 -1.3143190684 0.4914434633
H -3.1820309946 -1.9500950771 0.2776739162
H -2.2735280254 -1.1730371604 1.5763336558
C -2.4782670777 0.0190643435 -0.2142816556
H -2.6895834149 -0.1404454538 -1.2828329151
H -3.3145794231 0.5781514853 0.2102463377
H 0.2193760329 -1.0684562143 1.287612497
C -1.0677277935 -2.0001462882 -0.0068375168
H -1.1010034106 -2.1544490934 -1.0880703935
H -0.8817847368 -2.9547091283 0.4865205095
C 2.3155678112 0.5429513508 -0.5696893132
H 3.1361030038 1.2193619125 -0.3206509506
H 2.2257757384 0.5115739324 -1.6604939965

C 2.5800095647 -0.8617752203 -0.0279808975
H 3.4437321961 -1.3118750706 -0.5241073956
H 2.8045644069 -0.8308492745 1.0435102843
C 1.37200312 -1.7468265453 -0.2852593384
H 1.1970782288 -1.8745948404 -1.3561485367
H 1.4681468843 -2.7276308638 0.1824160594
C -1.4806889577 2.2055213843 -0.5695651678
H -0.5741800416 2.794165092 -0.4511782237
H -1.7543995488 2.1873709894 -1.6329094097
H -2.2901163286 2.6706228738 -0.0034552758
C 1.2069729542 1.6689147588 1.3265796557
H 1.9181831103 2.4968837037 1.2891578636
H 0.2411972731 2.0546134231 1.6556874064
H 1.5608949092 0.943539185 2.0734071827

10_rad

31

O 2

C -0.0001110132 -0.0000649611 0.076482661
N 0.5939660063 -1.2494148367 -0.2731412241
N 0.7849989991 1.1391089884 -0.2734478261
N -1.3789941942 0.1103083663 -0.2744619716
C -0.1747160671 -2.4239372293 0.1299961738
H 0.3236449813 -3.3042840384 -0.2860973245
H -0.1722829964 -2.5302795252 1.2310367689
C -1.603269781 -2.3267468776 -0.368234988
H -2.1876225291 -3.1742499212 0.0018453087
H -1.6200924669 -2.3526229148 -1.4631019233
C 2.8163264275 -0.2252786035 -0.3681051735
H 2.8461171968 -0.227915245 -1.4629810998
H 3.8427155865 -0.3073817527 0.0013202873
C 1.9900444733 -1.3947488943 0.130050684
H 2.3582950681 -2.3369436406 -0.2860778134
H 2.0709188697 -1.4638515368 1.2310944336
C -2.2032900435 -1.0260446122 0.1283342555
H -3.2029360661 -0.8739954036 -0.2889627637
H -2.3047569762 -1.0608676254 1.2292825895
C 2.1865643792 1.0608701584 0.1294432325
H 2.6995612983 1.932485204 -0.28727721
H 2.2775973365 1.1168244983 1.2304436338
C 0.2131087415 2.4209075863 0.1300419377
H 0.2331547179 2.5254966436 1.2310681919
H 0.8449497699 3.210731685 -0.2864270646
C -1.212977351 2.551925649 -0.3674034075
H -1.6550057127 3.481492678 0.0030530105
H -1.2260879046 2.5801029385 -1.4622325789
C -2.0118072262 1.363024252 0.1295012784
H -2.1054874199 1.4130237855 1.2305607317
H -3.0232521039 1.3720661852 -0.2868898094

10_H_rad

32

1 2

C -0.0044459547 0.0223879589 0.2047978563
N -1.2977281795 0.4634308303 -0.1109008573
N 1.0627906335 0.8746502768 -0.1139945148
N 0.2375824825 -1.3669742069 -0.3157022872
C -2.3938100789 -0.4146096195 0.3044409116
H -2.4564836322 -0.4654584521 1.4025127451
H -3.3214000262 0.0262414092 -0.0652471549
C -2.2014511595 -1.7998156096 -0.2834003878
H -2.3009043461 -1.7656211476 -1.3731842348
H -2.9617950221 -2.4840670509 0.0998585428

C -0.4810263153 2.751401528 -0.4044304276
H -0.6621483606 3.7940323163 -0.1321162335
H -0.4707360465 2.6799784543 -1.4965930964
C -1.5794892256 1.8742083278 0.1625971053
H -1.6785499559 2.0402333634 1.247347429
H -2.5417773213 2.1063197929 -0.2991803419
H 0.2311424387 -1.3198528056 -1.3442296273
C 0.8515569089 2.2980521758 0.1578990551
H 0.8929512621 2.4893237376 1.2422240674
H 1.6768989886 2.8412198627 -0.307804888
C -0.8391702988 -2.327507815 0.1071850367
H -0.7487663775 -2.4277587463 1.1912981178
H -0.6089926858 -3.283578308 -0.3635535559
C 1.5747025862 -1.9072998891 0.1098315457
H 1.6814495575 -2.8856636827 -0.3595701032
H 1.5224931799 -2.0313383277 1.1939990138
C 2.6788622022 -0.9508700165 -0.2816037838
H 3.6253120517 -1.336856807 0.1036485693
H 2.7620831519 -0.8886047252 1.3715345558
C 2.3914249928 0.4197303415 0.3018571346
H 2.4680207169 0.3967613223 1.3999946787
H 3.1154038332 1.1469055118 -0.0704457589

11_rad

21

O 2

C 0.9305217333 1.4533723412 -0.1849833964
N -0.2783702686 0.6713313525 0.0077591834
C -0.2708332277 -0.6654833712 -0.0788323426
N -1.5237408803 -1.1618787374 -0.1289180888
C -2.4638069983 -0.0816778774 0.2073074649
C -1.644235313 1.1663868059 -0.1488392855
H -1.8151715548 1.4880048493 -1.1837264521
H -1.8302849907 2.0033317199 0.5257436466
H -3.3764192697 -0.1666859296 -0.3823457769
H -2.7114973399 -0.1035427696 1.2735972552
N 0.8409736305 -1.3766322013 -0.1090764981
C 2.1592117522 -0.7461439575 -0.1801707701
H 2.491504153 -0.7294283026 -1.2237490904
H 2.8535317815 -1.3671166253 0.3904586387
H 0.8063802724 2.4039829315 0.3383947779
H 1.0754439837 1.6644264384 -1.2527462229
C 2.1103861937 0.6701428758 0.3876195418
H 2.0167220568 0.6265732041 1.4774285521
H 3.0420549602 1.1880207449 0.1471679113
H -1.6476737958 -2.1292238556 0.2068292885
H 0.7311311214 -2.4025746362 -0.0166463366

11_H_rad

22

1 2

C 0.2884715296 -0.775434643 0.4000083881
N 1.5482075489 -1.2076990275 -0.1400336303
C 2.4637338102 -0.0826013858 0.0830266743
C 1.5955959892 1.1715399612 -0.124639402
N 0.2784470488 0.6912523223 0.1852151161
C -0.9126112976 1.4778085387 0.3441537351
H -0.743002953 2.4641365969 -0.0893200909
H -1.0594721845 1.5941415165 1.4299440849
H 1.8349990874 2.0386467056 0.4989859589
H 1.5827201007 1.5010303051 -1.1751000683
H 2.842242549 -0.1105441663 1.1082370587
H 3.3021560276 -0.1257370636 -0.6099765908

H 0.2829982567 -0.8727091911 1.5021847772
 N -0.8535862216 -1.3667378721 -0.2429954076
 C -2.1120029841 -0.7274259625 0.1666189274
 H -2.2684595265 -0.7926961259 1.2544558785
 H -2.928350272 -1.2594519018 -0.3250773666
 C -2.1046426845 0.7319538357 -0.2687785328
 H -2.0469585236 0.7958076293 -1.359315369
 H -3.019249687 1.2314567705 0.0580444706
 H -0.8722833489 -2.356420854 -0.0120242545
 H 1.4243357351 -1.3582229883 -1.1406393568

12_rad

24

O 2

C 0.2163379506 -1.8702350662 0.0991527643
 N -0.6403719582 -0.8718709258 -0.5558049067
 C -0.2363429956 0.4901137827 -0.4854925728
 N -1.1516393151 1.1705481386 0.3931498148
 C -2.4417985983 0.5395693925 0.1025134467
 C -2.0378524645 -0.9255737843 -0.0948628636
 H -2.0897943941 -1.4647037138 0.8603504941
 H -2.6827529586 -1.4411061421 -0.8121126882
 H -3.1435068634 0.6698570652 0.9289017995
 H -2.8957842575 0.9444586844 -0.812438779
 N 1.138843154 0.7740518554 -0.4606717882
 C 2.000452767 -0.161013268 0.2689119359
 H 1.8618121471 -0.0626311618 1.3612888442
 H 3.0402479573 0.0937932514 0.041509323
 C 1.4678030232 2.1675625823 -0.22346029
 H 1.2837425592 2.4783736428 0.8184994418
 H 0.8812331589 2.8109308062 -0.8860603071
 H -0.0669070459 -2.8619330214 -0.2674458636
 H 0.0449414432 -1.8590662144 1.1908557632
 H 2.5273375058 2.3291686746 -0.4428326713
 C 1.6843073246 -1.5834501565 -0.1652735801
 H 1.9140086291 -1.7048129671 -1.2304286758
 H 2.2994549206 -2.2928518617 0.3961419669
 H -1.1769826893 2.173638407 0.2391373918

12_H_rad

25

1 2

C -0.2079959915 0.4284219959 1.2157952311
 N -1.2770813615 1.3548678515 1.0646745083
 C -2.1086341101 0.9337509175 -0.0852740633
 C -1.5846306748 -0.4536256358 -0.5126298545
 N -0.6239160948 -0.7823186394 0.5182183227
 C 0.2759965194 -1.9129921407 0.4476636607
 H -0.2032419828 -2.7014789712 -0.1358868778
 H 0.4468998223 -2.2707390064 1.4694036878
 H -2.3614836925 -1.223655112 -0.5280946932
 H -1.1098739709 -0.4335982288 -1.5041433942
 H -3.1556720625 0.8909398007 0.2171233598
 H -2.0157234434 1.6451302442 -0.9087768992
 H 0.0702337534 0.2256903864 2.2503497101
 N 0.9983885493 0.7966126043 0.4657395979
 C 2.0547804761 -0.2000402327 0.540320859
 H 2.2514368625 -0.4116901664 1.5975628654
 H 2.9559001182 0.2158220621 0.0851578251
 C 0.9058980382 1.5930191914 -0.7406764078
 H 1.8991557091 1.9924931723 -0.9552958168
 H 0.2099688302 2.4163374836 -0.58383276
 H 0.5839877128 0.9983464042 -1.6087349132

