

Supporting Information

The Cu_B site in particulate methane monooxygenase may be used to produce hydrogen peroxide

Kristoffer J. M. Lundgren,^a Lili Cao,^{ab} Magne Torbjörnsson,^a

Erik D. Hedegård,^a Ulf Ryde*^a

^a Department of Theoretical Chemistry, Lund University, Chemical Centre, P. O. Box 124,
SE-221 00 Lund, Sweden

^b Molecular AI, Discovery Sciences R&D AstraZeneca, Gothenburg, Sweden,
Pepparedsleden 1, SE-431 83 Mölndal, Sweden; lili.cao@astrazeneca.com

Correspondence to Ulf.Ryde@teokem.lu.se,

Tel: +46 – 46 2224502, Fax: +46 – 46 2228648

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Table S1. Coordinates of all intermediates discussed in the article.

1

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Energy = -4097.8991796111

C	-15.4948695	2.5087970	-0.1668285
H	-15.3019441	2.5596266	0.8774763
N	-16.6784546	2.0486177	-0.6924039
H	-17.4661218	1.6551870	-0.1500680
C	-16.6318861	2.2269585	-2.0211318
H	-17.4658237	2.0316244	-2.6915416
N	-15.4468545	2.7541018	-2.3615826
C	-14.7051649	2.9307034	-1.1980608
C	-13.3270589	3.5228790	-1.1228560
H	-12.5998187	2.9278012	-1.7091394
H	-13.0064732	3.5109492	-0.0661091
C	-13.3372615	4.9675616	-1.6383230
N	-13.6213484	4.9480707	-3.0883159
H	-13.7865300	5.9226033	-3.4015459
H	-12.7740940	4.5984345	-3.5676966
H	-14.1413762	5.5342090	-1.1405901
C	-11.9922605	5.7074477	-1.4979382
O	-10.9881434	5.2877887	-2.0827719
N	-12.0662021	6.8801140	-0.8109324
H	-12.9341605	7.1236937	-0.3203388
C	-10.9223731	7.7604159	-0.6528979
H	-10.6703211	7.8967596	0.4109303
H	-10.0923067	7.2437978	-1.1349339
C	-11.0501569	9.1530863	-1.2614392
O	-10.2370179	10.0323569	-0.9539856
N	-12.0659718	9.3284883	-2.1475413
H	-12.7921450	8.6041803	-2.1246680
C	-12.5729591	10.6911947	-2.3758451
H	-11.6835476	11.3179823	-2.5372340
C	-13.3930705	10.7495863	-3.6737861
H	-13.5275502	11.8051108	-3.9623955
H	-12.8173856	10.2958637	-4.5050470
C	-14.8222888	10.1596089	-3.6540495
H	-15.3088996	10.3310857	-2.6774717
H	-15.4032848	10.6773940	-4.4370566
C	-14.9099218	8.6814855	-3.9780140
O	-15.2375648	8.4002806	-5.1769495
O	-14.6988247	7.8085649	-3.0652471
H	-13.1302200	11.0027136	-1.4546556
H	-16.2779392	-0.2502530	-5.4812191
C	-16.5018864	0.4474260	-4.6394317
H	-17.1835770	-0.0934688	-3.9603982
H	-15.5744665	0.6688300	-4.0900990
C	-17.1633533	1.6919202	-5.1425345
N	-16.7228275	2.9914758	-4.9326676
C	-17.6177122	3.8061922	-5.5027236
H	-17.5393898	4.8902390	-5.6074432
N	-18.6046629	3.0797905	-6.0553222
H	-19.4081126	3.4632173	-6.5835552
C	-18.3443615	1.7531972	-5.8549433
H	-19.0057192	0.9776254	-6.2248235

H	-12.2885738	3.7381852	-9.0843505
C	-11.9651717	4.4639092	-8.3134959
H	-11.0099367	4.1284308	-7.8914732
H	-11.7717148	5.4502359	-8.7814070
C	-12.9774721	4.6518749	-7.2650353
N	-13.5428802	5.8900216	-7.0335246
H	-13.3920727	6.7485487	-7.5805497
C	-14.3950732	5.7843714	-5.9945742
H	-14.9212047	6.6414143	-5.5695503
N	-14.4022999	4.5278309	-5.5684708
C	-13.5193742	3.8015254	-6.3325775
H	-13.3019240	2.7547441	-6.1351703
Cu	-15.2082434	3.8967213	-3.9172188
O	-13.0267203	1.6456525	-3.8864852
H	-13.8841045	1.8277054	-3.4382593
H	-13.2842361	1.1291822	-4.7020283
O	-17.2675607	6.8976125	-6.0545255
H	-18.1225724	7.1998958	-5.6436895
H	-16.5852130	7.5850637	-5.7868557
O	-15.1911842	6.9668641	-0.2390369
H	-16.0989173	6.5935938	0.0279107
H	-15.2502787	7.4939492	-1.0706907
O	-16.4191027	5.8194058	-3.5326899
H	-16.8178512	6.1499462	-4.3844426
H	-15.7482741	6.5388724	-3.2938756

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Energy = -4097.9579962103

C	-15.4977497	2.9781440	-0.1762489
H	-15.7701944	3.8257811	0.4449584
N	-16.3573524	1.9423024	-0.4864808
H	-17.3002660	1.7776554	-0.1030163
C	-15.6907372	1.0939295	-1.3107542
H	-16.1198342	0.1768597	-1.7142701
N	-14.4513899	1.5253720	-1.5386633
C	-14.3083426	2.6993090	-0.8221520
C	-13.0398070	3.4992014	-0.8072407
H	-12.2818587	2.9856985	-1.4249524
H	-12.6456471	3.5896871	0.2232332
C	-13.2721043	4.9050756	-1.3802208
N	-13.7770162	4.7796661	-2.7681202
H	-13.9944519	5.7364549	-3.1087117
H	-12.9775049	4.4717397	-3.3463643
H	-14.0439558	5.4330682	-0.7989336
C	-11.9800724	5.7292408	-1.4271101
O	-10.9969659	5.3315070	-2.0657591
N	-12.0371513	6.9301213	-0.7797398
H	-12.8842378	7.1911770	-0.2636474
C	-10.8869412	7.8028896	-0.6747447
H	-10.5795978	7.9360616	0.3762971
H	-10.0906174	7.2783649	-1.2041257
C	-11.0326819	9.1979014	-1.2644940
O	-10.2436324	10.0946665	-0.9273495
N	-12.0357113	9.3618433	-2.1596637
H	-12.7343394	8.6066671	-2.1984437
C	-12.5736729	10.7093213	-2.3817912

