

Supporting Information For

Theoretical Exploring the Key Role of Residue Lys412 in the Conversion of N₂O to N₂ by Nitrous Oxide Reductase from *Achromobacter Cycloclaste*

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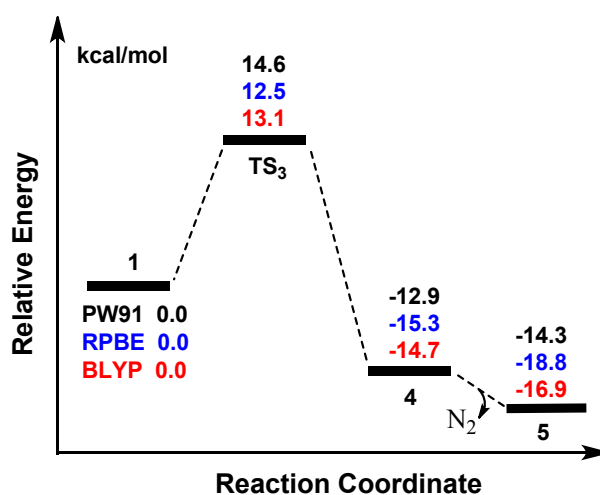


Fig. S1 The potential energy profiles for the N₂O reduction in Path A of nitrous oxide reductase in the protein environment calculated by PW91, RPBE and BLYP functionals.

Cartesian coordinates and electronic energies for all of the calculated structures

1				N	2.2245	1.5989	4.6319
SCF done:	-3346.550408			C	1.7233	-0.3175	3.7178
C	-1.7146	0.3573	4.5238	C	1.9116	1.8180	3.3309
C	-2.8914	0.5944	3.6520	N	1.5994	0.6631	2.7472
N	-2.8720	1.2834	2.4840	H	1.5595	-0.0316	6.9591
C	-4.2780	0.3080	3.9382	H	3.3000	-0.0849	6.6594
C	-4.2036	1.3844	2.1186	H	2.5282	2.3102	5.2919
N	-5.0629	0.8243	2.9912	H	1.5182	-1.3589	3.5069
H	-1.7022	1.0992	5.3394	H	1.9170	2.7922	2.8614
H	-0.7745	0.4399	3.9726	C	-0.7236	6.5603	3.8468
H	-4.6794	-0.1860	4.8189	C	-0.7095	5.4990	2.8170
H	-4.5207	1.9560	1.2531	N	-0.2129	5.6744	1.5352
C	2.3224	-0.3557	6.2388	C	-1.1602	4.2031	2.8415
C	2.1083	0.2467	4.9075	C	-0.3646	4.5227	0.8377

N	-0.9355	3.6054	1.6140	H	-5.0702	-4.7999	-5.1110
H	-1.4003	7.3801	3.5730	H	3.0415	-4.6604	-2.0189
H	0.2734	6.9923	4.0045	N	-0.1077	-0.9334	-3.1137
H	0.1684	6.5425	1.1682	N	-1.0842	-1.5426	-2.8473
H	-1.6509	3.6778	3.6502				
H	-0.0596	4.3867	-0.1912	2			
C	3.3134	4.2293	-5.7882	SCF done: -3346.549645			
C	2.3271	3.5602	-4.9192	C	-1.7841	0.3705	4.5458
N	1.0061	3.9497	-4.7828	C	-2.9863	0.6332	3.7179
C	2.4531	2.4624	-4.1082	N	-2.9682	1.2530	2.5122
C	0.3847	3.1059	-3.9226	C	-4.3658	0.3576	4.0143
N	1.2486	2.1896	-3.4918	C	-4.3014	1.3375	2.1395
H	3.0076	4.2091	-6.8430	N	-5.1531	0.8017	3.0230
H	4.2788	3.7218	-5.7148	H	-1.6840	1.1380	5.3297
H	0.5687	4.7277	-5.2693	H	-0.8718	0.3743	3.9422
H	3.3298	1.8502	-3.9498	H	-4.7688	-0.1197	4.9038
H	-0.6600	3.1820	-3.6489	H	-4.6184	1.8309	1.2265
C	5.5144	-2.3597	-4.0842	C	2.2529	-0.3425	6.2608
C	4.5811	-1.4789	-3.3369	C	2.0208	0.2466	4.9164
N	4.9923	-0.5972	-2.3503	N	2.1132	1.6024	4.6451
C	3.2180	-1.3023	-3.4106	C	1.6640	-0.3187	3.7153
C	3.9098	0.0708	-1.8738	C	1.8067	1.8226	3.3430
N	2.8125	-0.3398	-2.5017	N	1.5262	0.6654	2.7464
H	4.9598	-2.9754	-4.7980	H	1.5059	0.0008	6.9869
H	6.0652	-3.0343	-3.4154	H	3.2450	-0.0798	6.6483
H	5.9546	-0.4480	-2.0593	H	2.3911	2.3172	5.3128
H	2.5131	-1.7907	-4.0718	H	1.4810	-1.3619	3.4927
H	3.9625	0.8292	-1.1026	H	1.7944	2.8000	2.8799
C	2.2554	-4.7087	-1.2522	C	-0.7931	6.5735	3.8688
C	2.2581	-3.5045	-0.3947	C	-0.7808	5.5157	2.8485
N	3.3159	-3.1287	0.4166	N	-0.3438	5.6988	1.5488
C	1.3256	-2.5129	-0.2305	C	-1.1819	4.2078	2.9085
C	3.0086	-1.9577	1.0271	C	-0.4817	4.5363	0.8683
N	1.7973	-1.5567	0.6466	N	-0.9855	3.6106	1.6803
H	1.2951	-4.8009	-1.7665	H	-1.4848	7.3826	3.6007
H	2.4133	-5.6310	-0.6768	H	0.1982	7.0230	4.0122
H	4.1710	-3.6598	0.5579	H	-0.0133	6.5777	1.1590
H	0.3544	-2.4253	-0.6974	H	-1.6249	3.6783	3.7421
H	3.6655	-1.4444	1.7176	C	-0.2213	4.3957	-0.1719
C	-5.0376	-4.6437	-4.0272	H	3.2439	4.2425	-5.7662
C	-4.1079	-3.4976	-3.7132	C	2.3601	3.4826	-4.8492
N	-4.0401	-3.2357	-2.2208	N	0.9790	3.5789	-4.8447
H	-6.0672	-4.4415	-3.7037	C	2.6467	2.5710	-3.8621
H	-4.7020	-5.5830	-3.5703	C	0.4784	2.7526	-3.8933
H	-3.0787	-3.7018	-4.0264	N	1.4767	2.1251	-3.2772
H	-4.4282	-2.5593	-4.1762	H	3.0421	3.9985	-6.8173
H	-3.2449	-2.5665	-1.9965	H	4.2897	4.0004	-5.5603
H	-3.8784	-4.1148	-1.7135	H	0.4270	4.1594	-5.4709
H	-4.9239	-2.8498	-1.8623	H	3.6182	2.2087	-3.5543
C	-1.9826	-2.7737	1.8988	H	-0.5770	2.6290	-3.6891
C	-3.2659	-2.1361	1.5096	C	5.4449	-2.3465	-4.0622
N	-3.3454	-1.1372	0.5932	C	4.7203	-1.4015	-3.1765
C	-4.6126	-2.4653	1.8631	N	5.3395	-0.5482	-2.2766
C	-4.6962	-0.8831	0.4489	C	3.3803	-1.1351	-3.0399
N	-5.4781	-1.6969	1.1787	C	4.3941	0.1901	-1.6408
H	-2.0731	-3.2796	2.8660	N	3.1857	-0.1487	-2.0860
H	-1.1732	-2.0344	1.9600	H	4.7335	-2.8963	-4.6849
H	-4.9439	-3.2258	2.5647	H	6.0320	-3.0783	-3.4913
H	-5.0770	-0.1441	-0.2493	H	6.3432	-0.4652	-2.1377
S	-0.2850	1.1452	-0.6455	H	2.5487	-1.5753	-3.5738
O	-1.8930	-1.5687	-1.7858	H	4.6176	0.9432	-0.8963
Cu	-1.4541	1.7407	1.1964	C	2.1859	-4.6955	-1.2302
Cu	-1.8668	-0.2515	-0.2282	C	2.2477	-3.5020	-0.3638
Cu	0.9451	0.5064	-2.4493	N	3.3342	-3.1462	0.4172
Cu	0.9301	0.2303	0.9473	C	1.3408	-2.4929	-0.1782
H	3.4669	5.2800	-5.5085	C	3.0694	-1.9640	1.0281
H	6.2543	-1.7782	-4.6494	N	1.8582	-1.5404	0.6766
H	-1.0666	6.1531	4.8021	H	1.2081	-4.7538	-1.7157
H	2.2805	-1.4463	6.1724	H	2.3356	-5.6285	-0.6704
H	-1.7746	-0.6258	5.0063	H	4.1788	-3.6976	0.5444
H	-1.6738	-3.5350	1.1669	H	0.3561	-2.3952	-0.6136