C 1.6155149546 -1.4858403157 -0.1764581734
 H 1.4901142936 -1.2953957433 -1.2470432924
 H 2.3638621511 -2.2732550571 -0.0528068022
 H -1.821182406 1.3875571352 1.9181253199

13_rad

27

O 2

C 1.4825902561 -1.517134225 0.3328128376
 N 0.2153923832 -1.1475301422 -0.2712662734
 C -0.1964730472 0.1867815594 -0.0335272853
 N -1.5733934232 0.2956049586 -0.3837766239
 C -2.4247387722 1.0059035228 0.5717285062
 H -2.5365221022 0.4595082626 1.5216004907
 H -2.0105177445 1.990643533 0.7928841298
 H -3.4157692994 1.1471347466 0.1302186771
 C -2.0364615724 -1.0851667751 -0.6520509004
 C -0.9556872231 -1.9744873164 -0.037451702
 H -1.1321079452 -2.1442364524 1.0386249788
 H -0.8606224891 -2.941493945 -0.5375189617
 H -3.024311308 -1.2529232127 -0.2180363828
 H -2.0963485593 -1.2543896489 -1.7326531944
 N 0.7408143058 1.1622461119 -0.4611248983
 C 2.0664379638 0.9220310855 0.1210161749
 H 2.0485740556 1.1269984052 1.2068261973
 H 2.7653418908 1.6288116064 -0.3358888828
 C 0.3312733792 2.5509180102 -0.3385359539
 H 0.2079424964 2.869473865 0.7107529041
 H -0.6084242873 2.7144110916 -0.8702541871
 H 1.746923663 -2.5285318044 0.0099277006
 H 1.4088174515 -1.5202803615 1.4355630148
 H 1.0973834298 3.1807737261 -0.799006398
 C 2.5338568837 -0.5100025324 -0.1256626652
 H 2.7242029878 -0.6512352746 -1.19562349
 H 3.4739286262 -0.6793787941 0.4084381874

13_H_rad

28

1 2

C -0.1711311805 0.1357053023 0.3597727977
 N -1.6055707635 0.2426335237 0.0451303911
 C -2.373799058 1.4252377087 -0.2007850105
 H -2.3191768679 2.0830033042 0.67394424
 H -1.9522852565 1.9506284692 -1.0654217147
 H -3.4067313519 1.1422068661 -0.3959867896
 C -2.2062884803 -1.0726449523 0.0432536413
 C -1.0400151409 -1.9950358564 0.3724438216
 N 0.0817896166 -1.2085885114 -0.1147951148
 C 1.4188141895 -1.6932653221 0.1852788036
 H 1.5127413892 -2.7041890932 -0.218854089
 H 1.590692306 -1.7396167809 1.2754154009
 H -0.9821443442 -2.1780590829 1.4575120198
 H -1.1038263707 -2.9490609586 -0.1515164193
 H -3.0423102857 -1.0889469463 0.7504183567
 H -2.6110607161 -1.2387251873 -0.9647927371
 H -0.1477390087 0.1973628573 1.4794176361
 N 0.7152715244 1.1160642111 -0.2195359494
 C 2.1177193499 0.6846130023 0.0015231765
 H 2.360391842 0.7608365778 1.0763302793
 H 2.7521588058 1.3975810334 -0.5299665504
 C 0.5661684793 2.4498892505 0.3753969746
 H 0.6324496132 2.4219646025 1.4749167813
 H -0.3705602928 2.9233383216 0.0884960276

H 1.3748934916 3.0792661507 -0.0014122617
C 2.3973939834 -0.7328716054 -0.4709835798
H 2.2998443667 -0.7974647484 -1.5597554971
H 3.4252391601 -0.9949301364 -0.2041546349

14_rad

28

O 2

C 0.0023465846 0.1433894137 -0.0338858373
N -1.1216147056 0.9213483419 -0.3652095462
N -0.0273580254 -1.2295091193 -0.3425376234
N 1.1355462663 0.8838537802 -0.4153239431
C -0.7385015288 2.2976063191 -0.0416384365
H -1.1672058374 2.9947099025 -0.7659123244
H -1.0942261911 2.579688926 0.960309801
C -2.4867491186 -1.0655685265 -0.2500526763
H -2.6078594475 -1.1286324447 -1.3368862963
H -3.372325788 -1.5113594141 0.2121140664
C -2.3730424257 0.4038933099 0.1592969736
H -3.2023159009 0.9863039404 -0.2525401228
H -2.406669947 0.4956084196 1.2607385387
C 0.8132659841 2.2718551685 -0.0762297671
H 1.232200602 2.9548262433 -0.8194502784
H 1.2224342267 2.5413088203 0.9086553786
C -1.2478771184 -1.8556035646 0.1720667696
H -1.2952082669 -2.8780957767 -0.2142217154
H -1.2085062831 -1.9143043475 1.2753188548
C 1.1936111197 -1.8961825956 0.1170871385
H 1.2019951613 -1.9544542781 1.2210377046
H 1.1895659448 -2.9193722283 -0.2702343674
C 2.437783334 -1.1473623161 -0.36088194
H 3.3279867088 -1.6227422498 0.0611636722
H 2.5076535561 -1.2133965947 -1.452034653
C 2.3914869693 0.3246723759 0.0523742755
H 2.4778760235 0.4141556362 1.1511266459
H 3.2202011031 0.8796408585 -0.3967902915

14_H_rad

29

I 2

C 0.0560285264 0.1215961627 0.3656494473
N 1.1011762169 0.9209602125 -0.2050507628
N -0.0117133431 -1.1956532836 -0.1914787957
N -1.1237661909 0.9235538423 0.138195579
C 0.7632066684 2.2880188305 0.171220621
H 0.9694361646 2.5018566993 1.2321825899
H 1.2934986472 3.0097503549 -0.4495781591
C -0.7510970233 2.3021639076 -0.088993827
H -0.9931066508 2.5353140853 -1.1353728042
H -1.3387558752 2.961781612 0.5548687425
C 2.4440332311 -1.0827213462 -0.3393595597
H 3.3612257674 -1.5611897518 0.0140636969
H 2.4581009222 -1.0924427367 -1.433367918
C 2.4054556567 0.370767403 0.1455456441
H 2.5725008169 0.4198134708 1.2364138541
H 3.1821006782 0.9632297631 -0.3425845097
H 0.1292554119 0.0755777751 1.4900048135
C 1.2375874361 -1.8877489965 0.1549201526
H 1.3056239445 -2.0418488492 1.2468289896
H 1.2177033873 -2.87226393 -0.3181130134
C -2.4401843457 0.3596100564 0.26983818
H -3.1516323877 1.0108196924 -0.2398243722
H -2.6757930509 0.3812757059 1.3460106453

C -2.4464358116 -1.0847942394 -0.2529177512
H -3.3692420804 -1.5589468381 0.0862445449
H -2.4535416615 -1.0697290532 -1.3456448347
C -1.2337995039 -1.8741747448 0.237800048
H -1.2683634186 -1.9982434706 1.3345494274
H -1.2394801324 -2.8712943338 -0.2077446684

15_rad

35

O 2

C -1.1401257147 -1.6643211801 1.622791296
N -1.7768291831 -1.0290564249 0.4866096156
C -1.1600267947 0.127815629 -0.0930299268
N 0.0450638325 0.6211925327 0.4105212075
C 1.2064661163 0.1546232637 0.082390834
N 1.5944443379 -0.781170004 -0.8588365326
C 0.7847786311 -1.8778884075 -1.3529077315
H -0.2584221959 -1.5761757877 -1.4124616857
H 0.8700952947 -2.7607007301 -0.702050079
H 1.1370115624 -2.1496945867 -2.3517014323
C 3.0269618638 -1.027784592 -0.7403843922
C 3.516961857 0.2613515527 -0.0976808591
N 2.3536754373 0.6480015372 0.6858223248
C 2.3442106164 1.9564173441 1.3028083203
H 3.2585435174 2.0746176542 1.8887579453
H 2.2949478627 2.7613616472 0.5543217503
H 1.4814721498 2.0411184792 1.9634083167
H 3.7486058549 1.0224738997 -0.8590513143
H 4.3936247645 0.11934102 0.5374798498
H 3.4711774955 -1.2166189244 -1.7202053629
H 3.2160180031 -1.8971012838 -0.0924916816
N -2.1875884895 1.0987139382 -0.2961658805
C -3.4346856097 0.3511503893 -0.3736272532
C -3.1982656848 -0.7382759784 0.6611774496
H -3.3983082224 -0.3501925267 1.6744581073
H -3.8134727662 -1.628392474 0.5025373001
H -4.2936243225 0.9863771413 -0.1431087414
H -3.5810160245 -0.0883337496 -1.3764821617
C -1.9630464114 2.0314650947 -1.3839399996
H -1.9690793401 1.5298801465 -2.3677579511
H -2.7438976631 2.7974586056 -1.3758892916
H -0.9954906839 2.520578638 -1.2496625188
H -1.1343135831 -1.0209201873 2.5185919649
H -0.106778394 -1.9287633365 1.3871864379
H -1.678694114 -2.5860643396 1.859592076

15_H_rad

36

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C -2.6847295194 1.8923268834 -1.1580001326
N -2.4147532631 0.6990636376 -0.3803238359
C -1.2176551355 0.3555254242 0.1264962219
N -0.0866635308 1.0197613227 -0.1961492149
C 1.212002727 0.446015367 -0.3786421913
N 2.1466091229 0.5635032978 0.6680800966
C 2.5021268951 1.9002216388 1.1062248808
H 1.5957450207 2.4530683663 1.3640390742
H 3.0524203452 2.4564829839 0.3315012705
H 3.1255029832 1.8278526645 2.0001280927
C 3.2533888278 -0.3137275828 0.2957329116
C 2.5444954862 -1.45312376 -0.4511868514
N 1.2752799446 -0.856270474 -0.8770961413
C 0.7942317551 -1.134290889 -2.2171212708

H 1.4905880101 -0.7768420143 -2.9897182122
H 0.6557112323 -2.2114151082 -2.334156021
H -0.1733296775 -0.6497349412 -2.3691062958
H 2.3563465846 -2.3130367169 0.2010734708
H 3.1251881343 -1.7956476074 -1.3126479611
H 3.7906782215 -0.6545008273 1.183121098
H 3.9616775635 0.2103335321 -0.3651229754
N -1.3227038824 -0.6885255761 0.9483824949
C -2.6916373607 -1.2102725294 0.9044012644
C -3.4699993459 -0.0249875219 0.3297928207
H -4.2554241033 -0.3283355517 -0.3623726555
H -3.9007385648 0.6072097452 1.1151553485
H -2.734237011 -2.0898907408 0.252528919
H -3.0196321087 -1.4887121406 1.9061097981
C -0.2860889631 -1.3638396904 1.7049388323
H -0.6891894519 -1.6024724324 2.6916807457
H 0.0185887761 -2.2863252063 1.2031679988
H 0.58033257 -0.7117978854 1.8190154325
H -1.951859777 1.9957644282 -1.9614804028
H -2.6875500109 2.7940387635 -0.5357355945
H -3.6656218407 1.779351355 -1.6193805674
H -0.2289796537 1.9143347857 -0.6423764479