H	-11.7028355	11.3622195	-2.5478900
C	-13.4053299	10.7614512	-3.6745044
H	-13.6108792	11.8211780	-3.9141123
H	-12.8032541	10.3836890	-4.5253594
C	-14.7863762	10.0698315	-3.6775293
H	-15.2883494	10.2000758	-2.7006977
H	-15.3992213	10.5562695	-4.4580952
C	-14.7581921	8.5821587	-4.0135256
O	-15.0891033	8.2659895	-5.1957599
O	-14.4388718	7.7504738	-3.0918785
H	-13.1315708	11.0084945	-1.4570780
H	-16.2996577	-0.2510652	-5.4756850
C	-16.5576239	0.4323851	-4.6216913
H	-17.2656480	-0.1358119	-3.9921771
H	-15.6366297	0.5632399	-4.0343389
C	-17.1827576	1.7341484	-4.9868693
N	-16.9365350	2.9062031	-4.2744377
C	-17.7792130	3.8255628	-4.7624329
H	-17.8374042	4.8569984	-4.4300833
N	-18.5365741	3.3017087	-5.7502025
H	-19.2733330	3.7701782	-6.2971357
C	-18.1863574	1.9807147	-5.9027930
H	-18.7300194	1.3281516	-6.5822126
H	-12.3085315	3.7454930	-9.0571400
C	-12.0269653	4.4752433	-8.2519717
H	-11.0091645	4.2261976	-7.9072579
H	-11.9632609	5.4864465	-8.7038852
C	-12.9873380	4.5128673	-7.1202573
N	-13.7041693	5.6550726	-6.7939783
H	-13.6625793	6.5644794	-7.2673823
C	-14.5055509	5.3523361	-5.7381915
H	-15.1722651	6.0832267	-5.2904851
N	-14.3381802	4.0867262	-5.3706416
C	-13.3849215	3.5559412	-6.2067239
H	-13.0361492	2.5289513	-6.1041158
Cu	-15.2906671	3.5956071	-3.4423355
O	-13.8086655	-0.2310881	-3.4416847
H	-13.8322477	0.5215933	-2.7792947
H	-13.7411952	0.1845678	-4.3410270
O	-17.2542860	7.0608154	-6.2623367
H	-18.0786076	7.3322809	-5.7881188
H	-16.5206339	7.6359012	-5.9019035
O	-15.1958751	7.0927936	-0.2184037
H	-16.0840220	6.6486745	-0.0434782
H	-15.1396408	7.4133424	-1.1504143
O	-16.7694021	6.4412330	-3.2779605
H	-17.0047916	6.6068694	-4.2196596
H	-15.8252153	6.7475314	-3.2005987

³³

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Energy = -4248.2102599403

C	-15.3908778	2.8875572	-0.0040754
H	-15.4153684	3.4977262	0.8852372
N	-16.4314189	2.0868352	-0.4388503
H	-17.2888799	1.8309615	0.0767808
C	-16.0978052	1.6035616	-1.6491981

H	-16.7472915	0.9498706	-2.2258331
N	-14.8888052	2.0511339	-2.0201511
C	-14.4121217	2.8314012	-0.9636859
C	-13.0889611	3.5357601	-0.9319997
H	-12.3416539	2.9907496	-1.5311844
H	-12.7347868	3.5795051	0.1144820
C	-13.2269174	4.9701573	-1.4756610
N	-13.6573493	4.9105624	-2.8828262
H	-14.0037282	5.8439445	-3.1640689
H	-12.8161988	4.7123758	-3.4538761
H	-14.0118693	5.4959986	-0.9090652
C	-11.9127583	5.7561732	-1.4079504
O	-10.8891823	5.3552102	-1.9708098
N	-12.0067435	6.9620741	-0.7675617
H	-12.8717414	7.2149019	-0.2772805
C	-10.8695183	7.8444778	-0.6333371
H	-10.5987876	8.0028270	0.4245997
H	-10.0450425	7.3225731	-1.1206816
C	-11.0152739	9.2216694	-1.2593545
O	-10.2244832	10.1263917	-0.9522123
N	-12.0285256	9.3649056	-2.1506606
H	-12.7278534	8.6123873	-2.1367691
C	-12.5746959	10.7080389	-2.3828330
H	-11.7038017	11.3605367	-2.5485838
C	-13.3989569	10.7549435	-3.6811078
H	-13.5681780	11.8136350	-3.9478148
H	-12.8048159	10.3373602	-4.5185297
C	-14.8030254	10.1117551	-3.6817264
H	-15.3116766	10.2862090	-2.7156953
H	-15.3864015	10.5992801	-4.4843764
C	-14.8294876	8.6168874	-3.9812402
O	-15.0651443	8.2822374	-5.1771188
O	-14.6645645	7.7924313	-3.0092822
H	-13.1324012	11.0077895	-1.4577823
H	-16.3095788	-0.2590433	-5.4926476
C	-16.5920671	0.4194804	-4.6615173
H	-17.3257853	-0.1451732	-4.0607732
H	-15.6789936	0.5360319	-4.0588756
C	-17.1756150	1.7335334	-5.0543954
N	-16.7239395	2.9169867	-4.4905616
C	-17.5072007	3.8920106	-4.9575984
H	-17.3981827	4.9484466	-4.7034542
N	-18.4462923	3.3775807	-5.7874989
H	-19.1734780	3.8798207	-6.3157764
C	-18.2591656	2.0150954	-5.8646942
H	-18.9369605	1.3827240	-6.4351778
H	-12.3060907	3.7572960	-9.0770505
C	-12.0226464	4.5119480	-8.3004594
H	-11.0177870	4.2619723	-7.9175141
H	-11.9444934	5.5111517	-8.7761274
C	-13.0101181	4.5662116	-7.2037842
N	-13.6933459	5.7073395	-6.8094293
H	-13.6622463	6.6309329	-7.2562880
C	-14.4725488	5.3790990	-5.7454788
H	-15.1153091	6.1016721	-5.2459465
N	-14.3036439	4.0918866	-5.4488512
C	-13.4037694	3.5749518	-6.3411497

H	-13.0649039	2.5438866	-6.2863654
Cu	-14.7665525	3.1493439	-3.7483116
O	-12.7255661	2.2653130	-3.8286565
O	-11.7127792	2.9831343	-4.1032953
O	-13.8808525	-0.2618481	-3.3626204
H	-13.9960354	0.5444173	-2.8023782
H	-13.6725688	0.1271260	-4.2513641
O	-17.2579686	7.3274036	-6.5781233
H	-18.0179686	7.2188900	-5.9654416
H	-16.5054603	7.6495836	-6.0165069
O	-15.1896517	7.1117957	-0.2146080
H	-16.0641689	6.6417083	-0.0538488
H	-15.1321756	7.4388925	-1.1477331
O	-16.9162669	6.3976295	-3.3421245
H	-17.5526008	7.0471705	-3.7120535
H	-16.0292992	6.8544146	-3.2328700

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Energy = -4248.1628756174

C	-15.5447380	3.2038567	-0.5146013
H	-15.8484557	4.1885045	-0.1676665
N	-16.4345088	2.1613223	-0.6879647
H	-17.4291985	2.1467203	-0.4530972
C	-15.7274919	1.0964463	-1.1498013
H	-16.1883626	0.1420909	-1.4088040
N	-14.4377902	1.3856272	-1.2649649
C	-14.3003949	2.7125885	-0.8829026
C	-12.9814613	3.4416074	-0.8691831
H	-12.2614782	2.8859358	-1.4915716
H	-12.5887248	3.5035427	0.1661406
C	-13.1149232	4.8681962	-1.4363574
N	-13.4921561	4.7830101	-2.8625986
H	-13.5121335	5.7345952	-3.2720467
H	-12.7194230	4.2348377	-3.3554209
H	-13.9058667	5.4080973	-0.8900520
C	-11.8149918	5.6812552	-1.3501759
O	-10.7410135	5.2686700	-1.7963574
N	-11.9812048	6.9452669	-0.8292613
H	-12.8884674	7.2199656	-0.4382479
C	-10.8635024	7.8415204	-0.6411172
H	-10.6034914	7.9605623	0.4266020
H	-10.0253839	7.3468796	-1.1342488
C	-11.0150035	9.2527176	-1.1859303
O	-10.3133060	10.1737522	-0.7213179
N	-11.9354263	9.4293134	-2.1517172
H	-12.5231735	8.6268491	-2.4469456
C	-12.5238491	10.7507430	-2.3667804
H	-11.6928074	11.4536858	-2.5335108
C	-13.3464200	10.7864838	-3.6661600
H	-13.6312888	11.8402959	-3.8592567
H	-12.7018711	10.4968180	-4.5204701
C	-14.6590488	9.9882254	-3.7183100
H	-15.1401049	9.9626283	-2.7190020
H	-15.3603578	10.4879317	-4.4125895
C	-14.5173127	8.5354605	-4.1834282
O	-15.3581000	8.1748187	-5.0836032