H	3.7511	-1.4604	1.7014
C	-5.1071	-4.6305	-4.0052
C	-4.2074	-3.4457	-3.7541
N	-4.0580	-3.1876	-2.2723
H	-6.1299	-4.4513	-3.6503
H	-4.7225	-5.5404	-3.5286
H	-3.1944	-3.6119	-4.1366
H	-4.5958	-2.5241	-4.1990
H	-3.3276	-2.4693	-2.0943
H	-3.7818	-4.0470	-1.7814
H	-4.9280	-2.8692	-1.7933
C	-2.0521	-2.7605	1.9208
C	-3.2408	-2.2918	1.1557
N	-3.2458	-1.1484	0.3968
C	-4.5203	-2.8617	1.0195
C	-4.5124	-1.0591	-0.1238
N	-5.2976	-2.0929	0.1991
H	-2.3571	-3.4439	2.7202
H	-1.5172	-1.9136	2.3676
H	-4.9071	-3.7596	1.4927
H	-4.8311	-0.2362	-0.7564
S	-0.2788	1.4144	-0.5244
Cu	-1.5203	1.7586	1.3258
Cu	-1.7816	-0.1380	-0.2723
Cu	1.4030	0.7128	-1.8335
Cu	1.0286	0.2525	0.8430
H	3.1182	5.3255	-5.6415
H	6.1346	-1.8193	-4.7341
H	-1.1213	6.1686	4.8303
H	2.1940	-1.4336	6.2073
H	-1.8722	-0.5906	5.0673
H	-1.3383	-3.3071	1.2853
H	-5.1645	-4.8244	-5.0816
H	2.9494	-4.6581	-2.0200
N	-0.8188	-1.1855	-2.8151
N	-1.7147	-1.2464	-2.0404
O	0.2780	-0.6841	-3.0743

TS₃

SCF done: -3346.527161

C	4.4237	-0.4826	1.5374
C	4.6830	0.1247	0.2023
N	3.7703	0.2939	-0.7152
C	5.9699	0.7231	-0.2837
C	4.3663	1.2063	-1.7574
N	5.8212	1.3140	-1.4265
H	5.1117	-1.3156	1.7308
H	3.3967	-0.8316	1.6262
H	6.9146	0.6657	0.2374
H	4.2188	0.8208	-2.7652
C	3.2595	-2.5426	5.2987
C	2.5084	-2.5178	4.0068
N	2.5020	-3.5676	3.0813
C	1.7190	-1.5455	3.4476
C	1.7347	-3.2136	2.0052
N	1.2419	-1.9806	2.1936
H	4.3344	-2.6830	5.1360
H	2.9079	-3.3512	5.9505
H	2.9691	-4.4609	3.2090
H	1.4589	-0.5817	3.8454
H	1.5738	-3.8342	1.1430
C	4.2020	-5.8016	-1.8651
C	3.3064	-4.6062	-1.8274
N	1.9959	-4.6038	-2.3195
C	3.5123	-3.3339	-1.3557
C	1.4492	-3.3662	-2.1413
N	2.3490	-2.5659	-1.5505
H	4.3960	-6.1192	-2.8963
H	3.7650	-6.6491	-1.3242
H	1.5429	-5.3938	-2.7701
H	4.4034	-2.9215	-0.9182

H	0.4516	-3.0830	-2.4252
C	-6.1468	-3.5975	-3.4796
C	-4.9591	-2.7454	-3.1917
N	-3.9599	-2.4335	-4.1189
C	-4.5932	-2.1026	-2.0399
C	-3.0339	-1.6246	-3.5204
N	-3.3927	-1.4061	-2.2489
H	-6.7615	-3.1702	-4.2807
H	-6.7691	-3.6745	-2.5849
H	-3.9463	-2.7377	-5.0877
H	-5.1068	-2.0825	-1.0982
H	-2.1628	-1.2272	-4.0091
C	-7.0791	0.0365	2.6102
C	-5.7976	-0.3474	1.9485
N	-5.1780	-1.5886	2.1277
C	-4.9959	0.3292	1.0627
C	-4.0461	-1.6344	1.3582
N	-3.9064	-0.4791	0.6959
H	-7.3530	1.0553	2.3256
H	-7.0000	-0.0031	3.7031
H	-5.5332	-2.3390	2.7125
H	-5.1323	1.3151	0.6564
H	-3.3919	-2.4855	1.2965
C	-3.2412	2.9350	3.6242
C	-2.3524	1.7744	3.3514
N	-2.2814	0.6518	4.1803
C	-1.5099	1.5110	2.3021
C	-1.4210	-0.2520	3.6262
N	-0.9342	0.2425	2.4799
H	-3.0860	3.7076	2.8669
H	-3.0434	3.3806	4.6062
H	-2.7770	0.5414	5.0597
H	-1.2796	2.1190	1.4430
H	-1.1719	-1.2021	4.0642
C	-1.0614	7.5499	-2.2785
C	-1.1016	6.0202	-2.1196
N	-0.2042	5.5305	-0.9738
H	-0.0491	7.8999	-2.5069
H	-1.4179	8.0521	-1.3729
H	-2.1068	5.6623	-1.8895
H	-0.7490	5.5138	-3.0214
H	-0.2872	4.2991	-0.7971
H	-0.4849	6.0029	-0.1011
H	0.7717	5.7980	-1.1679
C	2.0578	2.8529	1.7409
C	2.8390	3.0282	0.4872
N	2.4947	2.5205	-0.6661
C	4.1705	3.6854	0.3456
C	3.7002	2.6514	-1.5792
N	4.6590	3.5216	-0.8419
H	2.1714	1.8188	2.0924
H	0.9937	3.0213	1.5437
H	4.6641	4.2529	1.1217
H	3.4409	3.0878	-2.5427
S	-0.2658	-0.3905	-1.1807
O	-0.4464	3.0085	-0.5833
Cu	2.0722	-0.6691	-1.0316
Cu	0.7905	1.6267	-0.9305
Cu	-2.6893	-0.0930	-0.9154
Cu	0.0577	-0.8065	1.0875
H	-5.8550	-4.6112	-3.7788
H	-7.8980	-0.6261	2.3061
H	5.1631	-5.5607	-1.4046
H	3.1158	-1.5979	5.8284
H	4.6190	0.2684	2.3147
H	2.4005	3.5299	2.5273
H	-1.7140	7.8455	-3.1056
H	-4.2966	2.6381	3.5912
N	-2.7009	1.8583	-1.0186
N	-2.2291	2.9003	-0.9805