16_rad

30

O 2

C 0.0000001027 -1.805518807 0.1163258822
N 1.1645124555 -1.0509428616 -0.3208694726
C 1.1210051118 0.3076486868 0.0410288374
N -0.0000003746 0.9802696944 0.2448317888
C -1.1210054944 0.3076479966 0.0410326471
N -1.1645129408 -1.0509427767 -0.3208672559
C -2.4939582661 -1.541805645 0.0312985515
C -3.3278280883 -0.2712998072 -0.1318202707
N -2.410774724 0.761902431 0.3449462239
C -2.7474164282 2.1330602056 0.0136588421
H -2.0044799945 2.8052095857 0.4462764449
H -2.780927339 2.2970583886 -1.076128187
H -3.7252342026 2.3748213675 0.4370990107
H -4.2469406381 -0.2848006456 0.4575356551
H -3.5865198628 -0.1139070064 -1.1919715473
H -2.5275401924 -1.8939177975 1.0739758991
H -2.8112377466 -2.351240012 -0.629182931
N 2.4107743701 0.7619029646 0.3449438425
C 3.3278276204 -0.2712993999 -0.1318225708
C 2.4939579035 -1.5418051809 0.0312968274
H 2.8112376568 -2.3512399672 -0.6291840279
H 2.5275397561 -1.8939166436 1.0739744252
H 3.5865191516 -0.1139069568 -1.1919739833
H 4.2469403266 -0.2848000271 0.4575331234
C 2.7474164167 2.13306037 0.0136550812
H 2.7809274993 2.2970574243 -1.076132141
H 2.0044800738 2.8052103786 0.4462718842
H 3.725234185 2.3748217912 0.4370951397
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H 0.0000010757 -1.9335189215 1.2169929108

16_H_rad

31

I 2

C 2.8114033646 2.146676482 -0.2901464278
N 2.4322653684 0.7458884411 -0.2782516022
C 1.1899059851 0.3013417277 -0.0462205578

N 0.0659933143 1.0162210703 -0.0800580082
C -1.147414122 0.3218652583 0.1702497519
N -2.3688119871 0.8968322401 -0.174313852
C -2.9026273283 1.9417085105 0.6922248992
H -2.1409218304 2.7044178602 0.8676584959
H -3.7477142997 2.419512194 0.1928384878
H -3.2335360955 1.5446189213 1.6622281776
C -3.279688381 -0.2165307691 -0.5130892398
C -2.4845928177 -1.4878572254 -0.1753588467
N -1.1102580945 -1.0061671322 -0.2984365248
C -0.0476848919 -1.8061986085 0.27373997
H 0.1051196248 -2.7002762369 -0.3376876089
H -0.2643381534 -2.1097421686 1.3087992879
H -2.6949965759 -1.8311210067 0.8482095875
H -2.6733620823 -2.3049976825 -0.8729229197
H -4.2028061034 -0.1511315635 0.0676788639
H -3.5316620006 -0.175982061 -1.5765390853
H 0.0818510754 2.0191121909 -0.1982924489
N 1.1707399018 -1.006379667 0.2514123599
C 2.5098856211 -1.5682988564 0.066485596
C 3.3812557651 -0.3060739991 0.1104587349
H 4.2156138305 -0.3437979566 -0.5896696012
H 3.7605978457 -0.1098760796 1.1198212162
H 2.5688268645 -2.0768030274 -0.9022481973
H 2.7495846603 -2.2725423913 0.8629398073
H 2.1338614475 2.7157500018 -0.9296885012
H 2.8162495058 2.5720853643 0.7192358846
H 3.811260589 2.2237461692 -0.717057699

17_rad

33

O 2

C -0.680634087 -2.1492913115 0.3349399236
N -1.5361870667 -1.0702694284 -0.1279873417
C -1.1756500561 0.268567168 0.1147844897
N -0.0000199056 0.8474842307 0.0000191948
C 1.175625162 0.2685996484 -0.1147582819
N 1.5361970338 -1.0702319844 0.1279914453
C 0.6806723096 -2.1492672024 -0.3349573098
H 0.5503501967 -2.1178323591 -1.4307997712
H 1.1850150967 -3.0865368638 -0.0819280029
C 2.9526572964 -1.2008396436 -0.2072730726
C 3.4727535459 0.196088703 0.0977843081
N 2.3480378619 1.0250756949 -0.3159002835
C 2.3624258136 2.4001020456 0.1379929955
H 1.5177916358 2.9391434999 -0.2930966777
H 2.2984828381 2.4736003637 1.2365818577
H 3.2906964171 2.872688428 -0.1925979475
H 4.3799066834 0.4490106455 -0.455712811
H 3.6723952148 0.3068816227 1.1772106134
H 3.0867995334 -1.4418169608 -1.2740641207
H 3.4269827292 -1.9797248437 0.3938138247
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C -3.4727770858 0.195999948 -0.097755367
C -2.9526432381 -1.2009198774 0.2072774168
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H -4.3799350373 0.4488885411 0.4557492103
H -3.6724253214 0.3068059658 -1.1771790138
C -2.362505786 2.4000418308 -0.1379327128
H -2.2985536667 2.4735591703 -1.23651981
H -3.2907942628 2.8725942535 0.1926561243

H -1.5178925578 2.9391022084 0.2931742418
H -0.5503124614 -2.1178745521 1.4307829915
H -1.1849531625 -3.0865688484 0.0818924622

17_H_rad

34

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C 1.2621275388 0.2470670738 -0.174810014
N 0.0665291707 0.7764803746 -0.4350339363
C -1.1767139602 0.2465754974 0.0144998463
N -2.2730529642 1.1046333861 -0.1306955645
C -2.2768403043 2.3437887073 0.6375161709
H -1.3793162268 2.9314853365 0.4348664157
H -3.1403509632 2.9394098028 0.3351766989
H -2.3342607556 2.1503727668 1.7191098626
C -3.4566033539 0.264513339 0.0770036383
C -3.0039244007 -1.1222313967 -0.3954523687
N -1.5342245346 -1.0519829641 -0.3699399376
C -0.807467335 -2.1358761718 0.2726292279
H -1.2507073704 -3.0792222345 -0.0550494836
H -0.8823522216 -2.0806928603 1.3691060201
H -3.3737933803 -1.9100551013 0.2659450498
H -3.3422767951 -1.3368512773 -1.4131526806
H -3.72663803 0.2485077545 1.1434049991
H -4.3043522606 0.6519679621 -0.4909339032
H 0.0497005871 1.7177885353 -0.8080720967
N 1.4579963466 -1.0138310859 0.2705821183
C 2.9135791274 -1.2477534015 0.3209797196
C 3.491667353 0.164853819 0.3202715215
H 4.408881917 0.2503674876 -0.262395418
H 3.669839122 0.5349866309 1.3362756715
H 3.2193382832 -1.8054640698 -0.5718275868
H 3.1767769057 -1.8183937036 1.2111585771
C 0.6488956369 -2.1653520599 -0.1538261118
H 1.1189060425 -3.0388448154 0.3019643167
H 0.715335249 -2.2698511942 -1.2443874368
H 3.521287804 2.6641783796 -0.4913038489
H 1.9459784644 2.7421016034 -1.2700919086
H 2.0665563703 2.8580490079 0.5147808207

18_rad

36

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N -1.1742470611 -1.0416810778 0.5357608013
C -1.1410548524 0.326229993 0.3008969954
N -0.0283953084 0.9688254609 0.0537861469
C 1.1509153092 0.2938364488 0.0204787111
N 1.1831941425 -1.0850928338 0.3759793245
C -0.0419033065 -1.7568636692 -0.0199407276
H -0.1183090594 -1.8313235803 -1.1236975945
H -0.0293728625 -2.7693434692 0.391235319
C 2.3604952148 -1.8104809557 -0.0997159076
C 3.6215257781 -1.0662804394 0.30553243
N 2.3368836994 1.0204240775 0.2815195272
C 2.2919345837 2.425759277 -0.0891951232
H 2.1985717288 2.5666847286 -1.1799897036
H 1.4471839075 2.9166654627 0.3923251712
H 3.2182566668 2.9010965429 0.2435366598
H 3.7196480681 -1.0697531846 1.3965611456
H 4.4982217959 -1.5669635569 -0.1153511154
H 2.3334538656 -1.9152020844 -1.2002086174

H 2.3407840955 -2.8158191333 0.3323470791
N -2.3498424009 0.9909605747 0.4011051399
C -3.35265045 -1.0601179677 -0.558212863
C -2.4760167804 -1.7030746354 0.5092942529
H -2.9527722418 -1.6167918727 1.4934682721
H -2.3177629923 -2.7653553692 0.3112176868
H -2.8553066236 -1.1594851807 -1.5296077695
H -4.3222676633 -1.5597607417 -0.6272349506
C -2.3239314834 2.439360213 0.3988438919
H -2.1306125282 2.8524354105 -0.6022262075
H -3.2964828398 2.8016432212 0.7434074247
H -1.5490611478 2.8009571926 1.0757522041
C 3.5525166256 0.3669670008 -0.1987956688
H 4.4113309314 0.9406377274 0.1615372749
H 3.5858163122 0.3741990114 -1.3051090961
C -3.5535488781 0.4104645836 -0.2088351501
H -4.3812900357 0.5225527582 0.5016660499
H -3.8163102095 0.9794270675 -1.1120950134