O	-13.6544747	7.7954318	-3.6551113
H	-13.1101009	11.0261558	-1.4496301
H	-16.2952446	-0.2497336	-5.4729365
C	-16.5438723	0.4341625	-4.6129867
H	-17.2861019	-0.1140665	-4.0046545
H	-15.6182692	0.5070937	-4.0122581
C	-17.1028581	1.7739587	-4.9589014
N	-16.7270002	2.9241525	-4.2671897
C	-17.5067703	3.9091472	-4.7270675
H	-17.4579458	4.9530152	-4.4163985
N	-18.3576915	3.4480867	-5.6799983
H	-19.0418878	3.9784759	-6.2313070
C	-18.1197694	2.0985208	-5.8390957
H	-18.7318956	1.4950020	-6.5082393
H	-12.2977199	3.7459241	-9.0741370
C	-11.9962732	4.4816726	-8.2880256
H	-11.0016177	4.1940337	-7.9090763
H	-11.8761332	5.4822292	-8.7561387
C	-12.9904767	4.5781361	-7.2010737
N	-13.6587696	5.7589760	-6.9109681
H	-13.5678416	6.6559487	-7.3995913
C	-14.5043230	5.5011514	-5.8772394
H	-15.1387923	6.2822248	-5.4665819
N	-14.4028619	4.2353494	-5.4996684
C	-13.4583643	3.6461510	-6.3042885
H	-13.1500285	2.6122225	-6.1571583
Cu	-14.8553971	3.3711287	-3.6219306
O	-13.1647272	2.1067066	-3.7885795
O	-11.9998126	2.7624396	-3.9088408
O	-13.9215523	-0.4060625	-3.3013914
H	-13.9125488	0.1367667	-2.4653576
H	-13.5694383	0.2807529	-3.9335337
O	-17.4121729	7.2995493	-6.6057207
H	-18.1295069	7.1643516	-5.9451496
H	-16.6737402	7.6797361	-6.0624109
O	-15.2779194	7.0285468	-0.2648175
H	-16.1197440	6.5849506	0.1076448
H	-15.3681252	6.8713626	-1.2456226
O	-16.1304793	6.2358160	-2.8555312
H	-15.9540400	6.8212864	-3.6342272
H	-15.5503482	5.4233703	-3.0135277

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Energy = -4248.7361929732

C	-15.4283890	2.4658789	-0.1964435
H	-15.1768776	2.4838918	0.8394141
N	-16.6512705	2.0562415	-0.6779719
H	-17.4280003	1.6678169	-0.1150538
C	-16.6664666	2.2951695	-2.0038380
H	-17.5332548	2.1407769	-2.6437311
N	-15.4946767	2.8148180	-2.3776719
C	-14.6866110	2.9105908	-1.2577919
C	-13.2900913	3.4626031	-1.2456942
H	-12.6248101	2.8691104	-1.9040302
H	-12.8979613	3.3934774	-0.2156014
C	-13.2981125	4.9309264	-1.7007354

N	-13.6017482	4.9798916	-3.1452344
H	-12.7783983	4.6686700	-3.7044197
H	-10.4074088	4.4794601	-3.1279290
H	-14.1046739	5.4683725	-1.1733220
C	-11.9807106	5.6808371	-1.4785129
O	-10.8951314	5.2707570	-1.9474086
N	-12.0841351	6.8570559	-0.8288853
H	-12.9809033	7.1070161	-0.3921767
C	-10.9484134	7.7494100	-0.6419248
H	-10.7373393	7.8893019	0.4296644
H	-10.0952800	7.2388200	-1.0882553
C	-11.0686430	9.1401740	-1.2588981
O	-10.2489530	10.0099866	-0.9452674
N	-12.0776750	9.3236859	-2.1491728
H	-12.8123151	8.6071441	-2.1504986
C	-12.5732044	10.6927215	-2.3762523
H	-11.6791887	11.3127555	-2.5362904
C	-13.3957380	10.7571348	-3.6715419
H	-13.5307277	11.8136464	-3.9540403
H	-12.8241269	10.3078858	-4.5076302
C	-14.8243114	10.1678791	-3.6480597
H	-15.3108265	10.3393440	-2.6714796
H	-15.4061549	10.6844399	-4.4308506
C	-14.9076050	8.6902243	-3.9731215
O	-15.2423513	8.4106271	-5.1676093
O	-14.6824343	7.8156990	-3.0621308
H	-13.1296882	11.0036942	-1.4544541
H	-16.2759976	-0.2507579	-5.4770794
C	-16.4961130	0.4442754	-4.6291640
H	-17.1998642	-0.0943543	-3.9693492
H	-15.5688496	0.6331994	-4.0613508
C	-17.1589877	1.6861892	-5.1368942
N	-16.7378699	2.9922978	-4.9350667
C	-17.6376576	3.7953783	-5.5135557
H	-17.5680316	4.8788966	-5.6239974
N	-18.6133742	3.0548373	-6.0657735
H	-19.4188835	3.4290850	-6.5967250
C	-18.3380888	1.7330899	-5.8550870
H	-18.9886144	0.9478609	-6.2233740
H	-12.2927434	3.7312078	-9.0813584
C	-11.9788609	4.4458269	-8.3018444
H	-11.0578507	4.0865212	-7.8309396
H	-11.7494815	5.4311497	-8.7544598
C	-13.0229273	4.6373855	-7.2864340
N	-13.5404805	5.8898059	-7.0284878
H	-13.3672380	6.7482444	-7.5682574
C	-14.3987656	5.7956289	-5.9942216
H	-14.9055740	6.6588033	-5.5603522
N	-14.4542593	4.5301849	-5.5983754
C	-13.6028070	3.7836279	-6.3791573
H	-13.4275935	2.7205236	-6.2127893
Cu	-15.2264814	3.9053797	-3.9452883
O	-10.0621826	4.0626138	-4.0177263
H	-13.8156151	5.9606145	-3.4086672
O	-11.1382801	4.0356086	-4.8068753
O	-14.1311152	-0.3262117	-2.1807126
H	-14.7287008	-1.1239733	-2.1989756

H	-14.6148054	0.3358861	-1.6433997
O	-17.2726326	6.8980077	-6.0663169
H	-18.1311658	7.1974298	-5.6618411
H	-16.5960086	7.5873751	-5.7968293
O	-15.1702392	6.9126671	-0.2670751
H	-16.0789972	6.5582919	0.0236981
H	-15.2549895	7.4673760	-1.0796777
O	-16.4376987	5.8347184	-3.5350880
H	-16.8307194	6.1535549	-4.3942737
H	-15.7635534	6.5494148	-3.3039811