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SCF done: -3346.570944

C	-1.7347	0.3423	4.4565
C	-2.9633	0.7124	3.7166
N	-2.9944	1.0237	2.4497
C	-4.3569	0.6870	4.2188
C	-4.4217	0.9763	2.0551
N	-5.2046	0.8765	3.2674
H	-1.5786	0.9917	5.3293
H	-0.8508	0.3764	3.8157
H	-4.6606	0.5410	5.2553
H	-4.7092	1.8596	1.4749
C	2.3023	-0.3707	6.1715
C	2.0749	0.2207	4.8272
N	2.2167	1.5698	4.5426
C	1.6724	-0.3383	3.6368
C	1.9058	1.7891	3.2402
N	1.5662	0.6416	2.6577
H	1.5850	0.0093	6.9104
H	3.3120	-0.1541	6.5442
H	2.5482	2.2760	5.1949
H	1.4562	-1.3777	3.4248
H	1.9404	2.7612	2.7670
C	-0.7437	6.5453	3.7795
C	-0.8717	5.4587	2.7820
N	-0.6532	5.6397	1.4268
C	-1.2017	4.1298	2.9048
C	-0.8456	4.4670	0.7804
N	-1.1801	3.5231	1.6590
H	-1.4194	7.3803	3.5541
H	0.2777	6.9456	3.8208
H	-0.4183	6.5243	0.9836
H	-1.4702	3.5908	3.8038
H	-0.7378	4.3338	-0.2872
C	3.2933	4.2143	-5.8555
C	2.3752	3.5065	-4.9310
N	0.9974	3.6503	-4.9414
C	2.6167	2.5975	-3.9291
C	0.4582	2.8550	-3.9847
N	1.4249	2.1995	-3.3468
H	3.1024	3.9436	-6.9022
H	4.3304	3.9533	-5.6270
H	0.4717	4.2416	-5.5800
H	3.5704	2.2036	-3.6048
H	-0.6042	2.7672	-3.7976
C	5.4943	-2.3747	-4.1515
C	4.7100	-1.4497	-3.2943
N	5.2797	-0.5676	-2.3901
C	3.3588	-1.2236	-3.1885
C	4.2973	0.1467	-1.7845
N	3.1080	-0.2325	-2.2505
H	4.8207	-2.9626	-4.7816
H	6.0998	-3.0723	-3.5583
H	6.2768	-0.4565	-2.2261
H	2.5617	-1.7106	-3.7335
H	4.4814	0.9114	-1.0415
C	2.2353	-4.7237	-1.3195
C	2.2232	-3.5131	-0.4736
N	3.2736	-3.1470	0.3517
C	1.2909	-2.5166	-0.3310
C	2.9707	-1.9746	0.9570
N	1.7672	-1.5663	0.5600
H	1.2829	-4.8182	-1.8486
H	2.3781	-5.6405	-0.7321
H	4.1197	-3.6886	0.5059
H	0.3214	-2.4110	-0.8134
H	3.6253	-1.4634	1.6508
C	-5.0577	-4.6587	-4.0945
C	-4.1406	-3.5209	-3.6451
N	-3.9172	-3.4509	-2.1801
H	-6.0592	-4.5666	-3.6559

H	-4.6471	-5.6367	-3.8103
H	-3.1562	-3.6161	-4.1206
H	-4.5497	-2.5524	-3.9606
H	-2.5820	-2.1897	-1.6700
H	-3.5581	-4.3542	-1.8575
H	-4.8200	-3.3323	-1.7111
C	-2.0027	-2.7887	1.8315
C	-3.2621	-2.0485	1.5966
N	-3.3404	-0.9676	0.8708
C	-4.5861	-2.2793	2.2099
C	-4.6555	-0.3580	1.1655
N	-5.4055	-1.3218	1.9401
H	-2.1317	-3.5780	2.5788
H	-1.2225	-2.0932	2.1646
H	-4.8739	-3.1458	2.8052
H	-5.1960	-0.0936	0.2501
S	-0.4010	1.2284	-0.6181
O	-1.7373	-1.6739	-1.5084
Cu	-1.5936	1.6393	1.2127
Cu	-1.9101	-0.3240	-0.2641
Cu	1.3311	0.6680	-2.0364
Cu	0.9526	0.2268	0.7846
H	3.1969	5.3045	-5.7699
H	6.1731	-1.8264	-4.8171
H	-1.0014	6.1773	4.7768
H	2.1940	-1.4581	6.1256
H	-1.8512	-0.6725	4.8615
H	-1.6406	-3.2422	0.8992
H	-5.1675	-4.6472	-5.1857
H	3.0347	-4.6853	-2.0728
N	0.1226	-0.6670	-3.4201
N	-0.2279	-0.9840	-4.4224

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SCF done: -3237.049124

C	-1.8282	0.3147	4.4122
C	-3.0095	0.6359	3.5754
N	-2.9736	1.1849	2.3460
C	-4.4123	0.5482	3.9500
C	-4.3109	1.3843	2.0043
N	-5.1802	1.0387	2.9919
H	-1.7195	1.0715	5.2047
H	-0.9048	0.2901	3.8275
H	-4.8171	0.1730	4.8871
H	-4.5962	2.0121	1.1670
C	2.2088	-0.3983	6.1272
C	2.0046	0.2075	4.7906
N	2.1346	1.5609	4.5226
C	1.6416	-0.3474	3.5877
C	1.8538	1.7881	3.2156
N	1.5471	0.6391	2.6166
H	1.4755	-0.0329	6.8574
H	3.2090	-0.1792	6.5236
H	2.4347	2.2666	5.1905
H	1.4394	-1.3867	3.3637
H	1.8825	2.7642	2.7509
C	-0.8372	6.5177	3.7352
C	-0.8539	5.4401	2.7232
N	-0.4585	5.6218	1.4079
C	-1.2332	4.1224	2.7943
C	-0.6006	4.4577	0.7333
N	-1.0693	3.5220	1.5576
H	-1.5308	7.3265	3.4719
H	0.1616	6.9588	3.8452
H	-0.1542	6.5040	1.0036
H	-1.6359	3.5881	3.6445
H	-0.3710	4.3257	-0.3153
C	3.1998	4.1867	-5.8998
C	2.3532	3.3933	-4.9796
N	0.9686	3.3563	-5.0270
C	2.6828	2.5685	-3.9314

C	0.5065	2.5465	-4.0443	N	-5.1472	0.7232	2.9859
N	1.5342	2.0536	-3.3551	H	-1.7472	1.1319	5.3462
H	3.0623	3.8811	-6.9451	H	-0.8636	0.4291	3.9746
H	4.2549	4.0497	-5.6477	H	-4.7587	-0.2389	4.8420
H	0.3888	3.8432	-5.7061	H	-4.6216	1.8326	1.2336
H	3.6701	2.3146	-3.5691	C	2.2458	-0.3429	6.2648
H	-0.5402	2.3345	-3.8714	C	2.0075	0.2604	4.9377
C	5.4008	-2.4023	-4.1958	N	2.1668	1.6032	4.6423
C	4.7422	-1.4387	-3.2741	C	1.5882	-0.3069	3.7606
N	5.4370	-0.6340	-2.3853	C	1.8543	1.8117	3.3388
C	3.4215	-1.1017	-3.0829	N	1.4989	0.6600	2.7741
C	4.5610	0.1436	-1.7025	H	1.5470	0.0419	7.0204
N	3.3183	-0.1234	-2.1042	H	3.2635	-0.1471	6.6274
H	4.6490	-2.9233	-4.7955	H	2.4991	2.3138	5.2893
H	5.9812	-3.1569	-3.6495	H	1.3174	-1.3388	3.5801
H	6.4482	-0.6069	-2.2826	H	1.9017	2.7764	2.8524
H	2.5492	-1.4969	-3.5872	C	-0.8002	6.5731	3.8728
H	4.8558	0.8662	-0.9535	C	-0.8462	5.5262	2.8293
C	2.1418	-4.7513	-1.3638	N	-0.4473	5.7280	1.5177
C	2.1902	-3.5472	-0.5135	C	-1.2508	4.2157	2.8739
N	3.2284	-3.2546	0.3553	C	-0.6048	4.5774	0.8213
C	1.3213	-2.4911	-0.4047	N	-1.0898	3.6358	1.6274
C	2.9794	-2.0666	0.9557	H	-1.4708	7.4094	3.6334
N	1.8235	-1.5788	0.5104	H	0.2096	6.9842	3.9964
H	1.1890	-4.7942	-1.8982	H	-0.1260	6.6117	1.1307
H	2.2376	-5.6765	-0.7804	H	-1.6712	3.6710	3.7090
H	4.0294	-3.8518	0.5425	H	-0.3641	4.4569	-0.2264
H	0.3777	-2.3305	-0.9233	C	3.2368	4.2421	-5.7622
H	3.6378	-1.6036	1.6789	C	2.3553	3.6775	-4.7262
C	-5.1512	-4.6863	-4.1388	N	0.9850	3.8671	-4.6717
C	-4.1667	-3.5506	-3.8309	C	2.6359	2.8449	-3.6748
N	-3.8579	-3.3971	-2.3935	C	0.4820	3.1631	-3.6316
H	-6.1131	-4.5240	-3.6364	N	1.4727	2.5292	-2.9987
H	-4.7529	-5.6572	-3.8187	H	2.9445	3.9109	-6.7676
H	-3.2176	-3.7168	-4.3562	H	4.2691	3.9198	-5.5963
H	-4.5670	-2.5929	-4.1854	H	0.4418	4.4348	-5.3173
H	-2.4305	-2.1212	-1.9192	H	3.5983	2.4515	-3.3805
H	-3.4966	-4.2778	-2.0177	H	-0.5697	3.1137	-3.3803
H	-4.7126	-3.1851	-1.8705	C	5.4378	-2.3469	-4.0582
C	-2.0962	-2.8163	1.7872	C	4.6196	-1.3639	-3.3083
C	-3.3029	-2.0323	1.4518	N	5.1435	-0.4804	-2.3791
N	-3.3296	-1.0478	0.5380	C	3.2717	-1.0923	-3.3315
C	-4.6594	-2.1648	1.9466	C	4.1439	0.2902	-1.8833
C	-4.6430	-0.5831	0.5280	N	2.9942	-0.0642	-2.4524
N	-5.4606	-1.2952	1.3456	H	4.8014	-2.9264	-4.7322
H	-2.2613	-3.4372	2.6735	H	5.9501	-3.0486	-3.3865
H	-1.2299	-2.1637	1.9597	H	6.1246	-0.4082	-2.1225
H	-5.0219	-2.8869	2.6741	H	2.4779	-1.5518	-3.9053
H	-5.0099	0.0828	-0.2458	H	4.2846	1.0581	-1.1341
S	-0.3185	1.2209	-0.6757	C	2.1788	-4.6959	-1.2262
O	-1.5918	-1.6016	-1.7491	C	2.1786	-3.5285	-0.3152
Cu	-1.5253	1.6467	1.1171	N	3.0318	-3.3539	0.7635
Cu	-1.8238	-0.3440	-0.4225	C	1.4239	-2.3843	-0.3535
Cu	1.6235	0.8419	-1.7821	C	2.7908	-2.1424	1.3238
Cu	1.0393	0.2167	0.7381	N	1.8153	-1.5245	0.6561
H	2.9758	5.2595	-5.8333	H	1.4071	-4.5666	-1.9894
H	6.0835	-1.8919	-4.8871	H	1.9797	-5.6386	-0.6981
H	-1.1442	6.1274	4.7095	H	3.7266	-4.0202	1.0904
H	2.1084	-1.4856	6.0660	H	0.7265	-2.0661	-1.1234
H	-1.9614	-0.6452	4.9270	C	3.3342	-1.7536	2.1749
H	-1.8275	-3.4812	0.9532	H	-5.1142	-4.6309	-4.0012
H	-5.3363	-4.7359	-5.2187	C	-4.3593	-3.3956	-3.5873
H	2.9456	-4.7526	-2.1139	N	-4.2794	-3.2931	-2.0822
				H	-6.1527	-4.6181	-3.6502
				H	-4.6267	-5.5487	-3.6495
				H	-3.3240	-3.4077	-3.9438
				H	-4.8313	-2.4727	-3.9373
				H	-3.6442	-2.5255	-1.8053
				H	-3.9219	-4.1660	-1.6734
				H	-5.1839	-3.0980	-1.6094
				C	-2.0592	-2.7609	1.9248
TS₆							
SCF done:	-3346.513971						
C	-1.7912	0.3701	4.5498				
C	-2.9819	0.5947	3.6962				
N	-2.9693	1.2566	2.5135				
C	-4.3588	0.2669	3.9674				
C	-4.2984	1.3108	2.1283				