18_H_rad

37

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C 2.2927410133 2.4934533661 -0.0566160818
N 2.3405263507 1.0389867305 0.0340128073
C 1.2159866933 0.3213532507 0.1452212476
C 3.6377937313 0.3626457203 0.1420979396
N 0.0282303348 0.9531735098 0.2562305236
N 1.2225179575 -1.018937995 0.1494153255
H 3.9110018556 0.2493962048 1.1976177734
H 4.3807241932 1.0019787231 -0.3344940017
C 3.5665455818 -0.9843853091 -0.557174764
C -1.2324755475 0.300482746 0.3020600071
H 4.5126167454 -1.5159968182 -0.4398397256
H 3.3928016471 -0.8308644719 -1.6262962786
N -1.1377068917 -1.0656418884 -0.0367214185
N -2.3015950748 1.0142941498 -0.2776121889
C 0.007513716 -1.6953046911 0.5833726389
C -3.5148342041 -1.1011973895 -0.5531898883
C -2.3622835167 2.4349024102 0.0481113081
C -3.5927579635 0.3442193732 -0.0857009149
H -4.4596656576 -1.6077612033 -0.3399704298
H -3.3495461499 -1.1304407016 -1.6349593675
H -3.8946615116 0.3852113102 0.9745732216
H -4.3376038801 0.8922199549 -0.6672512229
H 1.5643471656 2.807016865 -0.8085261884
H 3.2724205036 2.8479083073 -0.3716621284
H 2.0573817952 2.9553432222 0.9085562511
H 0.0614646011 -2.7304847224 0.2440640353
H -0.0517762554 -1.6852364623 1.6842210347
H -3.248599808 2.8565997943 -0.4279972108
H -2.4288587815 2.6177936091 1.1317572528
H -1.5001631121 2.9675469018 -0.3597792803
H 0.0517015925 1.910123439 0.5743017192
C -2.3790116081 -1.8191260804 0.1572943334
H -2.2300647851 -2.8201768309 -0.254877417
H -2.6070747018 -1.9197244816 1.2310889731
C 2.4467713348 -1.8142750412 0.0440319409
H 2.7218595727 -2.172714713 1.0426875257
H 2.2267330643 -2.6823807883 -0.5820473515

19_rad

39

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C 0.6608133355 -2.1375951275 -0.3719290432
 N 1.6257461316 -1.1803623349 0.1427141368
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 N -0.0000030796 0.6283764224 0.0000025866
 C -1.2293909347 0.1730519928 -0.0883371644
 N -1.6257358532 -1.180362796 -0.1426909876
 C -0.6608068162 -2.137575404 0.3719967143
 H -0.4719666724 -1.9907652918 1.449984306
 H -1.1134077455 -3.1255924492 0.253642471
 C -2.9761268286 -1.48989204 0.3367060406
 C -3.9969818522 -0.5428587527 -0.2598430916
 N -2.2191157934 1.1143113908 -0.4613524528
 C -1.8305168838 2.5117033813 -0.3712305447
 H -1.6573494942 2.8319072766 0.669485344
 H -0.916544625 2.6921736485 -0.9345733177
 H -2.6366205584 3.1179032767 -0.7923179159
 H -4.0612475789 -0.6950822429 -1.3427112361
 H -4.9822059149 -0.7410281718 0.171682135
 H -3.0146000409 -1.4285061956 1.4392389698
 H -3.1992033543 -2.5236871746 0.0577582377
 N 2.2191198834 1.1143206178 0.4613393445
 C 3.9969905801 -0.5428426466 0.2597774387
 C 2.9761206971 -1.4898819548 -0.3367375245
 H 3.014550827 -1.4284917474 -1.4392720966
 H 3.1992154549 -2.5236764419 -0.0578015703
 H 4.0612924295 -0.6950673891 1.3426433149
 H 4.9822019784 -0.7410056145 -0.1717800702
 C 1.8305189438 2.5117116522 0.3711991316
 H 0.916550961 2.6921906884 0.9345457526
 H 2.636625588 3.1179182244 0.792271795
 H 1.6573446814 2.831900472 -0.6695206692
 H 0.4719714179 -1.9908350533 -1.4499236398
 H 1.113410902 -3.1256086015 -0.2535291049
 C -3.5727130666 0.8824190287 0.0333722744
 H -4.2404384875 1.5921823923 -0.4628703988
 H -3.6319938161 1.0764791995 1.1206786734
 C 3.5727056689 0.8824337485 -0.033422638
 H 3.6319541149 1.0764957222 -1.1207309242
 H 4.2404423186 1.5921992654 0.462802226

19_H_rad

40

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C -2.0614565349 2.563792334 0.4324585595
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 C -3.6482060967 0.6340265245 0.0042946954
 N -0.0517188837 0.9107218683 -0.5095300183
 N -1.4890127259 -0.9365179728 -0.506216076
 H -3.9987091125 0.5300804906 -1.0290186163
 H -4.301450329 1.3409917483 0.5138290433
 C -3.6238310648 -0.7118291266 0.7153779526
 C 1.2179672537 0.2649340026 -0.3510264494
 C -0.4904271174 -1.7221119679 -1.2279310504
 H -4.622171131 -1.1526764936 0.7445291063
 H -3.287937527 -0.5639086349 1.7458231043
 N 1.1597321056 -0.9362147606 0.3961945083
 N 2.2592809248 1.1334843335 0.0287205635
 C 0.6835964721 -2.105907383 -0.3409491256
 C 3.6126750952 -0.9212009498 0.3317369953
 C 2.2077390055 2.5142726741 -0.4214499153
 C 3.6012317576 0.5482467659 -0.1114973413
 H 3.600888739 -1.5849888957 -0.5386633627

H 4.523110421 -1.1418209943 0.8948998686
 H 3.9538325884 0.6449146868 -1.149927691
 H 4.2654116019 1.1436264741 0.5215266775
 H -1.128334407 2.6356786409 0.9946686617
 H -2.8793689995 2.8721489817 1.0829944552
 H -2.0241752413 3.2420029307 -0.4260995861
 H 0.3754736793 -2.8579260677 0.3920365019
 H 1.4645048075 -2.5496882683 -0.9771235619
 H -0.9838863437 -2.6182114895 -1.6072778683
 H -0.1492808437 -1.1431665581 -2.0894093911
 H 3.1014012381 3.0245987912 -0.0583887981
 H 2.188081704 2.6040468147 -1.5196696707
 H 1.3489997488 3.0384514773 0.0049365702
 H -0.0437678302 1.8310333209 -0.9249753344
 C 2.3706282552 -1.1905510273 1.1787231602
 H 2.367338662 -0.5447315795 2.0624122456
 H 2.3378123242 -2.227063247 1.5211857334
 C -2.6851947279 -1.6436849626 -0.0334523465
 H -3.1856086961 -2.0613471905 -0.9132269525
 H -2.3654708872 -2.4753292636 0.6017596294

20_rad

44

0 2

C 0.018212 -3.24091 0.162126
 N 1.152025 -2.51502 -0.383504
 C 1.127412 -1.150127 -0.065656
 N 0.015132 -0.469231 0.105622
 C -1.119101 -1.142166 -0.040802
 N -1.184061 -2.533198 -0.255253
 C -2.44168 -2.991129 0.328562
 C -3.346975 -1.774356 0.154101
 N -2.406283 -0.652323 0.196892
 H -4.082352 -1.710604 0.958466
 H -3.87509 -1.794481 -0.808014
 H -2.315409 -3.223653 1.397094
 H -2.823661 -3.875913 -0.1835
 N 2.433631 -0.676727 0.017211
 C 3.340884 -1.76331 -0.351647
 C 2.492081 -3.004788 -0.082337
 H 2.763422 -3.847809 -0.719641
 H 2.5757 -3.307392 0.972389
 H 3.622749 -1.698178 -1.410841
 H 4.244554 -1.743194 0.260153
 H 0.002978 -4.256646 -0.239375
 H 0.080389 -3.296495 1.266839
 C 2.853821 0.649525 0.089449
 C 4.156846 0.991136 -0.318904
 C 2.020354 1.666415 0.594425
 C 4.60463 2.305801 -0.226012
 H 4.825157 0.237584 -0.719285
 C 2.483517 2.975894 0.671821
 H 1.020555 1.422392 0.924974
 C 3.774696 3.3123 0.265059
 H 5.614018 2.540908 -0.55027
 H 1.821238 3.741855 1.065096
 H 4.127066 4.336337 0.331645
 C -2.848235 0.655877 0.006561
 C -4.224251 0.945159 0.103153
 C -1.963994 1.716177 -0.277162
 C -4.690148 2.244617 -0.070264
 H -4.940641 0.159869 0.312836
 C -2.450622 3.008404 -0.449988

H -0.903876 1.521269 -0.356435
C -3.812014 3.291698 -0.347137
H -5.756507 2.433967 0.010559
H -1.745429 3.805089 -0.669782
H -4.180559 4.303282 -0.481773

20_H_rad

45

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C 0.153726 -3.26844 -0.051564
N 1.264964 -2.426988 -0.465695
C 1.264514 -1.151331 -0.035519
N 0.112851 -0.557038 0.252944
C -1.09442 -1.166959 -0.20306
N -1.095261 -2.566948 -0.309613
C -2.262035 -3.068738 0.43241
C -3.219134 -1.88308 0.396141
N -2.300063 -0.734081 0.351941
H -3.853859 -1.852139 1.281956
H -3.852496 -1.89665 -0.499063
H -1.981828 -3.308166 1.468182
H -2.67566 -3.960351 -0.040491
N 2.494721 -0.634693 0.053268
C 3.456765 -1.617989 -0.482901
C 2.648351 -2.922565 -0.434958
H 2.845156 -3.573389 -1.285878
H 2.825149 -3.471192 0.496947
H 3.725072 -1.338419 -1.50636
H 4.353138 -1.652967 0.134827
H 0.184753 -4.196557 -0.624493
H 0.253162 -3.507996 1.021006
C 2.769769 0.765647 0.128804
C 3.503846 1.249469 1.209445
C 2.318538 1.621956 -0.876326
C 3.788034 2.610487 1.284398
H 3.841261 0.563702 1.979603
C 2.592472 2.984403 -0.783518
H 1.763138 1.224803 -1.72058
C 3.328551 3.477398 0.293011
H 4.360239 2.994428 2.122105
H 2.238252 3.656779 -1.557519
H 3.545226 4.538411 0.359187
C -2.803551 0.555892 0.079333
C -3.945252 1.00281 0.758555
C -2.176331 1.409429 -0.837807
C -4.440889 2.281094 0.525417
H -4.439765 0.357159 1.476309
C -2.672679 2.694246 -1.050076
H -1.317785 1.06479 -1.405531
C -3.805305 3.139264 -0.37304
H -5.326626 2.610846 1.05924
H -2.172963 3.342495 -1.76318
H -4.19147 4.138396 -0.544691
H 0.107593 0.426298 0.496024

21_rad

52

0 2

C -0.0005576404 -3.9944909168 -0.1473233598
N -1.1899488159 -3.2592856541 0.2606351293
C -1.1149779844 -1.8759269727 -0.0102785465
N 0.0268634259 -1.2255805285 -0.2162373232
C 1.1325880876 -1.9091095125 -0.0274095673