6a

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Energy = -4248.7468389220

C	-15.5895038	3.0170291	-0.3772155
H	-15.9003854	3.9514156	0.0832178
N	-16.4582147	1.9671177	-0.6038920
H	-17.4218394	1.8672940	-0.2601205
C	-15.7417676	0.9710178	-1.1906824
H	-16.1779909	0.0214869	-1.5023827
N	-14.4699184	1.3154720	-1.3428666
C	-14.3519535	2.6016596	-0.8439003
C	-13.0507798	3.3583655	-0.8215819
H	-12.3171423	2.8234399	-1.4463566
H	-12.6605261	3.4237604	0.2135765
C	-13.2186656	4.7836816	-1.3764912
N	-13.6247016	4.6924024	-2.7982542
H	-13.6348835	5.6369298	-3.2064673
H	-12.8426678	4.1477877	-3.3112867
H	-14.0054767	5.3206316	-0.8237023
C	-11.9209252	5.6063981	-1.3385487
O	-10.8682875	5.2196701	-1.8442603
N	-12.0729154	6.8767403	-0.8065192
H	-12.9188333	7.0871845	-0.2678253
C	-10.9269163	7.7487856	-0.6434369
H	-10.6518299	7.8797229	0.4176042
H	-10.1092405	7.2198733	-1.1394371
C	-11.0379451	9.1405180	-1.2422129
O	-10.2275003	10.0288728	-0.9434204
N	-12.0578309	9.3172356	-2.1277424
H	-12.7790295	8.5916027	-2.0615172
C	-12.5448899	10.6829412	-2.3662934
H	-11.6352867	11.2881613	-2.4818789
C	-13.2742405	10.7550557	-3.7181949
H	-13.2584851	11.7797557	-4.1108520
H	-12.7078831	10.1634145	-4.4637578
C	-14.7605149	10.3445606	-3.7709130
H	-15.2996395	10.6390737	-2.8543026
H	-15.2258918	10.8471816	-4.6363786
C	-14.9772424	8.8763811	-3.9859774
O	-15.1955939	8.4559819	-5.1413392
O	-14.9929902	8.1189815	-2.9150055
H	-13.1223698	10.9982200	-1.4534720
H	-16.2867731	-0.2618204	-5.4732488
C	-16.5223216	0.4080024	-4.6118765
H	-17.2370001	-0.1477476	-3.9787154
H	-15.5924273	0.5167788	-4.0284974

C	-17.1425794	1.7021939	-4.9868879
N	-16.8513516	2.8933544	-4.3245128
C	-17.7342102	3.7865741	-4.7873559
H	-17.8378892	4.8164549	-4.4698401
N	-18.5425753	3.2401634	-5.7219943
H	-19.3006250	3.6968848	-6.2487228
C	-18.1888625	1.9193882	-5.8617925
H	-18.7572567	1.2455424	-6.4991709
H	-12.3037338	3.7378099	-9.0728677
C	-12.0117683	4.4616322	-8.2838474
H	-11.0391549	4.1518651	-7.8722401
H	-11.8556707	5.4592407	-8.7458797
C	-13.0264971	4.5918719	-7.2180553
N	-13.5593794	5.8278360	-6.8902546
H	-13.4201149	6.7072678	-7.4006800
C	-14.3808735	5.6412144	-5.8247416
H	-14.9070090	6.4664620	-5.3646237
N	-14.4092722	4.3674367	-5.4660119
C	-13.5589923	3.6975093	-6.3164436
H	-13.3430300	2.6385356	-6.1893332
Cu	-15.0082821	3.3825307	-3.6238512
O	-13.3086840	2.1189250	-3.8574574
H	-15.4838329	7.1311637	-3.1135548
O	-12.1531907	2.7902706	-3.9103103
O	-13.9298391	-0.4543181	-3.3694691
H	-13.8970233	0.1262743	-2.5596417
H	-13.6200848	0.1921372	-4.0586621
O	-17.1879656	6.7724243	-5.8938967
H	-18.0587977	7.0797101	-5.5211024
H	-16.5539263	7.5269463	-5.7569451
O	-15.1971988	6.9791899	-0.1865985
H	-16.1011255	6.5894892	0.0766604
H	-15.3133799	7.6842209	-0.8564766
O	-16.2997903	6.0758338	-3.3479847
H	-16.6163819	6.1745362	-4.3034774
H	-15.7832918	5.1568295	-3.3151788

TS6a/b

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Energy = -4248.7296744506

C	-15.6209723	3.0822799	-0.4336119
H	-15.9453989	4.0154373	0.0209171
N	-16.4619051	2.0000435	-0.6128995
H	-17.4179955	1.8822612	-0.2531458
C	-15.7253840	1.0086844	-1.1833093
H	-16.1381666	0.0391744	-1.4641249
N	-14.4675786	1.3861954	-1.3680824
C	-14.3788325	2.6911459	-0.9102814
C	-13.0911943	3.4710624	-0.8956341
H	-12.3508125	2.9628171	-1.5350763
H	-12.6904440	3.5163558	0.1371251
C	-13.2732951	4.9128781	-1.4013571
N	-13.7410496	4.8891461	-2.8149262
H	-13.6600612	5.8441881	-3.2032163
H	-12.9806433	4.3355233	-3.3453210
H	-14.0256506	5.4369512	-0.7895376
C	-11.9537771	5.7036721	-1.3715855

O	-10.9262934	5.2972669	-1.9145921
N	-12.0532924	6.9472038	-0.7878229
H	-12.8957019	7.1997428	-0.2610786
C	-10.8960104	7.8063261	-0.6546591
H	-10.6018102	7.9403203	0.4005634
H	-10.0936573	7.2700587	-1.1662967
C	-11.0233345	9.1973611	-1.2538788
O	-10.2329687	10.0963416	-0.9307713
N	-12.0291740	9.3611574	-2.1527405
H	-12.7313918	8.6118781	-2.1444976
C	-12.5612556	10.7110090	-2.3718891
H	-11.6860234	11.3564381	-2.5382634
C	-13.3927912	10.7685004	-3.6619471
H	-13.5510875	11.8255102	-3.9373649
H	-12.8187113	10.3332822	-4.5042085
C	-14.8083417	10.1515434	-3.6302945
H	-15.2859174	10.2951020	-2.6450708
H	-15.4114104	10.6647264	-4.3999162
C	-14.8581244	8.6763292	-3.9748247
O	-15.1985499	8.4237454	-5.1828328
O	-14.5978041	7.8038739	-3.0861441
H	-13.1239253	11.0115935	-1.4516210
H	-16.2862227	-0.2677737	-5.4709151
C	-16.5220092	0.3936558	-4.6056806
H	-17.2222169	-0.1694146	-3.9637328
H	-15.5888352	0.5216035	-4.0295396
C	-17.1654856	1.6682605	-4.9972090
N	-16.8571460	2.8873682	-4.3996895
C	-17.7412033	3.7631370	-4.8946655
H	-17.8170647	4.8174745	-4.6689567
N	-18.5682694	3.1753468	-5.7825152
H	-19.3321960	3.6180358	-6.3146950
C	-18.2267328	1.8482690	-5.8618067
H	-18.8061249	1.1463049	-6.4566367
H	-12.3014517	3.7364641	-9.0783552
C	-12.0053421	4.4601394	-8.2953660
H	-11.0336713	4.1518034	-7.8809680
H	-11.8496960	5.4577091	-8.7571778
C	-13.0229078	4.5899552	-7.2358504
N	-13.5224273	5.8302873	-6.8815118
H	-13.3640531	6.7190402	-7.3696858
C	-14.3370351	5.6477927	-5.8143952
H	-14.8035634	6.4968001	-5.3320699
N	-14.4015819	4.3675774	-5.4824538
C	-13.5751127	3.6918406	-6.3518095
H	-13.3806744	2.6274301	-6.2447121
Cu	-14.9913577	3.3201795	-3.7017628
O	-13.2708748	2.1934122	-3.8484115
H	-15.3199305	6.2441206	-3.1316032
O	-12.1845635	2.9726041	-3.9306308
O	-13.9129451	-0.3991015	-3.3637236
H	-13.8682725	0.2194475	-2.5814443
H	-13.6047498	0.2018829	-4.0910758
O	-17.0577843	6.7269969	-5.5367768
H	-17.9491321	7.0994787	-5.2797662
H	-16.3764442	7.5003282	-5.5281851
O	-15.2212158	7.1318103	-0.1869381

H	-16.0903866	6.6544835	0.0007767
H	-15.1591026	7.4145024	-1.1286036
O	-16.2403377	5.8181240	-3.3129307
H	-16.5839508	6.1706489	-4.2840221
H	-15.9361173	4.7631856	-3.3888043