C	-3.2931	-2.2740	1.2498
N	-3.3395	-1.1458	0.4749
C	-4.5907	-2.8350	1.2118
C	-4.6386	-1.0590	0.0342
N	-5.4111	-2.0793	0.4322
H	-2.3144	-3.4631	2.7256
H	-1.4975	-1.9261	2.3627
H	-4.9485	-3.7264	1.7188
H	-4.9878	-0.2509	-0.6018
S	-0.3156	1.3051	-0.5665
Cu	-1.5470	1.7546	1.2555
Cu	-1.8923	-0.1634	-0.3154
Cu	1.1743	0.7017	-2.2556
Cu	0.9246	0.2553	0.9176
H	3.2309	5.3409	-5.7599
H	6.2060	-1.8516	-4.6669
H	-1.1229	6.1626	4.8337
H	2.1124	-1.4270	6.2130
H	-1.8502	-0.5996	5.0585
H	-1.3830	-3.2844	1.2323
H	-5.1448	-4.6854	-5.0954
H	3.1430	-4.8099	-1.7396
N	-1.3960	-1.3234	-3.0063
N	-2.1363	-1.0787	-2.1742
O	0.4139	-0.8538	-2.6692

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SCF done: -3346.576235

C	-1.5239	0.5741	4.6508
C	-2.7058	0.6159	3.7539
N	-2.7001	1.0620	2.4691
C	-4.0470	0.1904	4.0288
C	-3.9996	0.8903	2.0311
N	-4.8252	0.3647	2.9468
H	-1.7236	1.1227	5.5830
H	-0.6374	1.0003	4.1715
H	-4.4328	-0.2170	4.9595
H	-4.3085	1.1659	1.0279
C	2.5131	-0.1389	6.3658
C	2.4511	0.4581	5.0176
N	2.9134	1.7217	4.6923
C	1.9314	-0.0336	3.8478
C	2.6668	1.9615	3.3796
N	2.0654	0.9049	2.8392
H	1.9576	0.4578	7.1019
H	3.5451	-0.2286	6.7295
H	3.3844	2.3603	5.3282
H	1.4530	-0.9900	3.6798
H	2.9266	2.8819	2.8735
C	-0.5329	6.7771	3.9738
C	-0.7532	5.6923	2.9761
N	-0.8691	5.9308	1.6167
C	-0.8938	4.3276	3.0990
C	-1.0634	4.7579	0.9695
N	-1.0822	3.7579	1.8486
H	-1.3484	7.5121	3.9562
H	0.4083	7.3108	3.7883
H	-0.8455	6.8478	1.1789
H	-0.8940	3.7351	4.0043
H	-1.1807	4.6669	-0.1019
C	3.5041	4.4461	-5.6612
C	2.4499	3.5308	-5.1630
N	1.1445	3.5081	-5.6288
C	2.4910	2.5513	-4.2052
C	0.4498	2.5508	-4.9694
N	1.2501	1.9484	-4.0916
H	3.6863	4.3080	-6.7346
H	4.4443	4.2542	-5.1366
H	0.7697	4.1001	-6.3657
H	3.3360	2.2382	-3.6105
H	-0.5930	2.3244	-5.1480

C	5.7051	-2.1429	-3.9572
C	4.6276	-1.3129	-3.3570
N	4.8365	-0.4716	-2.2757
C	3.2951	-1.1538	-3.6663
C	3.6748	0.1562	-1.9663
N	2.7178	-0.2454	-2.7962
H	5.3080	-2.7211	-4.7963
H	6.1269	-2.8497	-3.2312
H	5.7277	-0.3256	-1.8105
H	2.7304	-1.6300	-4.4578
H	3.5639	0.8679	-1.1589
C	2.4461	-4.4919	-1.1252
C	2.4661	-3.2903	-0.2609
N	3.3861	-3.0765	0.7548
C	1.6747	-2.1693	-0.2593
C	3.1384	-1.8748	1.3291
N	2.0986	-1.2963	0.7288
H	1.6473	-4.4022	-1.8667
H	2.2715	-5.4122	-0.5515
H	4.1099	-3.7278	1.0466
H	0.8537	-1.9249	-0.9246
H	3.7062	-1.4693	2.1565
C	-4.8469	-4.4269	-3.9002
C	-5.6254	-5.1937	-2.8485
N	-6.2196	-4.2464	-1.8398
H	-4.0074	-3.8768	-3.4611
H	-5.4912	-3.7269	-4.4483
H	-6.4389	-5.7801	-3.2893
H	-4.9772	-5.8757	-2.2884
H	-6.6993	-4.7554	-1.0883
H	-6.9213	-3.6388	-2.2798
H	-5.4052	-3.5923	-1.3867
C	-1.7919	-2.5569	2.0258
C	-2.6653	-2.4286	0.8361
N	-2.4839	-1.5240	-0.1891
C	-3.7579	-3.2272	0.4875
C	-3.4416	-1.8160	-1.1054
N	-4.2359	-2.8371	-0.7290
H	-2.3028	-3.1017	2.8265
H	-1.4991	-1.5695	2.4064
H	-4.2012	-4.0379	1.0567
H	-3.5467	-1.2786	-2.0405
S	0.1007	1.6424	-0.3185
Cu	-1.3119	1.8138	1.3458
Cu	-1.1655	-0.0959	-0.5043
Cu	0.8200	0.4377	-2.9025
Cu	1.3403	0.5210	1.0464
H	3.2403	5.4995	-5.5004
H	6.5249	-1.5226	-4.3418
H	-0.4889	6.3559	4.9821
H	2.0788	-1.1425	6.3525
H	-1.2944	-0.4594	4.9491
H	-0.8672	-3.1034	1.7833
H	-4.4442	-5.1327	-4.6347
H	3.3933	-4.6174	-1.6666
N	-2.3451	1.7082	-2.5403
N	-2.5833	1.1500	-1.6150
O	-0.5249	-0.5227	-2.2147