N 1.1481988419 -3.2584832425 0.3513093148
C 2.4807747896 -3.7736190023 0.0573287587
C 3.3405901765 -2.5275671546 0.2632073973
N 2.4418870997 -1.4574230498 -0.1628937075
H 4.2468840778 -2.5432367072 -0.3454329741
H 3.6202492311 -2.4140297994 1.3198188675
H 2.5506488067 -4.1226661472 -0.9840264426
H 2.7519460182 -4.5902218503 0.7283213518
N -2.3979777107 -1.3887490483 -0.2861030064
C -3.3476014493 -2.4942845488 -0.1565281113
C -2.4584249462 -3.7271124919 -0.291569002
H -2.8441736863 -4.5869099985 0.2590439858
H -2.3469337984 -4.0028763663 -1.3516979035
H -3.8484691998 -2.4607847421 0.8207835233
H -4.1064180347 -2.4645507066 -0.9412927662
H -0.0182898229 -4.9939508708 0.2932596255
H 0.043961756 -4.0933199799 -1.2500921077
C -2.8285500015 -0.067679779 -0.1102999356
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C -1.9302614896 0.9947781752 0.1154814695
C -4.6585544331 1.5460473857 -0.0151980323
H -4.9303652358 -0.5414648979 -0.3341891359
C -2.3933787236 2.2929934018 0.2698044447
H -0.868344139 0.797304286 0.1639532886
C -3.7579727957 2.5864677892 0.2045939943
H -5.726030311 1.7248725785 -0.0680578065
H -1.6892340003 3.100935687 0.4442167479
C 2.8634849777 -0.1251059041 -0.242118802
C 4.138879102 0.2395788661 0.2046332075
C 2.0492417003 0.875947998 -0.8064529572
C 4.5953187671 1.5559354601 0.1023866943
H 4.8016399358 -0.4958583541 0.6461652987
C 2.4988132966 2.1838813562 -0.8955144001
H 1.0644970561 0.6211936106 -1.1734648628
C 3.7736798801 2.5398975257 -0.4435495937
H 5.5907041502 1.7872978626 0.46255601
H 1.8622001609 2.948382793 -1.3301019491
O -4.105568449 3.8981464397 0.3670901074
C -5.4814949956 4.2299920106 0.3026207329
H -5.5394221672 5.3078531848 0.4509002364
H -5.9072079202 3.9748218488 -0.6748317069
H -6.0505670126 3.7243697807 1.0914555143
O 4.1182972078 3.8536207602 -0.5816534166
C 5.4032537966 4.2516604116 -0.1352857868
H 5.4733121805 5.3207411873 -0.3329731105
H 5.5240888123 4.0724230351 0.9393061059
H 6.1947267603 3.7284542344 -0.684234183

21_H_rad

53

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N 0.1222831702 -1.3564593574 -0.1424997882
C 1.2331301897 -2.0578795408 0.0474434495
N 1.1647895162 -3.3712846259 0.3287627976
C 2.5132339269 -3.9399555059 0.2022336317
C 3.3973264732 -2.6984637849 0.3953845352
N 2.491675848 -1.6063562442 -0.0101117913
H 4.2865689836 -2.7098334414 -0.2337706266
H 3.6880991444 -2.5627602223 1.4420649262
H 2.6424555264 -4.3749151564 -0.7951479037

H 2.6836872862 -4.7036986878 0.9599832658
 N -2.2862292922 -1.4191521774 -0.3773040545
 C -3.3052393408 -2.4708014674 -0.2301843325
 C -2.4621044956 -3.7383179473 -0.3054738527
 H -2.9065520783 -4.5782403807 0.2300674868
 H -2.2960397943 -4.0260729284 -1.3530485713
 H -3.8139538009 -2.3822717512 0.7388039759
 H -4.0441969384 -2.4144635194 -1.029454751
 H -0.037141656 -5.0679838978 0.3567175071
 H -0.0055447426 -4.2004466216 -1.2045525039
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 H -1.4882183891 0.213363403 1.6370927839
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 C 2.646809523 0.4793312119 1.2691427798
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 H 3.4768048534 -0.1256566591 -1.9695926427
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 H 2.2507838727 -0.0313543207 2.1416243923
 C 3.4833321842 2.4815596537 0.2092818791
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 H 2.8267808343 2.3849857524 2.2536192884
 O -3.7582485102 3.900534789 0.4767292189
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 H -4.7762932544 5.5687706853 -0.00347525
 H -4.2867329627 4.5953042018 -1.4147657159
 H -5.6493310332 4.0610717425 -0.3822737637
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 C 4.2831738267 4.5216653683 -0.7320295797
 H 4.4290856238 5.5395658554 -0.374401576
 H 5.2426049937 4.1085868883 -1.0600137089
 H 3.5745853688 4.5255004925 -1.5667309975
 H 0.1912952288 -0.3510676644 -0.2504640897

22_rad

44

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C 0.043429 -4.033782 0.149423
 N 1.153859 -3.299438 -0.432395
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 N 0.026486 -1.25929 0.100879
 C -1.107759 -1.938882 -0.002211
 N -1.175659 -3.327299 -0.218885
 C -2.411937 -3.792804 0.403735
 C -3.327041 -2.577315 0.269965
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 H -4.026486 -2.516786 1.105883
 H -3.895038 -2.595078 -0.668703
 H -2.248574 -4.033638 1.46508
 H -2.808921 -4.674161 -0.102492
 N 2.439386 -1.456275 -0.076881
 C 3.340235 -2.537259 -0.479038
 C 2.506998 -3.784194 -0.185239
 H 2.757723 -4.621668 -0.837893
 H 2.631723 -4.092747 0.863452

H 3.58603 -2.465859 -1.546424
 H 4.262738 -2.514043 0.103703
 H 0.016971 -5.046255 -0.259266
 H 0.146011 -4.096969 1.250385
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 C 2.029865 0.874024 0.541904
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 H 4.807624 -0.517046 -0.86517
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 H 1.040784 0.624164 0.898472
 C 3.757084 2.513025 0.185761
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 H 1.831627 2.948217 1.046276
 C -2.833979 -0.146735 0.11002
 C -4.201827 0.147049 0.27731
 C -1.964304 0.912225 -0.219817
 C -4.679818 1.443598 0.130577
 H -4.911378 -0.633251 0.523324
 C -2.447179 2.207113 -0.367447
 H -0.910119 0.718955 -0.357342
 C -3.800121 2.471201 -0.189671
 H -5.737095 1.644868 0.264373
 H -1.760741 3.007237 -0.623625
 Cl 4.320507 4.173357 0.297939
 Cl -4.403261 4.111619 -0.37373

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45

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C -0.569529 -4.029366 -0.082371
 N 0.742958 -3.432489 -0.285175
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 N -1.591584 -3.089527 -0.514828
 C -3.013596 -3.4616 -0.543254
 C -3.702131 -2.090295 -0.605365
 N -2.677855 -1.200509 -0.020899
 H -4.620713 -2.052009 -0.021497
 H -3.905213 -1.779077 -1.634603
 H -3.274085 -4.000687 0.374226
 H -3.23348 -4.084078 -1.409555
 N 2.077879 -1.717558 0.436282
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 H 2.188226 -4.958924 0.018068
 H 1.496582 -4.26903 1.510576
 H 3.560262 -3.003633 -0.358837
 H 3.486153 -2.973579 1.42132
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 H -0.724358 -4.277935 0.981271
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 C 3.857829 -0.139385 0.909465
 C 2.168592 0.445561 -0.713214
 C 4.471492 1.091684 0.716707
 H 4.283219 -0.833311 1.625526
 C 2.77152 1.686583 -0.896212
 H 1.297871 0.190377 -1.307934
 C 3.918794 2.001791 -0.179885
 H 5.369019 1.342161 1.270957
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 C -2.822777 0.217842 0.046283
 C -3.504942 0.77809 1.123212

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 H -3.907795 0.137119 1.899721
 C -2.430572 2.405565 -0.883974
 H -1.777038 0.57578 -1.804654
 C -3.115527 2.955615 0.195438
 H -4.189321 2.606454 2.030866
 H -2.017246 3.04212 -1.657452
 Cl 4.684418 3.562357 -0.410807
 Cl -3.296147 4.691349 0.294278
 N -0.306368 -1.33041 0.256065
 H -0.225778 -0.354603 0.515152

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 C 0.0024011548 -3.6385895584 0.2106868898
 N 1.1490324546 -2.9267695047 -0.3269569569
 C 1.1241516399 -1.5570305606 -0.0356505306
 N 0.0132322686 -0.868270654 0.1037263053
 C -1.1217948002 -1.5393655996 -0.0559843679
 N -1.1895093647 -2.93429675 -0.2418509802
 C -2.4586796364 -3.3746324083 0.3312927875
 C -3.3551957164 -2.1567397215 0.1213165176
 N -2.4090473898 -1.0393293056 0.1616551296
 H -4.1034386066 -2.0769952019 0.9123585847
 H -3.867043671 -2.190339741 -0.8493379724
 H -2.3497497008 -3.5879850891 1.4056438623
 H -2.8379297765 -4.2666057853 -0.1701261235
 N 2.4300607253 -1.0874323956 0.0646382001
 C 3.3399801834 -2.1816130038 -0.2724263956
 C 2.4825694101 -3.4157730945 0.0044526596
 H 2.7611673733 -4.270203898 -0.6141286154
 H 2.5479091868 -3.7005019645 1.0652855353
 H 3.6373132414 -2.1356498126 -1.3285359721
 H 4.23445619 -2.1532877915 0.352605667
 H -0.0091639822 -4.6614069327 -0.1723699425
 H 0.0440985391 -3.6737612719 1.3170970329
 C 2.8479672379 0.24194633 0.102617588
 C 4.151121769 0.5760601637 -0.3075548912
 C 2.0089594202 1.267869448 0.5777468553
 C 4.6038367597 1.8911873882 -0.2486249472
 H 4.8257410546 -0.18327619 -0.6844076083
 C 2.457557036 2.5835943946 0.6264253179
 H 1.0082641551 1.0306489262 0.9100941517
 C 3.7467882416 2.8739984701 0.2134736165
 H 5.6085264507 2.1458359533 -0.5671915187
 H 1.8106141055 3.3736789699 0.9918964065
 C -2.8391602415 0.2647167191 -0.0850672558
 C -4.2114869516 0.5703234071 -0.0036550033
 C -1.9438282676 1.3025280843 -0.41078256
 C -4.6738884851 1.862832852 -0.2309826843
 H -4.9369629248 -0.1967329046 0.2376227405
 C -2.4070235419 2.5948011566 -0.6393652918
 H -0.8852464942 1.0959854416 -0.4793754557
 C -3.7623954859 2.8560274745 -0.5437445584
 H -5.7321841634 2.0904731926 -0.1672110164
 H -1.7142673308 3.3906731683 -0.8909664241
 F 4.1842983521 4.1622749867 0.2656026941
 F -4.2125084184 4.1227116128 -0.76602847