6b

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Energy = -4248.7781024448

C	-15.5039875	3.2069401	-0.3766450
H	-15.8402920	4.1404692	0.0667803
N	-16.3505773	2.1395507	-0.6111655
H	-17.3296756	2.0436068	-0.3168875
C	-15.6040170	1.1460803	-1.1658080
H	-16.0170821	0.1846052	-1.4745024
N	-14.3333955	1.5083804	-1.2901909
C	-14.2466697	2.8027688	-0.8009561
C	-12.9408742	3.5582860	-0.7289540
H	-12.1945441	3.0297547	-1.3416181
H	-12.5799836	3.5962934	0.3175920
C	-13.0570963	5.0065858	-1.2347357
N	-13.4652119	4.9973013	-2.6693064
H	-13.6102340	5.9623055	-3.0729192
H	-12.7396306	4.3632500	-3.2524231
H	-13.8310060	5.5518591	-0.6709603
C	-11.7403246	5.7929794	-1.2359832
O	-10.7311865	5.3554007	-1.7876914
N	-11.8620109	7.0352521	-0.6881440
H	-12.7422178	7.3254176	-0.2482276
C	-10.7567320	7.9565454	-0.5846802
H	-10.4903281	8.1451408	0.4691954
H	-9.9100326	7.4685573	-1.0617290
C	-10.9634950	9.3177659	-1.2191941
O	-10.2351334	10.2542181	-0.8572477
N	-11.9402694	9.4323321	-2.1427953
H	-12.5768956	8.6330471	-2.2863585
C	-12.5425721	10.7503182	-2.3715720
H	-11.7126555	11.4475980	-2.5569898
C	-13.3968776	10.7648275	-3.6482298
H	-13.6669867	11.8163006	-3.8665948
H	-12.7886019	10.4393665	-4.5161380
C	-14.7268019	9.9805981	-3.6252773
H	-15.1596929	9.9681099	-2.6069270
H	-15.4361341	10.4835341	-4.3060887
C	-14.5812728	8.5418197	-4.1136197
O	-15.1351330	8.2999833	-5.2432101
O	-13.9248338	7.7227440	-3.4108579
H	-13.1154582	11.0275070	-1.4499596
H	-16.3105433	-0.2762167	-5.4765690
C	-16.5954603	0.3731121	-4.6221250
H	-17.2793234	-0.2149743	-3.9895793
H	-15.6765006	0.5515843	-4.0303339
C	-17.2604012	1.6284929	-5.0477872
N	-16.7780689	2.8611008	-4.6370533
C	-17.5667070	3.7914946	-5.1938644
H	-17.4308843	4.8724557	-5.1832208
N	-18.5339232	3.1943798	-5.9188521

H	-19.2742189	3.6625307	-6.4641648
C	-18.3628529	1.8330864	-5.8503827
H	-19.0427840	1.1483740	-6.3478640
H	-12.2967284	3.7500755	-9.0826682
C	-11.9910933	4.4951042	-8.3125432
H	-10.9890923	4.2235365	-7.9410993
H	-11.8893067	5.4914874	-8.7908867
C	-12.9563303	4.6015586	-7.2041156
N	-13.5908076	5.7881510	-6.8715989
H	-13.5264478	6.6858629	-7.3667493
C	-14.3334396	5.5603934	-5.7605609
H	-14.8873119	6.3615246	-5.2818375
N	-14.2028455	4.3003626	-5.3725058
C	-13.3456029	3.6854854	-6.2606414
H	-13.0373777	2.6465451	-6.1444377
Cu	-14.9213505	2.8817647	-4.0379989
O	-13.1056884	2.2514826	-3.6931521
H	-14.3616949	4.4754293	-2.7537613
O	-12.0685177	3.1004739	-3.7672614
O	-13.9172226	-0.3068774	-3.3316479
H	-13.7739788	0.3423734	-2.5871782
H	-13.6111214	0.2045417	-4.1214587
O	-17.1683477	6.8186266	-5.8966175
H	-18.0065154	7.1612816	-5.4848991
H	-16.4478586	7.5023894	-5.7002925
O	-15.2703098	7.0240908	-0.2687204
H	-16.1358375	6.5868396	0.0546143
H	-15.2938169	7.0077594	-1.2526933
O	-16.3710850	5.9262531	-3.2543710
H	-16.6230348	6.3353611	-4.1260433
H	-16.0482036	5.0328434	-3.5206933

TS6b/c

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Energy = -4248.7773915409

C	-15.5049465	3.1955384	-0.3503387
H	-15.8401314	4.1238641	0.1044744
N	-16.3507673	2.1302955	-0.5980337
H	-17.3285383	2.0281332	-0.3004129
C	-15.6042234	1.1457939	-1.1682191
H	-16.0158252	0.1870308	-1.4872847
N	-14.3343377	1.5127223	-1.2915177
C	-14.2477566	2.7994339	-0.7813775
C	-12.9441429	3.5573285	-0.6974468
H	-12.1900615	3.0229109	-1.2944215
H	-12.5986764	3.6040597	0.3536892
C	-13.0571875	4.9991705	-1.2239881
N	-13.4558990	4.9632343	-2.6568118
H	-13.5736280	5.9191221	-3.0772869
H	-12.6943656	4.2400799	-3.2519401
H	-13.8272690	5.5515372	-0.6609447
C	-11.7398971	5.7837963	-1.2301234
O	-10.7287501	5.3422933	-1.7760226
N	-11.8625063	7.0308536	-0.6925976
H	-12.7445252	7.3232668	-0.2582205
C	-10.7574604	7.9520428	-0.5873905
H	-10.4883544	8.1363170	0.4666488

H	-9.9119947	7.4662988	-1.0684785
C	-10.9659613	9.3163884	-1.2142128
O	-10.2453002	10.2543744	-0.8402237
N	-11.9368894	9.4328741	-2.1432697
H	-12.5642966	8.6292782	-2.3061547
C	-12.5413804	10.7496765	-2.3716852
H	-11.7132881	11.4494746	-2.5570098
C	-13.3939905	10.7613805	-3.6495283
H	-13.6725844	11.8115951	-3.8645358
H	-12.7805905	10.4444314	-4.5171262
C	-14.7161489	9.9634069	-3.6314822
H	-15.1430568	9.9316716	-2.6104659
H	-15.4352376	10.4690032	-4.3000254
C	-14.5592614	8.5319822	-4.1405573
O	-15.1316467	8.2944331	-5.2635731
O	-13.8796023	7.7136436	-3.4624752
H	-13.1151903	11.0268468	-1.4502183
H	-16.3104087	-0.2755757	-5.4769333
C	-16.5953328	0.3743985	-4.6230649
H	-17.2798009	-0.2138078	-3.9910518
H	-15.6762440	0.5490646	-4.0303749
C	-17.2584647	1.6336670	-5.0415811
N	-16.7862971	2.8603481	-4.6015663
C	-17.5742403	3.7979215	-5.1461372
H	-17.4461836	4.8784717	-5.1051533
N	-18.5308033	3.2113619	-5.8941920
H	-19.2694666	3.6843329	-6.4373682
C	-18.3547149	1.8490068	-5.8500831
H	-19.0308596	1.1713560	-6.3628665
H	-12.2970841	3.7510014	-9.0813815
C	-11.9929370	4.4970187	-8.3102016
H	-10.9906554	4.2270147	-7.9381665
H	-11.8927879	5.4935232	-8.7883790
C	-12.9599453	4.5998305	-7.2024370
N	-13.5983674	5.7825002	-6.8635924
H	-13.5310607	6.6859180	-7.3478807
C	-14.3497640	5.5451589	-5.7610358
H	-14.9091720	6.3433714	-5.2834459
N	-14.2217677	4.2807705	-5.3841349
C	-13.3555303	3.6752068	-6.2704674
H	-13.0457829	2.6362226	-6.1602041
Cu	-14.9162828	2.8839675	-4.0371318
O	-13.0996970	2.2631700	-3.7037366
H	-14.3668220	4.4700329	-2.7224001
O	-12.0778931	3.1407667	-3.7381614
O	-13.9123117	-0.2956591	-3.3307144
H	-13.7705460	0.3568270	-2.5882565
H	-13.6061550	0.2067818	-4.1258976
O	-17.1730058	6.8286910	-5.9142675
H	-18.0141238	7.1784150	-5.5170151
H	-16.4511061	7.5131659	-5.7228319
O	-15.2751772	7.0250963	-0.2749855
H	-16.1386606	6.5887814	0.0558903
H	-15.3054782	6.9934180	-1.2585494
O	-16.4042590	6.0218727	-3.2346584
H	-16.6622521	6.4194039	-4.1101784
H	-15.9950033	5.1687155	-3.5056400