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SCF done: -3237.054468

C	-1.6091	0.5938	4.6197
C	-2.7937	0.6469	3.7287
N	-2.7943	1.1184	2.4537
C	-4.1345	0.2181	4.0025
C	-4.0967	0.9577	2.0191
N	-4.9178	0.4159	2.9283
H	-1.8019	1.1371	5.5566
H	-0.7230	1.0200	4.1396
H	-4.5157	-0.2070	4.9271
H	-4.4130	1.2569	1.0255

C	2.4279	-0.1192	6.3347	H	-2.3948	-3.0731	2.7968
C	2.3618	0.4789	4.9871	H	-1.5830	-1.5475	2.3676
N	2.8265	1.7415	4.6615	H	-4.2475	-4.0582	1.0076
C	1.8360	-0.0100	3.8189	H	-3.6662	-1.2492	-2.0599
C	2.5729	1.9845	3.3508	S	0.0103	1.6537	-0.3456
N	1.9665	0.9302	2.8115	Cu	-1.4015	1.8479	1.3154
H	1.8591	0.4670	7.0689	Cu	-1.2538	-0.0885	-0.5282
H	3.4593	-0.1935	6.7032	Cu	0.7394	0.4659	-2.9271
H	3.2975	2.3798	5.2978	Cu	1.2666	0.5393	1.0092
H	1.3561	-0.9656	3.6508	H	3.1468	5.5192	-5.5472
H	2.8332	2.9048	2.8448	H	6.4581	-1.5088	-4.3407
C	-0.6181	6.7968	3.9427	H	-0.6296	6.3795	4.9537
C	-0.8238	5.7133	2.9425	H	2.0087	-1.1293	6.3175
N	-0.8819	5.9476	1.5787	H	-1.3822	-0.4422	4.9115
C	-0.9955	4.3521	3.0656	H	-0.9534	-3.0900	1.7623
C	-1.0709	4.7757	0.9289	H	-4.5361	-5.0813	-4.6990
N	-1.1444	3.7808	1.8111	H	3.3136	-4.6098	-1.6851
H	-1.4130	7.5520	3.8872	O	-0.5582	-0.5431	-2.2117
H	0.3427	7.3068	3.7969				
H	-0.8202	6.8613	1.1380				
H	-1.0471	3.7639	3.9722	9			
H	-1.1527	4.6836	-0.1456	SCF done:	-2937.987202		
C	3.4189	4.4658	-5.6923	C	-4.2656	-0.8313	-0.5660
C	2.3650	3.5504	-5.1922	N	-3.6648	0.2483	-0.9899
N	1.0584	3.5310	-5.6551	C	-5.7342	-0.6975	-0.8201
C	2.4075	2.5672	-4.2387	C	-4.6975	1.0499	-1.7395
C	0.3640	2.5728	-4.9970	N	-6.0174	0.3978	-1.4533
N	1.1650	1.9661	-4.1227	H	-6.4835	-1.4115	-0.5100
H	3.6129	4.3148	-6.7620	H	-4.6222	1.9987	-2.2684
H	4.3550	4.2867	-5.1558	C	-2.5578	-1.4697	4.2367
H	0.6825	4.1288	-6.3869	N	-2.4276	-0.1022	4.4969
H	3.2540	2.2503	-3.6483	C	-1.8263	-1.6888	3.0993
H	-0.6783	2.3454	-5.1770	C	-1.6405	0.4610	3.5236
C	5.6199	-2.1232	-3.9883	N	-1.2557	-0.4812	2.6555
C	4.5453	-1.2884	-3.3886	H	-2.8359	0.3865	5.2872
N	4.7546	-0.4579	-2.2990	H	-1.6810	-2.6098	2.5659
C	3.2149	-1.1179	-3.7024	H	-1.3973	1.5059	3.4680
C	3.5959	0.1753	-1.9893	C	-3.1740	4.3108	2.0206
N	2.6404	-0.2120	-2.8276	N	-1.8497	4.6353	1.7064
H	5.2295	-2.6741	-4.8486	C	-3.4077	3.1109	1.4023
H	6.0143	-2.8536	-3.2700	C	-1.3250	3.6441	0.9211
H	5.6458	-0.3176	-1.8322	N	-2.2522	2.7009	0.7241
H	2.6508	-1.5825	-4.5014	H	-1.3731	5.4860	1.9872
H	3.4865	0.8811	-1.1766	H	-4.3159	2.5356	1.3855
C	2.3609	-4.4722	-1.1563	H	-0.3254	3.6221	0.5226
C	2.3844	-3.2724	-0.2901	C	5.2683	3.8163	-0.5438
N	3.2963	-3.0671	0.7348	N	4.6442	4.1768	-1.7415
C	1.6024	-2.1453	-0.2963	C	4.7433	2.5952	-0.2185
C	3.0540	-1.8628	1.3061	C	3.7704	3.1809	-2.0982
N	2.0261	-1.2749	0.6944	N	3.8086	2.2044	-1.1882
H	1.5740	-4.3702	-1.9088	H	4.8268	5.0242	-2.2683
H	2.1644	-5.3911	-0.5871	H	4.9721	1.9747	0.6273
H	4.0109	-3.7251	1.0340	H	3.1543	3.2048	-2.9788
H	0.7902	-1.8920	-0.9695	C	5.7256	-1.6215	1.2085
H	3.6166	-1.4624	2.1396	N	4.9343	-1.1668	2.2690
C	-4.9321	-4.4072	-3.9313	C	5.0710	-1.2174	0.0714
C	-5.6411	-5.2213	-2.8672	C	3.8445	-0.5107	1.7546
N	-6.2641	-4.3104	-1.8431	N	3.8987	-0.5259	0.4201
H	-4.0936	-3.8399	-3.5131	H	5.1526	-1.2832	3.2525
H	-5.6200	-3.7163	-4.4352	H	5.3555	-1.3646	-0.9549
H	-6.4289	-5.8533	-3.2908	H	3.0648	-0.0722	2.3500
H	-4.9439	-5.8674	-2.3236	C	2.2155	-3.9692	0.5773
H	-6.7027	-4.8440	-1.0886	N	1.8431	-4.1091	1.9165
H	-7.0045	-3.7387	-2.2674	C	1.6268	-2.8079	0.1543
H	-5.4700	-3.6185	-1.4023	C	1.0540	-3.0439	2.2628
C	-1.8771	-2.5372	1.9947	N	0.9005	-2.2353	1.2063
C	-2.7466	-2.4171	0.7993	H	2.1109	-4.8769	2.5234
N	-2.5917	-1.4929	-0.2140	H	1.7325	-2.3183	-0.7949
C	-3.8250	-3.2304	0.4475	H	0.6298	-2.8975	3.2394
C	-3.5493	-1.7921	-1.1290	C	-2.4777	-2.6881	-2.7189
N	-4.3189	-2.8338	-0.7614	N	-2.2071	-1.4478	-3.0147
				C	-3.6827	-3.1217	-3.4839

C	-3.3741	-0.9444	-3.8404
N	-4.1939	-2.1479	-4.1642
H	-4.0766	-4.1282	-3.4944
H	-3.5801	0.0315	-4.2764
S	0.3891	0.9389	-0.8067
Cu	-1.9734	1.0516	-0.3523
Cu	-0.7745	-0.3614	-2.2371
Cu	2.7239	0.5050	-0.8855
Cu	-0.0624	-0.4346	1.0356
N	1.8644	-1.0067	-3.3870
N	0.7255	-0.9740	-3.6396
O	2.8477	-0.7894	-2.5800
H	2.8541	-4.6504	0.0549
H	6.6441	-2.1531	1.3455
H	-1.9956	-3.2728	-1.9635
H	-3.7419	-1.6687	-0.1545
H	-3.1266	-2.1515	4.8337
H	5.9944	4.4115	-0.0305
H	-3.8182	4.9192	2.6204