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 C 1.1478644986 -1.5084783776 -0.2151906105
 N -0.0862838256 -0.9621474144 0.2407561567
 C -1.2074819211 -1.6177549056 -0.0331956223
 N -1.1489761011 -2.8949575899 -0.4497419153
 C -2.5061922339 -3.4569995662 -0.4102527597
 C -3.3757001566 -2.1926338832 -0.4726998129
 N -2.4622312366 -1.159053189 0.0556685664
 H -4.2704885359 -2.2638071992 0.1441537473
 H -3.6546654705 -1.937366291 -1.4996821345
 H -2.6553658608 -4.0022110654 0.528274308
 H -2.672531233 -4.1261474519 -1.2534268173
 N 2.3314316605 -1.0259708451 0.3497429378
 C 3.3196504082 -2.1169462689 0.2981176108
 C 2.4349600717 -3.3571126226 0.3383035717
 H 2.8802094958 -4.2115275404 -0.1728105333
 H 2.2080870448 -3.6363935631 1.3770201591
 H 3.899497596 -2.0615991174 -0.6313522354
 H 4.0006332579 -2.0759603282 1.1482023627
 H 0.0215100716 -4.6057637092 -0.617123006
 H -0.0485769934 -3.9056278183 1.023970614
 C 2.7533704823 0.3009733549 0.0991959789
 C 3.8236254406 0.8240806908 0.8364211438
 C 2.1147961998 1.1096580422 -0.8482634599
 C 4.2510740823 2.1303916278 0.6311617552
 H 4.321003664 0.2139137258 1.5822998275
 C 2.5234837805 2.4273589142 -1.0447626757
 H 1.3071266793 0.7100188504 -1.4529882189
 C 3.5856313192 2.9104644124 -0.3024967589
 H 5.0793915502 2.5426207702 1.1959751925
 H 2.031949058 3.0608470236 -1.7743410211
 C -2.7943681834 0.2290420784 0.0959555215
 C -3.4966007883 0.7244330962 1.1929228313
 C -2.4266125206 1.067336599 -0.957980848
 C -3.8387330326 2.0715884522 1.2427008283
 H -3.7698698688 0.0574300614 2.0031879622
 C -2.7496558353 2.4194086488 -0.9102764001
 H -1.8898685231 0.6663395871 -1.8118563285
 C -3.4516814643 2.8874615693 0.1900708235
 H -4.3847932907 2.4856377256 2.0819665121
 H -2.4715971639 3.095265676 -1.7102076264
 F 3.9925143634 4.1908500755 -0.493535756
 F -3.7729762464 4.1979137306 0.2388311613
 H -0.1311261924 0.0213116634 0.4791818507

24_rad 36

O 2
 C 0.0140628451 2.9424551851 0.4476759292
 N -1.1595735944 2.3736755733 -0.2016973189
 C -1.0908951151 0.9742625213 -0.3958300593
 N 0.0587046739 0.2726999367 -0.3462059528
 C 1.147525205 0.9876368455 -0.288873637
 N 1.1756312469 2.3759190907 -0.2167710655
 C 2.5172171744 2.7719118239 0.2031303274
 C 3.363234709 1.6355271477 -0.3757057541
 N 2.4482695163 0.498071426 -0.2655856296
 C 2.7539507707 -0.754174573 -0.8985279099
 H 1.8341514641 -1.2121923169 -1.271295897
 H 3.4482664833 -0.6265076074 -1.7375536304
 H 4.2794712235 1.4660197815 0.1907971872

H 3.6198624786 1.8294173824 -1.4270280306
H 2.5979332885 2.7961217442 1.2996106529
H 2.7887731618 3.7492453671 -0.1986027026
N -2.3463846547 0.3977771728 -0.0874211435
C -3.3102702276 1.5003992125 -0.1000511372
C -2.4595448823 2.6643143644 0.4023562185
H -2.8415103 3.6369419362 0.0858424794
H -2.3983941255 2.6446175609 1.5012351798
H -3.676393626 1.6935779164 -1.1205884487
H -4.1614621668 1.293839384 0.5491681015
C -2.6888913319 -0.8067515471 -0.8020156088
H -3.3252284254 -0.6154100336 -1.6781137933
H -1.773504486 -1.2976259354 -1.1402339798
H 0.0150484949 4.0282843526 0.3287790432
H 0.0268132602 2.7025623973 1.5288793213
C -3.41295724 -1.7974713119 0.0868960115
F -4.5658225841 -1.3029861942 0.5890933139
F -2.6693430638 -2.1902192294 1.1389836827
F -3.7351423263 -2.9108093876 -0.6069069591
C 3.3834417417 -1.7328834308 0.0754876801
F 3.6861020667 -2.8943093165 -0.5418289895
F 2.5683971716 -2.0311452465 1.1053770813
F 4.5296681738 -1.2600829919 0.6105154375

24_H_rad

37
1 2
C -0.084507 2.99007 0.451243
N -1.182533 2.339123 -0.244846
C -1.138537 0.997858 -0.341599
N 0.03421 0.379245 -0.30979
C 1.224323 1.14146 -0.472451
N 1.170467 2.490233 -0.089251
C 2.36455 2.769361 0.724021
C 3.338892 1.700577 0.248769
N 2.442533 0.57701 -0.062661
C 2.998144 -0.511674 -0.842004
H 2.502597 -0.614797 -1.813061
H 4.06313 -0.348128 -1.025015
H 4.058931 1.416825 1.017128
H 3.878599 2.029484 -0.648859
H 2.137166 2.640812 1.791485
H 2.728183 3.783428 0.554022
N -2.359763 0.455474 -0.468158
C -3.355366 1.539951 -0.557244
C -2.575475 2.748047 -0.021717
H -2.799794 3.667107 -0.561255
H -2.750431 2.897485 1.049148
H -3.650123 1.674072 -1.602374
H -4.232338 1.306666 0.045207
C -2.633927 -0.886095 -0.918535
H -3.546725 -0.884865 -1.516583
H -1.828799 -1.275899 -1.547781
H -0.155178 4.066376 0.288561
H -0.158281 2.784682 1.532997
C -2.834215 -1.833197 0.255812
F -3.845332 -1.444973 1.050101
F -1.727887 -1.898715 1.026799
F -3.102343 -3.074353 -0.176582
C 2.867303 -1.833787 -0.108653
F 3.38641 -2.840167 -0.833194
F 1.568105 -2.1501 0.1305
F 3.487107 -1.829127 1.082554

H 0.097029 -0.629365 -0.368127

25_rad

50
0 2
C -3.09764 0.62446 0.
N -2.540177 -0.045727 1.165047
C -1.141014 -0.174114 1.120274
N -0.439091 -0.213087 0.
C -1.141014 -0.174114 -1.120274
N -2.540177 -0.045727 -1.165047
C -2.876826 0.459953 -2.493274
C -1.742845 -0.128719 -3.331651
N -0.609236 -0.052485 -2.410857
C 0.559536 -0.853016 -2.740583
H 1.255746 -0.770166 -1.90101
H 0.288073 -1.917618 -2.841047
H -1.549315 0.437898 -4.244428
H -1.96235 -1.174477 -3.602125
H -2.845378 1.560081 -2.521554
H -3.864856 0.1228 -2.812706
N -0.609236 -0.052485 2.410857
C -1.742845 -0.128719 3.331651
C -2.876826 0.459953 2.493274
H -3.864856 0.1228 2.812706
H -2.845378 1.560081 2.521554
H -1.96235 -1.174477 3.602125
H -1.549315 0.437898 4.244428
C 0.559536 -0.853016 2.740583
H 0.288073 -1.917618 2.841047
H 1.255746 -0.770166 1.90101
H -4.185764 0.525312 0.
H -2.838413 1.701626 0.
C 1.21957 -0.370888 4.01231
C 2.447537 0.53978 6.36441
C 1.684776 0.945243 4.107748
C 1.373158 -1.221477 5.107449
C 1.98653 -0.771594 6.278413
C 2.293964 1.399157 5.274022
H 1.560098 1.61501 3.261235
H 1.007638 -2.243452 5.047851
H 2.098018 -1.445413 7.122394
H 2.651163 2.422743 5.334294
H 2.92256 0.893086 7.274405
C 1.21957 -0.370888 -4.01231
C 2.447537 0.53978 -6.36441
C 1.684776 0.945243 -4.107748
C 1.373158 -1.221477 -5.107449
C 1.98653 -0.771594 -6.278413
C 2.293964 1.399157 -5.274022
H 1.560098 1.61501 -3.261235
H 1.007638 -2.243452 -5.047851
H 2.098018 -1.445413 -7.122394
H 2.651163 2.422743 -5.334294
H 2.92256 0.893086 -7.274405

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51
1 2
C -0.05915 2.973906 0.815523
N -1.19961 2.468185 0.073315
C -1.184864 1.160057 -0.259351
N -0.017679 0.535818 -0.391913

C 1.186779 1.292242 -0.456141
 N 1.154646 2.576302 0.120111
 C 2.39939 2.746184 0.883841
 C 3.322894 1.729458 0.227793
 N 2.395974 0.651587 -0.136269
 C 2.924897 -0.309976 -1.105448
 H 2.11881 -0.990632 -1.396389
 H 3.261122 0.20676 -2.017184
 H 4.096664 1.361709 0.902917
 H 3.803519 2.150523 -0.668079
 H 2.236836 2.494411 1.941488
 H 2.768489 3.770387 0.813243
 N -2.415926 0.658156 -0.402681
 C -3.382664 1.761453 -0.298095
 C -2.57334 2.836928 0.433694
 H -2.804871 3.846813 0.097502
 H -2.705926 2.77033 1.519771
 H -3.679577 2.084389 -1.302335
 H -4.265479 1.444098 0.256379
 C -2.766284 -0.578082 -1.091657
 H -2.969206 -0.363106 -2.147255
 H -1.91189 -1.25764 -1.048594
 H -0.121145 4.062402 0.857521
 H -0.077053 2.574786 1.844897
 C -3.963393 -1.235289 -0.441969
 C -6.171605 -2.448477 0.771783
 C -3.901768 -1.633288 0.896977
 C -5.135974 -1.446066 -1.166079
 C -6.237485 -2.05449 -0.562272
 C -5.000561 -2.235352 1.502086
 H -2.991287 -1.465521 1.466307
 H -5.192821 -1.132443 -2.204813
 H -7.145795 -2.214482 -1.134362
 H -4.944395 -2.541221 2.541938
 H -7.028288 -2.919085 1.243599
 C 4.06052 -1.108381 -0.507975
 C 6.157692 -2.583843 0.621662
 C 3.831374 -1.933684 0.59793
 C 5.347641 -1.028766 -1.039713
 C 6.393465 -1.764715 -0.479715
 C 4.871991 -2.666631 1.160771
 H 2.831621 -1.995661 1.019275
 H 5.536809 -0.38536 -1.894967
 H 7.390574 -1.693254 -0.902896
 H 4.681939 -3.304609 2.018343
 H 6.969664 -3.155692 1.059879
 H 0.002522 -0.417366 -0.725997