6c

79

Energy = -4248.8139860172

C	-15.4383443	2.8744097	0.0046366
H	-15.4707953	3.4838418	0.8924016
N	-16.4673512	2.0679497	-0.4434412
H	-17.3256507	1.8038901	0.0657372
C	-16.1185020	1.5906924	-1.6516382
H	-16.7563955	0.9342612	-2.2371890
N	-14.9102354	2.0494296	-2.0039173
C	-14.4522500	2.8295030	-0.9444997
C	-13.1354211	3.5341799	-0.9107110
H	-12.4198225	2.9791734	-1.5381092
H	-12.7675071	3.5697282	0.1314353
C	-13.2914095	4.9766533	-1.4271822
N	-13.8096861	4.9864416	-2.8041987
H	-13.0251451	4.8064756	-3.4519711
H	-11.3852477	3.8265696	-3.1905651
H	-14.0295343	5.5002025	-0.7998980
C	-11.9672078	5.7310884	-1.4111151
O	-10.9644963	5.2852697	-2.0042123
N	-12.0083846	6.9395076	-0.7881652
H	-12.8655348	7.2140709	-0.2950203
C	-10.8653133	7.8187747	-0.6792157
H	-10.5649360	7.9564254	0.3732397
H	-10.0602983	7.3040398	-1.2012189
C	-11.0245252	9.2106539	-1.2727617
O	-10.2360257	10.1094479	-0.9411612
N	-12.0340327	9.3690185	-2.1615856
H	-12.7375074	8.6184818	-2.1932655
C	-12.5725356	10.7164013	-2.3830710
H	-11.6987484	11.3671392	-2.5385436
C	-13.3872934	10.7838595	-3.6871868
H	-13.5610258	11.8454758	-3.9345891
H	-12.7814877	10.3866667	-4.5264591
C	-14.7888119	10.1407504	-3.7203688
H	-15.3190988	10.3178912	-2.7658096
H	-15.3592557	10.6209114	-4.5363779
C	-14.7879148	8.6437720	-3.9956984
O	-15.1064386	8.2763496	-5.1670957
O	-14.4968814	7.8549760	-3.0310961
H	-13.1320151	11.0106261	-1.4578524
H	-16.3054652	-0.2651551	-5.4920503
C	-16.5808055	0.4045269	-4.6567636
H	-17.3368839	-0.1495641	-4.0741583
H	-15.6673566	0.4881669	-4.0433571
C	-17.1319573	1.7356308	-5.0350987
N	-16.6488690	2.8962895	-4.4504943
C	-17.4224048	3.8935060	-4.8807796
H	-17.3129331	4.9353779	-4.5951154
N	-18.3810129	3.4215590	-5.7138136
H	-19.0980972	3.9533135	-6.2245472
C	-18.2190137	2.0571952	-5.8268646
H	-18.9147199	1.4521756	-6.4060214
H	-12.3042781	3.7546913	-9.0759201
C	-12.0168467	4.5047231	-8.2969361

H	-11.0048984	4.2606627	-7.9289497
H	-11.9529063	5.5078177	-8.7668401
C	-12.9888075	4.5418546	-7.1862250
N	-13.6858677	5.6770279	-6.7938928
H	-13.6651198	6.5986595	-7.2434894
C	-14.4463189	5.3458594	-5.7181691
H	-15.0923674	6.0601837	-5.2139183
N	-14.2537276	4.0642802	-5.4188102
C	-13.3497994	3.5523343	-6.3078037
H	-12.9752015	2.5358400	-6.2082462
Cu	-14.6516869	3.0540058	-3.7542241
O	-12.6884987	2.4496688	-3.6648721
H	-15.8957517	6.8440761	-3.1441473
O	-11.6947921	3.4133788	-4.0539010
O	-13.8205059	-0.1606043	-3.3720362
H	-13.8911411	0.6394995	-2.7980961
H	-13.6045617	0.2347284	-4.2580158
O	-17.2522924	7.0547593	-6.2754594
H	-18.0812121	7.3320114	-5.8145085
H	-16.5163090	7.6114806	-5.8929483
O	-15.1971633	7.1212661	-0.2022331
H	-16.0804799	6.6630863	-0.0443917
H	-15.1524661	7.4896617	-1.1170255
O	-16.8532677	6.5790728	-3.1800132
H	-17.1290434	6.7654686	-4.1038736
H	-14.1412509	5.9399428	-3.0275228

6d

79

Energy = -4248.7890372711

C	-15.4457316	2.9575071	-0.1341514
H	-15.6809557	3.7489085	0.5688393
N	-16.3341482	1.9684023	-0.5096729
H	-17.2702300	1.7875001	-0.1157891
C	-15.7157198	1.1970647	-1.4333690
H	-16.1898190	0.3383607	-1.9035960
N	-14.4714437	1.6280432	-1.6669448
C	-14.2826766	2.7280333	-0.8387553
C	-13.0235979	3.5394527	-0.8099760
H	-12.2390216	3.0348653	-1.3958193
H	-12.6646851	3.6503818	0.2304878
C	-13.2721200	4.9377881	-1.4005380
N	-13.7759922	4.8095368	-2.7884832
H	-12.9769839	4.5068776	-3.3718756
H	-13.3838115	1.7768331	-3.1263121
H	-14.0462567	5.4632919	-0.8199255
C	-11.9809919	5.7636552	-1.4417160
O	-11.0000705	5.3789674	-2.0873772
N	-12.0358064	6.9522453	-0.7706608
H	-12.8803360	7.2080185	-0.2472988
C	-10.8828282	7.8195224	-0.6610751
H	-10.5835590	7.9594970	0.3913356
H	-10.0828220	7.2903482	-1.1806873
C	-11.0248394	9.2074128	-1.2655824
O	-10.2305992	10.1052122	-0.9478369
N	-12.0368938	9.3627094	-2.1545941
H	-12.7399751	8.6130264	-2.1518359