TS₁₀

SCF done: -2937.943695

C	-4.2084	-0.6585	0.4199
N	-3.5541	-0.1124	-0.5715
C	-5.4823	-1.2428	-0.0678
C	-4.2602	-0.6358	-1.8236
N	-5.5664	-1.1709	-1.3618
H	-6.2649	-1.6491	0.5553
H	-4.3565	0.1055	-2.6113
C	-1.9765	1.2809	4.8526
N	-1.7026	2.5346	4.3095
C	-1.6248	0.3696	3.8954
C	-1.1944	2.3582	3.0514
N	-1.1255	1.0500	2.7685
H	-1.8564	3.4239	4.7735
H	-1.6812	-0.7029	3.9261
H	-0.9127	3.1581	2.3925
C	-2.4549	5.2848	0.0977
N	-1.2318	5.1797	-0.5649
C	-2.9440	4.0094	0.1938
C	-1.0025	3.8665	-0.8502
N	-2.0245	3.1232	-0.3979
H	-0.6318	5.9578	-0.8179
H	-3.8693	3.6678	0.6209
H	-0.1263	3.4776	-1.3370
C	5.3615	2.4417	-2.5552
N	4.3506	2.5406	-3.5110
C	4.8984	1.5795	-1.6023
C	3.3092	1.7468	-3.1206
N	3.6125	1.1498	-1.9614
H	4.3966	3.0876	-4.3640
H	5.3825	1.2311	-0.7107
H	2.3934	1.6259	-3.6700
C	5.7615	-1.5570	1.5046
N	5.2232	-0.5046	2.2464
C	4.9662	-1.6849	0.3957
C	4.1310	-0.0221	1.5793
N	3.9499	-0.7175	0.4503
H	5.5946	-0.1523	3.1218
H	5.0369	-2.3809	-0.4202
H	3.5171	0.7887	1.9265
C	1.9503	-3.3683	2.5398
N	1.7008	-2.8136	3.7953
C	1.4054	-2.5164	1.6215
C	1.0169	-1.6447	3.6144
N	0.8191	-1.4348	2.3031
H	1.9721	-3.2165	4.6857
H	1.4463	-2.5570	0.5412
H	0.6949	-1.0032	4.4145
C	-2.8366	-3.1511	-0.5297
N	-2.3620	-2.1750	-1.2459

C	-3.9745	-3.7891	-1.2599
C	-3.3758	-1.9294	-2.3342
N	-4.2670	-3.1273	-2.3373
H	-4.4823	-4.6932	-0.9607
H	-2.9223	-1.7397	-3.3037
S	0.3976	0.7794	-0.8232
Cu	-2.0240	1.1420	-0.5218
Cu	-0.7609	-1.0595	-1.2568
Cu	2.5861	-0.2837	-1.0166
Cu	0.0065	0.1503	1.3550
N	1.1001	-2.5045	-2.6096
N	0.0367	-2.1451	-2.9067
O	1.8045	-1.9736	-1.2676
H	2.4957	-4.2756	2.3915
H	6.6388	-2.0905	1.8207
H	-2.5002	-3.3306	0.4838
H	-3.7776	-0.7962	1.4006
H	-2.3617	1.1413	5.8431
H	6.2949	2.9638	-2.6228
H	-2.8488	6.2255	0.4313

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SCF done: -2938.026917

C	4.2329	0.1461	-0.8819
N	3.4482	-0.6743	-0.2337
C	5.3995	-0.5919	-1.4296
C	3.9401	-2.0652	-0.6290
N	5.2843	-1.8695	-1.2273
H	6.2573	-0.1416	-1.9065
H	3.9436	-2.7736	0.1945
C	2.3763	4.8914	0.8925
N	2.1529	4.4932	2.2085
C	1.7922	3.9426	0.1029
C	1.4437	3.3233	2.1891
N	1.2028	2.9648	0.9215
H	2.4591	4.9940	3.0362
H	1.7392	3.8874	-0.9685
H	1.1451	2.7772	3.0645
C	2.7987	0.3212	5.1011
N	1.5338	-0.2659	5.1373
C	3.1601	0.3592	3.7810
C	1.1566	-0.5660	3.8614
N	2.1236	-0.1950	3.0076
H	1.0005	-0.4632	5.9777
H	4.0694	0.7213	3.3367
H	0.2207	-1.0161	3.5820
C	-5.3109	-2.1879	2.6112
N	-4.6879	-3.4179	2.3921
C	-4.6769	-1.2945	1.7937
C	-3.7037	-3.2458	1.4617
N	-3.6710	-1.9621	1.0779
H	-4.9418	-4.2957	2.8327
H	-4.8680	-0.2493	1.6507
H	-3.0584	-4.0238	1.0971
C	-5.5883	1.7339	-1.4785
N	-4.9035	2.4700	-0.5107
C	-4.9325	0.5330	-1.5707
C	-3.8643	1.7056	-0.0486
N	-3.8527	0.5226	-0.6716
H	-5.1520	3.4007	-0.1950
H	-5.1477	-0.3093	-2.2027
H	-3.1570	2.0342	0.6906
C	-1.8884	2.5420	-3.4544
N	-1.6140	3.8352	-3.0066
C	-1.4183	1.6880	-2.4979
C	-0.9859	3.7418	-1.7971
N	-0.8477	2.4496	-1.4596
H	-1.8377	4.6928	-3.4997
H	-1.4759	0.6080	-2.4339
H	-0.6593	4.5874	-1.2189
C	2.6830	-0.8421	-3.2380

N	2.1020	-1.3657	-2.1923
C	3.6677	-1.8136	-3.7975
C	2.9423	-2.5716	-1.8353
N	3.7876	-2.8550	-3.0309
H	4.2005	-1.6971	-4.7290
H	2.3464	-3.4216	-1.5185
S	-0.4269	-0.5342	0.8514
Cu	1.9718	-0.4059	1.0319
Cu	0.3736	-1.0829	-1.2737
Cu	-2.4678	-1.1393	-0.2913
Cu	-0.0349	1.5915	0.1732
N	-0.9194	-4.2932	-0.2327
N	0.0677	-4.0382	-0.6728
O	-1.4025	-1.2472	-1.7800
H	-2.3890	2.3283	-4.3742
H	-6.4538	2.1198	-1.9867
H	2.5313	0.1898	-3.5325
H	3.9714	1.1699	-1.1115
H	2.8932	5.7872	0.6242
H	-6.1271	-2.0499	3.2969
H	3.3105	0.6456	5.9874

Int₁_C

SCF done: -3347.143245

C	-1.7832	0.3357	4.4358
C	-2.9850	0.6746	3.6376
N	-2.9664	1.2231	2.4052
C	-4.3771	0.5934	4.0349
C	-4.3041	1.4362	2.0923
N	-5.1597	1.0853	3.0840
H	-1.6429	1.0788	5.2362
H	-0.8796	0.3142	3.8213
H	-4.7704	0.2171	4.9762
H	-4.6032	2.0490	1.2489
C	2.2538	-0.3773	6.1508
C	2.0083	0.2180	4.8122
N	2.1060	1.5734	4.5382
C	1.6286	-0.3450	3.6171
C	1.7911	1.7927	3.2378
N	1.4922	0.6382	2.6456
H	1.5286	-0.0187	6.8925
H	3.2582	-0.1367	6.5228
H	2.3990	2.2877	5.1999
H	1.4340	-1.3874	3.4010
H	1.7834	2.7697	2.7738
C	-0.7922	6.5387	3.7588
C	-0.8205	5.4559	2.7481
N	-0.4189	5.6293	1.4329
C	-1.2130	4.1410	2.8198
C	-0.5697	4.4637	0.7612
N	-1.0485	3.5340	1.5856
H	-1.4777	7.3537	3.4924
H	0.2112	6.9692	3.8677
H	-0.1047	6.5071	1.0271
H	-1.6252	3.6118	3.6688
H	-0.3337	4.3246	-0.2851
C	3.2448	4.2077	-5.8762
C	2.3946	3.4166	-4.9554
N	1.0092	3.4489	-4.9577
C	2.7164	2.5444	-3.9442
C	0.5410	2.6335	-3.9823
N	1.5631	2.0671	-3.3433
H	3.0672	3.9410	-6.9261
H	4.3005	4.0251	-5.6588
H	0.4350	3.9902	-5.5991
H	3.7006	2.2352	-3.6192
H	-0.5088	2.4864	-3.7661
C	5.4458	-2.3813	-4.1722
C	4.7664	-1.4281	-3.2518
N	5.4424	-0.6284	-2.3437
C	3.4417	-1.0994	-3.0753