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56
 0 2
 C -0.000649 3.965351 -0.988282
 N 1.165195 3.543899 -0.226165
 C 1.119713 2.195499 0.166377
 N 0.000205 1.512757 0.337388
 C -1.119638 2.194355 0.165605
 N -1.166064 3.542824 -0.226156
 C -2.493543 3.776465 -0.78912
 C -3.333616 2.773858 0.001468
 N -2.410265 1.649263 0.148552
 C -2.740267 0.650488 1.146894
 H -1.876668 -0.015128 1.241044
 H -2.904895 1.11461 2.133607

H -4.242122 2.473453 -0.524294
 H -3.611169 3.187572 0.984304
 H -2.519124 3.53765 -1.863451
 H -2.814154 4.810015 -0.64533
 N 2.410631 1.650837 0.148174
 C 3.333284 2.775899 0.000302
 C 2.492247 3.777858 -0.790044
 H 2.812538 4.811597 -0.64687
 H 2.517238 3.538656 -1.86431
 H 3.611197 3.189998 0.98288
 H 4.241654 2.475869 -0.525919
 C 2.741769 0.652767 1.146821
 H 2.907152 1.117525 2.133121
 H 1.878383 -0.012967 1.24222
 H -0.001162 5.052765 -1.09423
 H -0.000467 3.509246 -1.997872
 C 3.956934 -0.156897 0.75369
 C 6.169925 -1.706545 0.040146
 C 4.101108 -0.626768 -0.556723
 C 4.937178 -0.468403 1.694422
 C 6.04145 -1.244442 1.346001
 C 5.19817 -1.396543 -0.915607
 H 3.348222 -0.374618 -1.296648
 H 4.845276 -0.100591 2.712124
 H 6.79593 -1.476964 2.088636
 H 5.29877 -1.754699 -1.935202
 C -3.955683 -0.158903 0.754046
 C -6.169433 -1.70733 0.040381
 C -4.097782 -0.632395 -0.55532
 C -4.938315 -0.46621 1.693616
 C -6.043086 -1.241565 1.345102
 C -5.195187 -1.401594 -0.914254
 H -3.342945 -0.383609 -1.294405
 H -4.847953 -0.095633 2.710448
 H -6.799484 -1.470807 2.086804
 H -5.29417 -1.762699 -1.932967
 C -7.341997 -2.548984 -0.370821
 F -6.964095 -3.791225 -0.7579
 F -8.005212 -2.018085 -1.424927
 F -8.246031 -2.710832 0.613575
 C 7.341493 -2.54984 -0.370537
 F 8.24732 -2.708725 0.612721
 F 8.002817 -2.022775 -1.427658
 F 6.96249 -3.793361 -0.752612

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57
 1 2
 C -0.119709 3.757345 -1.292301
 N 1.105508 3.557848 -0.533565
 C 1.161703 2.452734 0.335724
 N -0.036273 1.701129 0.489491
 C -1.211433 2.262816 0.220679
 N -1.247459 3.4412 -0.434513
 C -2.629764 3.695754 -0.856181
 C -3.418433 2.833937 0.135133
 N -2.435501 1.804912 0.507648
 C -2.769465 0.775017 1.477546
 H -1.885402 0.161547 1.668243
 H -3.05474 1.2431 2.426287
 H -4.300839 2.376091 -0.311954
 H -3.712297 3.398195 1.027038
 H -2.774567 3.355932 -1.888006

H -2.868687 4.755887 -0.782364
 N 2.368209 1.756077 0.149192
 C 3.282381 2.721382 -0.471899
 C 2.340693 3.553119 -1.331911
 H 2.701445 4.567923 -1.505128
 H 2.16789 3.062688 -2.300155
 H 3.774459 3.341181 0.292184
 H 4.04688 2.208139 -1.056849
 C 2.91587 1.037798 1.296075
 H 3.302239 1.739095 2.050775
 H 2.11167 0.466021 1.770573
 H -0.194976 4.800371 -1.603159
 H -0.141397 3.113784 -2.188875
 C 4.004364 0.079306 0.868688
 C 5.991898 -1.724552 0.103288
 C 3.789278 -0.799812 -0.198032
 C 5.22482 0.046512 1.540273
 C 6.220154 -0.853546 1.16401
 C 4.775176 -1.697083 -0.58334
 H 2.844194 -0.772342 -0.731013
 H 5.407437 0.729098 2.364691
 H 7.164973 -0.868503 1.69515
 H 4.597348 -2.374809 -1.411751
 C -3.88323 -0.114446 0.968349
 C -5.906595 -1.796215 0.051675
 C -3.815226 -0.662763 -0.315231
 C -4.973726 -0.410011 1.783336
 C -5.986435 -1.252257 1.330508
 C -4.822532 -1.499128 -0.776732
 H -2.97199 -0.430191 -0.958475
 H -5.039946 0.017813 2.778871
 H -6.830279 -1.476812 1.97283
 H -4.760891 -1.921582 -1.773631
 C -7.016842 -2.66432 -0.470096
 F -6.563136 -3.64603 -1.276876
 F -7.910156 -1.955075 -1.201887
 F -7.717544 -3.258258 0.515396
 C 7.063998 -2.673054 -0.350828
 F 8.035867 -2.841802 0.566073
 F 7.673645 -2.243259 -1.482746
 F 6.574105 -3.900232 -0.633035
 H -0.000618 0.869922 1.062232

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O 2

C -0.0003653687 4.3050054437 -0.6253671118
 N -1.1659704215 3.6265502678 -1.1725793996
 C -1.1190189233 2.2305196199 -1.0298208859
 N -0.0001904138 1.5334658976 -0.9323281135
 C 1.1184868314 2.230681427 -1.0299056178
 N 1.1652079222 3.6266953133 -1.1728802465
 C 2.4934740744 4.0547080474 -0.740995187
 C 3.3338833887 2.8293200345 -1.0993371654
 N 2.4102414557 1.7311996342 -0.8139654813
 C 2.7346746385 0.4298407367 -1.3587184942
 H 1.8532090525 -0.2071156123 -1.235752515
 H 2.9463269275 0.4886653371 -2.4390285546
 H 4.2426272611 2.7499098979 -0.4991457385
 H 3.6112060977 2.8439291147 -2.1652570595
 H 2.5210971211 4.2362840399 0.344287439
 H 2.8132149701 4.9585020357 -1.2628942986
 N -2.4106329782 1.7308651343 -0.8133173304

C -3.3345045759 2.8288483015 -1.0985059653
 C -2.4941905858 4.0543668711 -0.7403927312
 H -2.8142102902 4.9580954492 -1.2622436089
 H -2.5215967992 4.2359877219 0.3448872929
 H -3.6120793002 2.8433744984 -2.1643634957
 H -4.2430796826 2.7492818848 -0.4980851871
 C -2.7350823798 0.4294635911 -1.358002342
 H -2.9468656209 0.4882070982 -2.4382894011
 H -1.8535725434 -0.2074390501 -1.235085726
 H -0.0004685381 5.3519394041 -0.9375911014
 H -0.0001994201 4.2627974732 0.481373846
 C -3.9085001606 -0.206871188 -0.6461501852
 C -6.0508014676 -1.4533808902 0.6857554604
 C -4.107596857 -0.0063660395 0.7190193275
 C -4.7923760634 -1.0294008545 -1.3403872898
 C -5.8490302823 -1.6496037768 -0.6756386203
 C -5.1694661263 -0.6244719972 1.3732077378
 H -3.4277583181 0.6462707421 1.2582199811
 H -4.6566079464 -1.1852625327 -2.4066711976
 H -6.8763387379 -1.9307596142 1.1979885425
 C 3.9081825584 -0.2065483956 -0.6470582049
 C 6.0505442443 -1.4533368593 0.684486219
 C 4.1079455168 -0.0055058808 0.7179290986
 C 4.7914112137 -1.0297662492 -1.341308291
 C 5.8480899248 -1.6501062519 -0.6767333526
 C 5.1698428751 -0.6237586944 1.3719389798
 H 3.4285523173 0.6476020512 1.2571282855
 H 4.6551045735 -1.1860491422 -2.4074593831
 H 6.8760921217 -1.9308360286 1.1965824439
 C -6.7780501723 -2.5277388942 -1.4687578876
 F -7.7410832428 -3.0851480263 -0.7141142156
 F -6.1170376439 -3.5395694549 -2.073683526
 F -7.3986449381 -1.8401466046 -2.4534433296
 C -5.3564471867 -0.3609138595 2.8425554341
 F -6.345528685 -1.0945934898 3.3829298459
 F -5.6539694028 0.9361429428 3.0835733253
 F -4.2362389562 -0.6290380987 3.5481397714
 C 5.3575294377 -0.3596422802 2.8410910262
 F 6.3463501652 -1.0937078561 3.3814250489
 F 4.2374249004 -0.6267404123 3.54721519
 F 5.6559794719 0.9373395455 3.0813889937
 C 6.7764306884 -2.528955676 -1.4698752843
 F 7.7392320921 -3.0868559704 -0.7153297021
 F 7.3973288436 -1.8418862817 -2.4547635613
 F 6.1147073431 -3.5404435949 -2.0745485003

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1 2

C -0.1783907841 -4.091008517 -1.4532062488
 N -1.289672745 -3.9066286386 -0.5369416452
 C -1.304500526 -2.7716861844 0.1912860457
 N -0.1616265544 -2.1414957068 0.445818454
 C 1.077805823 -2.7989458719 0.2055874972
 N 1.0614625542 -3.847138586 -0.732647623
 C 2.2545285742 -3.7004347397 -1.5800866404
 C 3.175298588 -2.861467017 -0.7054917354
 N 2.2261493121 -2.0087717355 0.0206069354
 C 2.7774381002 -1.3328804385 1.1899870037
 H 1.9605702097 -0.869928142 1.7523522857
 H 3.2698426584 -2.0474424886 1.865631343
 H 3.8731331361 -2.2564619476 -1.2862113956
 H 3.7452652543 -3.4926574712 -0.0081484163