C	-12.5751864	10.7093824	-2.3817018
H	-11.7025309	11.3587374	-2.5509744
C	-13.4093988	10.7555083	-3.6722185
H	-13.5869702	11.8139774	-3.9357686
H	-12.8226525	10.3419509	-4.5168083
C	-14.8089398	10.1029047	-3.6529252
H	-15.3022672	10.2615851	-2.6765072
H	-15.4092444	10.5957125	-4.4390034
C	-14.8374311	8.6128798	-3.9756761
O	-15.1140389	8.3065169	-5.1688652
O	-14.6393237	7.7661163	-3.0267974
H	-13.1313039	11.0092089	-1.4565830
H	-16.2885180	-0.2497857	-5.4743233
C	-16.5248943	0.4371670	-4.6190332
H	-17.2084571	-0.1301728	-3.9589982
H	-15.5791642	0.5915555	-4.0759507
C	-17.1778450	1.7250966	-4.9927022
N	-16.9115439	2.9235787	-4.3381857
C	-17.7487034	3.8341063	-4.8531781
H	-17.7492070	4.8895358	-4.5824748
N	-18.5337282	3.2702713	-5.7969154
H	-19.2726110	3.7242631	-6.3543450
C	-18.2005351	1.9401283	-5.8959625
H	-18.7592994	1.2638948	-6.5389584
H	-12.3090951	3.7452204	-9.0593643
C	-12.0285178	4.4754572	-8.2565620
H	-11.0277492	4.2027334	-7.8845305
H	-11.9295981	5.4818213	-8.7137497
C	-13.0124360	4.5471976	-7.1482662
N	-13.7109632	5.7106393	-6.8543911
H	-13.6595244	6.6029257	-7.3595941
C	-14.5282885	5.4478252	-5.8009961
H	-15.1969117	6.1958569	-5.3805925
N	-14.3781251	4.1876360	-5.4042609
C	-13.4306265	3.6147581	-6.2210708
H	-13.0936657	2.5883573	-6.0762465
Cu	-15.2708346	3.6437341	-3.5348466
O	-12.5797194	1.9833598	-3.7243075
H	-14.0176964	5.7635941	-3.1204629
O	-11.5832611	1.2341630	-3.2502609
O	-14.0478480	-0.7427619	-3.0674332
H	-14.6636308	-1.3801032	-2.6017136
H	-13.8802304	-0.0057277	-2.4318324
O	-17.2815771	7.3700904	-6.6159686
H	-18.0337649	7.2121314	-6.0060974
H	-16.5415782	7.7068294	-6.0471150
O	-15.1916387	7.1180122	-0.2199317
H	-16.0703749	6.6567106	-0.0574081
H	-15.1221556	7.4232139	-1.1602491
O	-16.9012871	6.3757055	-3.3487592
H	-17.5217038	7.0151066	-3.7603992
H	-16.0073695	6.8231531	-3.2615892

7c

79

Energy = -4248.7534221946

C	-15.6211329	3.1049383	-0.4211308
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H	-15.9396824	4.0753301	-0.0497397
N	-16.4999535	2.0604305	-0.6355315
H	-17.4817951	2.0031884	-0.3503674
C	-15.7824903	1.0246096	-1.1443040
H	-16.2296506	0.0752376	-1.4407359
N	-14.5010988	1.3411162	-1.2632182
C	-14.3784646	2.6509233	-0.8271159
C	-13.0662235	3.3819561	-0.8395866
H	-12.4138504	2.8240580	-1.5330478
H	-12.6146290	3.4032476	0.1740273
C	-13.2345852	4.8322024	-1.3295938
N	-13.7503873	4.8627409	-2.7098470
H	-12.9950730	4.5464609	-3.3554495
H	-11.4158918	3.4646792	-3.1736988
H	-13.9671371	5.3518863	-0.6904467
C	-11.9243014	5.6184776	-1.3207994
O	-10.8822371	5.1888343	-1.8428483
N	-12.0315774	6.8905625	-0.8013023
H	-12.8927715	7.1529172	-0.3110048
C	-10.8953751	7.7739552	-0.6901953
H	-10.5736986	7.9072901	0.3588919
H	-10.0982176	7.2556034	-1.2260950
C	-11.0447993	9.1752223	-1.2621298
O	-10.2601460	10.0759007	-0.9074057
N	-12.0426867	9.3524643	-2.1586504
H	-12.7392188	8.5950206	-2.2307228
C	-12.5670509	10.7046977	-2.3772725
H	-11.6861919	11.3485683	-2.5289008
C	-13.3838068	10.7830254	-3.6783064
H	-13.5528328	11.8490762	-3.9164959
H	-12.7821851	10.3897795	-4.5227379
C	-14.7850618	10.1442099	-3.7081156
H	-15.3009037	10.2874228	-2.7394926
H	-15.3696132	10.6505434	-4.4981027
C	-14.8028506	8.6530060	-4.0369707
O	-15.2018254	8.3521900	-5.2026826
O	-14.4637820	7.8278306	-3.1274847
H	-13.1295611	11.0063206	-1.4558726
H	-16.2945221	-0.2626999	-5.4758172
C	-16.5441798	0.4035802	-4.6150843
H	-17.2954929	-0.1438922	-4.0173216
H	-15.6151778	0.4740575	-4.0120843
C	-17.0810574	1.7519058	-4.9430394
N	-16.6648028	2.8572618	-4.2095240
C	-17.4155179	3.8821048	-4.6204825
H	-17.3411550	4.9015176	-4.2436854
N	-18.2853133	3.4886436	-5.5923753
H	-18.9510080	4.0600949	-6.1214010
C	-18.0880531	2.1382151	-5.8101080
H	-18.7157513	1.5858915	-6.5088043
H	-12.3089294	3.7487159	-9.0644233
C	-12.0299613	4.4866562	-8.2662214
H	-11.0362520	4.2049441	-7.8767421
H	-11.9136922	5.4883683	-8.7334746
C	-13.0314886	4.5712571	-7.1776076
N	-13.6864750	5.7538922	-6.8468320
H	-13.6146284	6.6542277	-7.3321344

C	-14.5060778	5.4779319	-5.7902111
H	-15.1467561	6.2355482	-5.3465364
N	-14.3965606	4.2056142	-5.4387907
C	-13.4755013	3.6300742	-6.2769580
H	-13.1509948	2.6007233	-6.1225275
Cu	-14.7406308	3.1098622	-3.6388799
O	-12.8917908	2.2320604	-3.5896227
H	-15.9630291	6.8710783	-3.1415751
O	-11.8418137	3.2286565	-4.0356193
O	-13.8534435	-0.2648714	-3.3296430
H	-13.8667462	0.2797278	-2.4914248
H	-13.4893023	0.4083253	-3.9701283
O	-17.3402083	7.3386598	-6.5825422
H	-18.0880857	7.2613769	-5.9490564
H	-16.5796456	7.7041707	-6.0550739
O	-15.1972731	7.1524407	-0.2050496
H	-16.0604050	6.6575668	-0.0700123
H	-15.1049356	7.3987336	-1.1553158
O	-16.9365321	6.7882501	-2.9450827
H	-17.4002204	7.0253096	-3.7750823
H	-13.9932474	5.8291315	-2.9764269

7d

79

Energy = -4248.7702008130

C	-15.4736729	3.0040438	-0.4830368
H	-15.8418980	3.9534703	-0.0984982
N	-16.3058994	1.9220727	-0.6966237
H	-17.2936545	1.8440498	-0.4353197
C	-15.5373234	0.9252643	-1.2243265
H	-15.9532660	-0.0405368	-1.5146472
N	-14.2670151	1.2882557	-1.3365315
C	-14.2109980	2.6048542	-0.8939988
C	-12.9345672	3.4048388	-0.9133860
H	-12.2389435	2.9164120	-1.6165180
H	-12.4787505	3.4424585	0.0977861
C	-13.1619882	4.8486303	-1.4025732
N	-13.6509186	4.8335178	-2.7896424
H	-12.9284661	4.3922144	-3.3833669
H	-10.6626251	4.4404199	-3.4758681
H	-13.9259161	5.3456230	-0.7814686
C	-11.8816731	5.6849617	-1.3679747
O	-10.8221573	5.3267627	-1.9115964
N	-12.0093490	6.9187268	-0.7812469
H	-12.8793480	7.1589410	-0.2948953
C	-10.8843464	7.8159619	-0.6509426
H	-10.5969369	7.9615640	0.4056523
H	-10.0643280	7.3046335	-1.1579468
C	-11.0357403	9.2060535	-1.2441734
O	-10.2616866	10.1151068	-0.8892483
N	-12.0247974	9.3673633	-2.1527290
H	-12.7136081	8.6033703	-2.2313601
C	-12.5627878	10.7130864	-2.3766650
H	-11.6904315	11.3664159	-2.5352423
C	-13.3866691	10.7780983	-3.6733910
H	-13.5655239	11.8425673	-3.9143337
H	-12.7859461	10.3873389	-4.5195689