C	4.5502	0.1359	-1.6654
N	3.3151	-0.1312	-2.0885
H	4.7069	-2.9050	-4.7856
H	6.0252	-3.1343	-3.6229
H	6.4517	-0.5952	-2.2250
H	2.5811	-1.4933	-3.5999
H	4.8302	0.8539	-0.9062
C	2.1868	-4.7303	-1.3402
C	2.2106	-3.5320	-0.4801
N	3.2409	-3.2172	0.3892
C	1.3228	-2.4937	-0.3672
C	2.9643	-2.0339	0.9897
N	1.8001	-1.5693	0.5449
H	1.2334	-4.7918	-1.8719
H	2.3034	-5.6581	-0.7649
H	4.0549	-3.7966	0.5771
H	0.3796	-2.3580	-0.8849
H	3.6112	-1.5567	1.7144
C	-5.1062	-4.6653	-4.1152
C	-4.1244	-3.5351	-3.8308
N	-3.7817	-3.3650	-2.3818
H	-6.0626	-4.5086	-3.6009
H	-4.7008	-5.6370	-3.8054
H	-3.1790	-3.7002	-4.3635
H	-4.5269	-2.5741	-4.1741
H	-2.7247	-2.4086	-2.1153
H	-3.5000	-4.2764	-2.0042
H	-4.6336	-3.1176	-1.8659
C	-2.0512	-2.7953	1.8108
C	-3.2781	-2.0292	1.4896
N	-3.3385	-1.0474	0.5665
C	-4.6119	-2.1759	2.0200
C	-4.6578	-0.6119	0.5873
N	-5.4438	-1.3189	1.4314
H	-2.1880	-3.3905	2.7195
H	-1.1888	-2.1291	1.9491
H	-4.9458	-2.8930	2.7654
H	-5.0525	0.0655	-0.1629
S	-0.3428	1.2517	-0.7064
O	-1.8494	-1.7249	-1.9256
Cu	-1.5271	1.6497	1.1440
Cu	-1.8781	-0.3073	-0.4643
Cu	1.6108	0.8378	-1.7621
Cu	0.9870	0.2288	0.7475
H	3.0623	5.2847	-5.7688
H	6.1330	-1.8605	-4.8513
H	-1.1045	6.1541	4.7336
H	2.1703	-1.4663	6.0990
H	-1.9048	-0.6317	4.9393
H	-1.7923	-3.4894	0.9978
H	-5.3129	-4.7203	-5.1904
H	2.9891	-4.7076	-2.0915
H	-1.5672	-1.3853	-2.7913

Int₂_C

SCF done: -3347.669073

C	-2.0220	-0.5916	3.8461
C	-3.1580	0.0652	3.1768
N	-3.0465	1.0824	2.2865
C	-4.5774	-0.0409	3.5008
C	-4.3421	1.5203	2.0976
N	-5.2714	0.8682	2.8248
H	-1.7611	0.0178	4.7311
H	-1.1246	-0.6281	3.2276
H	-5.0381	-0.7105	4.2233
H	-4.5816	2.3544	1.4436
C	2.2589	-0.3433	6.1787
C	2.0209	0.2505	4.8422
N	2.1385	1.6025	4.5645
C	1.6470	-0.3139	3.6451
C	1.8445	1.8238	3.2620

N	1.5376	0.6680	2.6708	O	-2.2601	-0.5230	-2.2627
H	1.5368	0.0242	6.9193	Cu	-1.5334	1.7658	1.2238
H	3.2632	-0.1054	6.5530	Cu	-1.4684	-0.0785	-0.4247
H	2.4397	2.3136	5.2279	Cu	1.7436	0.9511	-1.6996
H	1.4596	-1.3578	3.4302	Cu	1.2056	0.3030	0.7387
H	1.8707	2.7976	2.7918	H	3.2729	5.3113	-5.6004
C	-0.7871	6.5727	3.7867	H	6.1640	-1.8739	-4.8310
C	-0.9490	5.5500	2.7444	H	-0.8801	6.1228	4.7788
N	-0.8788	5.8130	1.3889	H	2.1697	-1.4319	6.1326
C	-1.1890	4.2003	2.8324	H	-2.2835	-1.5717	4.2470
C	-1.0621	4.6640	0.7018	H	-1.7618	-3.6294	1.3394
N	-1.2533	3.6637	1.5614	H	-4.5463	-4.4824	-5.4979
H	-1.5525	7.3566	3.7085	H	3.0375	-4.7810	-2.0080
H	0.1918	7.0657	3.7282	H	-2.5884	0.2826	-2.7030
H	-0.7455	6.7339	0.9763	H	-1.6087	-0.8754	-2.8962
H	-1.3439	3.6030	3.7215				
H	-1.0477	4.5905	-0.3764				
C	3.2499	4.2417	-5.8483	Int₁_D			
C	2.4115	3.4852	-4.8958	SCF done:	-3347.180754		
N	1.0631	3.7207	-4.6934	C	-1.6000	0.6072	4.6467
C	2.7213	2.4665	-4.0248	C	-2.8254	0.7317	3.8197
C	0.6016	2.8860	-3.7348	N	-2.8626	1.2084	2.5458
N	1.5949	2.1046	-3.3058	C	-4.1740	0.3778	4.1566
H	2.8834	4.1468	-6.8783	C	-4.1907	1.1297	2.1768
H	4.2780	3.8712	-5.8244	N	-4.9955	0.6289	3.1250
H	0.5058	4.4064	-5.1991	H	-1.7222	1.1378	5.6017
H	3.6749	1.9769	-3.8867	H	-0.7217	1.0060	4.1305
H	-0.4182	2.8787	-3.3762	H	-4.5336	-0.0321	5.0967
C	5.4509	-2.3473	-4.1443	H	-4.5400	1.4552	1.2026
C	4.8270	-1.3511	-3.2362	C	2.4370	-0.1058	6.3617
N	5.5383	-0.5483	-2.3597	C	2.3179	0.4848	5.0132
C	3.5140	-0.9857	-3.0455	N	2.7162	1.7690	4.6815
C	4.6821	0.2553	-1.6848	C	1.8005	-0.0291	3.8516
N	3.4315	0.0068	-2.0793	C	2.4356	1.9982	3.3740
H	4.6830	-2.8358	-4.7510	N	1.8747	0.9152	2.8421
H	5.9904	-3.1245	-3.5885	H	1.8676	0.4646	7.1076
H	6.5518	-0.5378	-2.2614	H	3.4798	-0.1449	6.7031
H	2.6377	-1.3691	-3.5512	H	3.1690	2.4274	5.3104
H	4.9946	0.9887	-0.9535	H	1.3585	-1.0040	3.6911
C	2.1919	-4.6963	-1.3123	H	2.6379	2.9310	2.8643
C	2.2940	-3.4871	-0.4730	C	-0.6090	6.8102	3.9697
N	3.3125	-3.2347	0.4299	C	-0.8644	5.7323	2.9756
C	1.4938	-2.3766	-0.4092	N	-0.9865	5.9708	1.6169
C	3.1166	-2.0210	0.9987	C	-1.0310	4.3712	3.1033
N	2.0094	-1.4723	0.5020	C	-1.2089	4.8013	0.9729
H	1.2745	-4.6654	-1.9068	N	-1.2412	3.8050	1.8558
H	2.1683	-5.6162	-0.7141	H	-1.4091	7.5624	3.9631
H	4.0774	-3.8685	0.6528	H	0.3407	7.3252	3.7747
H	0.5911	-2.1718	-0.9703	H	-0.9487	6.8866	1.1775
H	3.7716	-1.5878	1.7434	H	-1.0398	3.7807	4.0099
C	-4.5195	-4.2691	-4.4234	H	-1.3360	4.7091	-0.0970
C	-4.1460	-2.8267	-4.2112	C	3.4280	4.4792	-5.6653
N	-4.1260	-2.5003	-2.7238	C	2.3584	3.5939	-5.1480
H	-5.5228	-4.4929	-4.0385	N	1.0378	3.6360	-5.5665
H	-3.8007	-4.9579	-3.9634	C	2.3919	2.5954	-4.2104
H	-3.1400	-2.6009	-4.5778	C	0.3276	2.6955	-4.9001
H	-4.8527	-2.1305	-4.6721	N	1.1316	2.0422	-4.0617
H	-3.5403	-1.6690	-2.5375	H	3.5874	4.3378	-6.7420
H	-3.7302	-3.2885	-2.1946	H	4.3715	4.2617	-5.1569
H	-5.0685	-2.3346	-2.3395	H	0.6642	4.2628	-6.2747
C	-1.9793	-2.7069	1.9050	H	3.2446	2.2357	-3.6532
C	-3.0884	-1.9784	1.2488	H	-0.7285	2.5150	-5.0487
N	-2.9357	-1.1047	0.2042	C	5.6290	-2.1098	-3.9613
C	-4.4967	-2.1326	1.4393	C	4.5472	-1.2933	-3.3539
C	-4.2208	-0.7304	-0.1275	N	4.7510	-0.4511	-2.2730
N	-5.1767	-1.3697	0.5544	C	3.2118	-1.1498	-3.6556
H	-2.2430	-3.0351	2.9107	C	3.5821	0.1614	-1.9581
H	-1.0494	-2.1333	1.9151	N	2.6232	-0.2512	-2.7814
H	-5.0044	-2.8021	2.1290	H	5.2366	-2.6827	-4.8063
H	-4.4284	0.0164	-0.8893	H	6.0569	-2.8201	-3.2421
S	-0.0721	1.5826	-0.5487	H	5.6414	-0.2981	-1.8085
				H	2.6529	-1.6324	-4.4474