H 2.002292718 -3.1611070324 -2.503731602
H 2.6766999765 -4.67258317 -1.8379051095
N -2.5418063885 -2.4235030177 0.5577940201
C -3.4839042245 -3.4606453163 0.1115392716
C -2.6662648116 -4.2182921646 -0.9412972849
H -2.8415032532 -5.2930372477 -0.9215851942
H -2.8537622535 -3.8329871701 -1.9497838346
H -3.7524546809 -4.0966940621 0.9610893615
H -4.3850593809 -3.0067819796 -0.3020416406
C -2.9235539972 -1.4320029501 1.5422731181
H -3.4539565591 -1.9328532869 2.3585142325
H -2.0271397373 -0.9879853104 1.9823003786
H -0.1942725826 -5.1174491521 -1.8226895212
H -0.2830927789 -3.4011106766 -2.3088947534
C -3.7904663198 -0.3400493204 0.9467154457
C -5.3592437424 1.7325505602 -0.1097594281
C -3.580731167 0.1077999481 -0.3559592797
C -4.7890990077 0.2485136023 1.7165879098
C -5.5618321221 1.2813829393 1.1888082204
C -4.3612267989 1.1359095765 -0.8747674243
H -2.8100369719 -0.3500776973 -0.9677490004
H -4.966070029 -0.0975975096 2.7304964401
H -5.965110951 2.5318292694 -0.5177560999
C 3.7513807409 -0.2538044863 0.7740343818
C 5.5328574183 1.7779175919 0.0119341319
C 3.3941802815 0.6652263075 -0.2161148904
C 5.0005012803 -0.1520987197 1.3733206166
C 5.8823280697 0.8625896313 0.9935503956
C 4.278067796 1.6689301994 -0.5886422183
H 2.4235118739 0.5805352315 -0.692920429
H 5.2915756568 -0.86644052 2.137564932
H 6.2199254419 2.5618876864 -0.2825762302
H -0.1604351234 -1.3347080749 1.0541157952
C 3.9086564142 2.6250957004 -1.6907469968
F 4.3998566394 3.8617616784 -1.4770029895
F 2.576811719 2.7481792045 -1.8398224681
F 4.3963268058 2.2202210424 -2.8863844746
C 7.2257543599 0.9347956602 1.6676768726
F 7.9767189251 1.9579435086 1.2256373817
F 7.9428667488 -0.1939830457 1.4732546263
F 7.1061684086 1.0820697697 3.0054180998
C -6.6439908207 1.8808756233 2.0470576722
F -7.2144178129 2.9596443456 1.484493367
F -6.1714802104 2.2645823317 3.2517092649
F -7.6339901289 0.9937960943 2.2911069338
C -4.1446266027 1.5670565582 -2.3009975227
F -4.634429401 2.7948708149 -2.5478603893
F -4.7463816254 0.7245410392 -3.1713764657
F -2.8376513916 1.5863774797 -2.6300094829

28_rad

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O 2

C -0.0000001461 2.6293872779 -0.0107528114
N 1.1673076046 1.8404072514 0.3556080568
C 1.1109253618 0.518179723 -0.088261403
N -0.0000007026 -0.1409154938 -0.3445624779
C -1.1109262233 0.5181803192 -0.0882617242
N -1.1673076051 1.8404073212 0.3556090307
C -2.4909914149 2.3603482999 0.0261661689
C -3.3542086355 1.1057201356 0.1381245426
N -2.4265142049 0.0574835823 -0.3399818227
H -4.2426192823 1.1492263566 -0.4894527882

H -3.6440893663 0.9257166257 1.1792275217
H -2.5171336202 2.7602918513 -0.9977053005
H -2.7994325405 3.1393176404 0.7245543808
N 2.4265130014 0.057482461 -0.339983094
C 3.3542082177 1.1057196979 0.1381203689
C 2.4909908558 2.3603477314 0.0261621113
H 2.7994333447 3.1393179286 0.7245487696
H 2.5171311653 2.760290023 -0.9977099113
H 3.6440908255 0.9257174528 1.1792230401
H 4.2426177583 1.1492251809 -0.4894585872
H 0.0000001124 3.5669235187 0.5484049922
H -0.0000005987 2.8556253622 -1.0931875154
C -2.7533634525 -1.2706784537 -0.0426899554
F -4.0635055305 -1.4782903366 -0.2595962001
F -2.5183737925 -1.631886421 1.2505249373
F -2.0661329735 -2.1386000961 -0.7991605875
C 2.7533626216 -1.2706788172 -0.0426880498
F 4.0635041515 -1.4782917274 -0.2595967722
F 2.0661301224 -2.1386024961 -0.7991544275
F 2.51837595 -1.6318828992 1.2505285074

28_H_rad

31

I 2

C 0.0204575484 2.6149098586 0.0210279842
N 1.1844868068 1.8365640118 0.4240702566
C 1.1492181359 0.4556650635 0.2561920235
N -0.0349995671 -0.120755396 -0.2485708808
C -1.1752658308 0.5387207961 -0.1126162131
N -1.1752572003 1.8228461022 0.2461550668
C -2.5248475695 2.381393257 0.117273883
C -3.3955508315 1.1211619458 0.1615399723
N -2.4478777435 0.0729942364 -0.2995591852
H -4.2485708485 1.1761188716 -0.5103465349
H -3.7263005935 0.8959212992 1.1783481531
H -2.6178890802 2.9072354691 -0.8378364663
H -2.7384747148 3.0640717581 0.9382351765
N 2.403158333 0.0026276864 -0.2207234379
C 3.3698300226 1.1003411195 0.0234896223
C 2.4780197256 2.3307298148 -0.0721085481
H 2.8415237238 3.1580716039 0.5372804246
H 2.3811559047 2.6615521171 -1.1141357641
H 3.8135809385 1.0097984162 1.0196361361
H 4.1519235406 1.0897159534 -0.733313222
H -0.0433540479 3.5224317412 0.622076067
H 0.0831806595 2.8874917864 -1.0437774572
C -2.7971371587 -1.2929952504 -0.1724993328
F -4.0264901463 -1.481958136 -0.6413128855
F -2.7750832607 -1.7270336367 1.1005104986
F -1.9394839409 -2.0575181254 -0.8654255832
C 2.8176695443 -1.2837400821 0.1774764442
F 3.971613491 -1.59736017 -0.4172842861
F 1.891597517 -2.1987666945 -0.1724996448
F 3.0094276005 -1.4291134072 1.5088523437
H -0.0384951781 -1.1102370699 -0.4636868907

29_rad

30

O 2

C -0.0000000699 2.616331124 -0.1624869621
N 1.1685669635 1.8617966033 0.2711699217
C 1.1117525543 0.5058773879 -0.0607615138
N -0.0000000641 -0.1758776816 -0.2566412267

C -1.1117526515 0.5058773006 -0.0607599354
 N -1.168566826 1.861796743 0.2711709866
 C -2.494424205 2.3473843254 -0.1095475151
 C -3.3552016296 1.0964779743 0.0813725768
 N -2.4155141601 0.0314803964 -0.3013194583
 H -4.234284896 1.0895357307 -0.562467844
 H -3.6639414311 0.9907058618 1.127142257
 H -2.5104113363 2.6713523446 -1.1604211175
 H -2.8129007236 3.1748806485 0.5258937878
 N 2.4155139158 0.0314804965 -0.3013212412
 C 3.355201659 1.0964778349 0.081370624
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 F -3.0347658224 -1.5338811142 1.2992340419
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 C 2.7079796152 -1.3064620577 -0.0348878935
 F 3.0347683019 -1.5338828359 1.299229235
 F 3.8254879113 -1.6843991832 -0.7265598324
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 H -1.8736189965 -1.9597729874 -0.2856355273

29_H_rad

31
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 C 0.0014454274 2.6119623109 -0.106528231
 N 1.179497185 1.857753122 0.3020773353
 C 1.1564193321 0.470755885 0.1453019379
 N -0.0483555077 -0.1210998457 -0.2852976559
 C -1.1895695233 0.5322977204 -0.1207453863
 N -1.179575365 1.8290031691 0.2088533385
 C -2.5378984992 2.3704450862 0.1094513949
 C -3.3871711145 1.1012607824 0.2335274718
 N -2.4569079378 0.0536272571 -0.2537653592
 H -4.2807407603 1.1309216754 -0.3852923942
 H -3.6589142071 0.8998333559 1.2742389346
 H -2.6752083296 2.8571264996 -0.8615156356
 H -2.7297655703 3.0832940586 0.9102093537
 N 2.3821911379 0.0211695183 -0.3983216504
 C 3.3484733327 1.114431826 -0.150433766
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 H 3.802766518 1.01457045 0.8431677769
 H 4.1294238361 1.1115420177 -0.9085914302
 H -0.0434526935 3.5524411795 0.4436346751
 H 0.0260186128 2.8248265981 -1.1871987737
 C -2.7915697858 -1.3241077625 -0.0366308314
 F -4.0414674392 -1.5185666632 -0.5052077151
 F -1.9393866124 -2.0931803308 -0.7682525183
 C 2.8236482526 -1.2606019393 0.0497120124
 F 3.9498817739 -1.5856693105 -0.6318576067
 F 1.8655525339 -2.1836595729 -0.2735679892
 H -0.0518694324 -1.1139494396 -0.4857758699
 H 3.0260606444 -1.3477226921 1.1227092927
 H -2.7469739352 -1.650694688 1.0059199126

30_rad

30
 0 2
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 N -1.1758278683 2.4408309097 -0.2649845948
 C -1.1163561931 1.1286591174 -0.7559508241
 N -0.0012567649 0.4747730762 -1.0152847673
 C 1.1138028277 1.1295148562 -0.7565352903
 N 1.1722733234 2.4420658309 -0.2660169995
 C 2.4788477414 2.5960283186 0.3753964781
 C 3.3538441421 1.6577568337 -0.4657834878
 N 2.4122837405 0.6206298081 -0.9107026335
 C 2.6717653435 -0.7371833983 -0.7025227436
 H 1.9088789921 -1.3499196854 -1.1811430048
 H 3.676784253 -0.9974892302 -1.0327470228
 H 4.1702793025 1.224585634 0.1128004258
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 C -2.4820103778 2.5931272171 0.3776863083
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 H -2.4455388267 2.2566032837 1.4250202272
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30_H_rad

31
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 C 1.2435022519 1.1636637925 -0.4916389506
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 C 3.3555486089 1.7359665626 0.2037558969
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 H 4.0057216688 -0.6951678296 -0.4545826158
 H 4.0896357289 1.4814704244 0.9687085216
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 H 2.7403302652 3.8281230481 0.4391754952
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 H -0.1715431899 4.0541605152 0.3435284692

H -0.1259893296 2.7350388537 1.5480980763
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F -2.8200043626 -1.6693356652 0.2022817575
F 2.2117213506 -1.6401269747 -0.4753016236

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