H	3.4673	0.8673	-1.1463	C	-0.7169	6.8076	3.8977
C	2.3700	-4.4588	-1.1293	C	-0.7525	5.7211	2.9019
C	2.3709	-3.2578	-0.2637	N	-0.2711	5.8547	1.6108
N	3.2784	-3.0396	0.7620	C	-1.2184	4.4327	2.9721
C	1.5734	-2.1414	-0.2672	C	-0.4471	4.6879	0.9476
C	3.0187	-1.8396	1.3349	N	-1.0194	3.8019	1.7575
N	1.9824	-1.2664	0.7246	H	-1.2446	7.7029	3.5442
H	1.5769	-4.3775	-1.8783	H	0.3116	7.1053	4.1436
H	2.1986	-5.3815	-0.5586	H	0.1138	6.7084	1.2159
H	4.0028	-3.6873	1.0604	H	-1.7037	3.9359	3.8022
H	0.7562	-1.8957	-0.9346	H	-0.1657	4.5190	-0.0825
H	3.5758	-1.4317	2.1683	C	3.3201	4.4766	-5.7373
C	-4.9230	-4.3938	-3.9043	C	2.4759	3.8224	-4.7099
C	-5.6681	-5.1617	-2.8270	N	1.2001	4.2411	-4.3708
N	-6.2828	-4.2200	-1.8305	C	2.7103	2.7378	-3.9020
H	-4.0968	-3.8098	-3.4828	C	0.7117	3.4323	-3.3975
H	-5.5930	-3.7247	-4.4590	N	1.6157	2.5056	-3.0876
H	-6.4613	-5.7855	-3.2542	H	2.8419	4.4659	-6.7252
H	-4.9930	-5.8165	-2.2653	H	4.2759	3.9543	-5.8255
H	-6.7803	-4.7374	-1.0964	H	0.7064	5.0242	-4.7908
H	-6.9805	-3.6198	-2.2858	H	3.5957	2.1180	-3.8617
H	-5.4575	-3.5288	-1.3213	H	-0.2664	3.5409	-2.9477
C	-1.8680	-2.5238	2.0217	C	5.5211	-2.1124	-4.0333
C	-2.7888	-2.4056	0.8609	C	4.8004	-1.1393	-3.1687
N	-2.7023	-1.4289	-0.1164	N	5.4391	-0.2110	-2.3599
C	-3.8437	-3.2378	0.5116	C	3.4605	-0.9119	-2.9629
C	-3.6898	-1.7080	-1.0046	C	4.5067	0.5317	-1.7111
N	-4.3995	-2.7962	-0.6602	N	3.2869	0.1256	-2.0582
H	-2.3323	-3.1096	2.8226	H	4.8034	-2.7341	-4.5763
H	-1.6160	-1.5326	2.4202	H	6.1727	-2.7761	-3.4508
H	-4.2214	-4.1078	1.0370	H	6.4454	-0.0922	-2.2788
H	-3.8923	-1.1025	-1.8814	H	2.6111	-1.4172	-3.4034
S	-0.0563	1.7076	-0.2922	H	4.7478	1.3337	-1.0257
Cu	-1.4786	1.8674	1.3571	C	2.2621	-4.4614	-1.2013
Cu	-1.3914	-0.0194	-0.4061	C	2.3565	-3.2475	-0.3694
Cu	0.7508	0.4768	-2.9477	N	3.4470	-2.9032	0.4112
Cu	1.1822	0.5291	1.0305	C	1.4730	-2.2137	-0.2130
H	3.1957	5.5390	-5.4984	C	3.2069	-1.7047	1.0005
H	6.4453	-1.4808	-4.3394	N	2.0088	-1.2609	0.6315
H	-0.5634	6.3880	4.9775	H	1.2915	-4.4927	-1.7035
H	2.0498	-1.1289	6.3588	H	2.3588	-5.3809	-0.6090
H	-1.4056	-0.4435	4.9057	H	4.2808	-3.4679	0.5477
H	-0.9275	-3.0215	1.7418	H	0.4981	-2.0966	-0.6673
H	-4.5060	-5.1014	-4.6293	H	3.8957	-1.2062	1.6698
H	3.3224	-4.5747	-1.6634	C	-5.0309	-4.3964	-3.9763
O	-0.7294	-0.4905	-2.2346	C	-5.9390	-5.0932	-2.9763
H	-1.1346	-1.2569	-2.6712	N	-6.5056	-4.1040	-1.9931
Int₂_D							
SCF done: -3347.717189							
C	-1.7079	0.6046	4.5747	H	-6.7720	-5.5965	-3.4790
C	-2.9093	0.6007	3.7019	H	-5.3914	-5.8394	-2.3916
N	-2.9464	1.1367	2.4470	H	-7.0918	-4.5739	-1.2949
C	-4.2125	0.0873	3.9606	H	-7.1109	-3.4281	-2.4737
C	-4.2463	0.9249	2.0144	H	-5.6485	-3.5441	-1.4550
N	-5.0202	0.2912	2.8961	C	-1.9759	-2.5264	1.9497
H	-1.7852	1.3857	5.3477	C	-2.8618	-2.4943	0.7564
H	-0.7963	0.7800	3.9954	N	-2.7765	-1.5287	-0.2364
H	-4.5658	-0.3977	4.8660	C	-3.9136	-3.3293	0.4143
H	-4.5897	1.2588	1.0406	C	-3.7701	-1.8175	-1.1195
C	2.3291	-0.1084	6.2897	N	-4.4739	-2.9001	-0.7653
C	2.0833	0.4739	4.9451	H	-2.2085	-3.3962	2.5736
N	2.1399	1.8328	4.6754	H	-2.1102	-1.6248	2.5635
C	1.7408	-0.0990	3.7428	H	-4.2903	-4.1929	0.9506
C	1.8365	2.0447	3.3713	H	-3.9699	-1.2258	-2.0062
N	1.5843	0.8820	2.7737	S	-0.2484	1.6180	-0.4594
H	1.5869	0.2349	7.0214	Cu	-1.5629	1.9596	1.3887
H	3.3237	0.1580	6.6704	Cu	-1.6251	-0.0376	-0.2942
H	2.3986	2.5532	5.3443	Cu	1.5324	1.0095	-1.7312
H	1.5820	-1.1460	3.5200	Cu	1.1302	0.4846	0.8558
H	1.8031	3.0216	2.9086	H	3.5333	5.5230	-5.4821
				H	6.1458	-1.6013	-4.7780

H	-1.1996	6.4852	4.8245
H	2.2729	-1.1997	6.2424
H	-1.6068	-0.3478	5.1099
H	-0.9143	-2.5892	1.6694
H	-4.6495	-5.1355	-4.6893
H	3.0424	-4.4854	-1.9749
O	0.3126	-0.5017	-3.1440
H	-0.5862	-0.5639	-2.7706
H	0.1902	-0.0647	-4.0058

H₂O

SCF done: -76.4089533

O	0.4043	0.2268	0.0000
H	1.3643	0.2268	0.0000
H	0.0838	1.1317	0.0000

N₂O

SCF done: -184.6602738

N	0.0000	0.0000	0.0692
N	0.0000	0.0000	1.2021
O	0.0000	0.0000	-1.1124

N₂

SCF done: -109.5241291

N	0.4043	0.2268	0.0000
N	-0.2326	1.3301	0.0000

H

SCF done: -0.5002728

H	0.7396	0.7396	0.0000
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