C	-14.7817097	10.1243888	-3.6902087
H	-15.2858141	10.2494318	-2.7129776
H	-15.3833746	10.6334409	-4.4652968
C	-14.7873640	8.6374210	-4.0403466
O	-15.2165422	8.3532371	-5.2004235
O	-14.4065926	7.8017093	-3.1587154
H	-13.1270284	11.0103156	-1.4549942
H	-16.2792285	-0.2537974	-5.4679165
C	-16.4984445	0.4262301	-4.5996710
H	-17.1690469	-0.1355170	-3.9224056
H	-15.5501979	0.6339534	-4.0658902
C	-17.1275267	1.7342813	-4.9460956
N	-16.7702895	2.8793062	-4.2412742
C	-17.5721591	3.8522752	-4.6850697
H	-17.5453836	4.8851197	-4.3414416
N	-18.4141121	3.3856444	-5.6489871
H	-19.1159023	3.9038939	-6.1900854
C	-18.1493899	2.0424053	-5.8245969
H	-18.7437020	1.4386906	-6.5094837
H	-12.3046867	3.7456724	-9.0614414
C	-12.0173269	4.4769469	-8.2587018
H	-11.0382564	4.1802254	-7.8518521
H	-11.8808599	5.4785371	-8.7206244
C	-13.0212651	4.5766241	-7.1746389
N	-13.6924274	5.7603261	-6.8907089
H	-13.6090145	6.6501713	-7.3934549
C	-14.5229554	5.5130911	-5.8372699
H	-15.1703788	6.2788374	-5.4196478
N	-14.4042324	4.2538550	-5.4454507
C	-13.4630684	3.6565314	-6.2505044
H	-13.1277815	2.6386024	-6.0391479
Cu	-14.8879701	3.2224808	-3.6915757
O	-10.6213499	2.6045495	-4.0626690
H	-15.8969484	6.7698762	-3.1823339
O	-10.6077521	4.0410210	-4.3867423
O	-13.1196420	2.2310718	-3.7251785
H	-13.2237447	1.4977597	-3.0818041
H	-11.6785539	2.4230427	-3.9847094
O	-17.3470622	7.3593994	-6.5932559
H	-18.0917250	7.2702375	-5.9575043
H	-16.5898167	7.7339312	-6.0668695
O	-15.1894100	7.1274410	-0.2184529
H	-16.0534218	6.6364872	-0.0744280
H	-15.0984246	7.3573548	-1.1728259
O	-16.8759694	6.7167061	-3.0068103
H	-17.3019630	6.9808115	-3.8478724
H	-13.8116587	5.7973102	-3.1239826

8b

80

Energy = -4249.3393925889

C	-15.4998439	2.8147609	-0.0609110
H	-15.4089842	3.1897172	0.9378860
N	-16.5977198	2.1572137	-0.5626187
H	-17.4003880	1.7888798	-0.0233114
C	-16.4252020	2.0307951	-1.8910011
H	-17.1734909	1.5951834	-2.5478603

N	-15.2506440	2.5528064	-2.2515416
C	-14.6382121	3.0331768	-1.1015343
C	-13.2863705	3.6738952	-1.0031711
H	-12.5676626	3.1286640	-1.6326227
H	-12.9572209	3.6146292	0.0502116
C	-13.3094654	5.1638673	-1.3590520
N	-13.8250867	5.4302754	-2.7453828
H	-13.1799308	5.0060290	-3.4698233
H	-11.4401527	4.1541785	-3.1868116
H	-14.0140101	5.6936619	-0.7008037
C	-11.9348678	5.8323666	-1.3272886
O	-10.9632296	5.3463597	-1.9330441
N	-11.9347253	7.0223608	-0.6882880
H	-12.7740157	7.3219192	-0.1761553
C	-10.7933226	7.9093847	-0.6118958
H	-10.5177788	8.0986577	0.4377206
H	-9.9684830	7.3903841	-1.0918233
C	-10.9744549	9.2630852	-1.2832283
O	-10.1641449	10.1603090	-1.0371551
N	-12.0214307	9.3826690	-2.1409069
H	-12.7491938	8.6676466	-2.0460357
C	-12.5650212	10.7293436	-2.3819083
H	-11.6884089	11.3732518	-2.5329595
C	-13.3567698	10.7881225	-3.7012325
H	-13.4491639	11.8356406	-4.0201573
H	-12.7707406	10.2985419	-4.5040528
C	-14.8050148	10.2547753	-3.7317866
H	-15.3451420	10.5212115	-2.8057454
H	-15.3204847	10.7167030	-4.5921240
C	-14.8635560	8.7585129	-3.9112220
O	-15.1122107	8.3135246	-5.0684471
O	-14.6635072	8.0189416	-2.8728318
H	-13.1282140	11.0168234	-1.4567659
H	-16.2998516	-0.2783661	-5.4857918
C	-16.5703532	0.3755760	-4.6422319
H	-17.2929717	-0.1926243	-4.0349744
H	-15.6661654	0.5514654	-4.0289522
C	-17.1941237	1.6435723	-5.1096469
N	-16.6078615	2.8688594	-4.8648223
C	-17.4144825	3.8057297	-5.3744701
H	-17.2304158	4.8785689	-5.4323798
N	-18.4934406	3.2156673	-5.9314987
H	-19.2623760	3.6797697	-6.4440622
C	-18.3753796	1.8554669	-5.7914905
H	-19.1220755	1.1768030	-6.1885314
H	-12.2925802	3.7566639	-9.0930987
C	-11.9811403	4.5140852	-8.3395170
H	-10.9919521	4.2401775	-7.9386458
H	-11.8669341	5.5040344	-8.8261903
C	-12.9714276	4.6231682	-7.2612395
N	-13.5865853	5.8042729	-6.8849401
H	-13.5166109	6.7092902	-7.3683719
C	-14.3600480	5.5470664	-5.8014342
H	-14.9350207	6.3147770	-5.2890615
N	-14.2534012	4.2594303	-5.4896637
C	-13.3983467	3.6681073	-6.3820383
H	-13.0875119	2.6295002	-6.2808746

Cu	-14.7489390	3.0274094	-4.0644628
O	-12.7779043	2.8159719	-3.7268476
H	-15.9275126	6.8627853	-3.0779722
O	-11.9059602	3.9343157	-4.0564433
H	-13.9377204	6.4759468	-2.9064049
O	-13.5538329	0.3741178	-3.4349857
H	-12.9557928	1.1504189	-3.2887144
H	-13.6042532	0.3457794	-4.4342456
O	-17.1944315	6.8864713	-6.0065034
H	-18.0549949	7.1910354	-5.6109931
H	-16.5081369	7.5618671	-5.7367185
O	-15.2310338	7.0507851	-0.1761391
H	-16.1412248	6.6609245	0.0743109
H	-15.2953114	7.6867061	-0.9253677
O	-16.4799065	6.0652529	-3.3106880
H	-16.8134417	6.2535703	-4.2260605
H	-14.8023930	5.0781147	-2.8866424

TS8b/d

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Energy = -4249.3211217857

C	-15.5173889	2.7878023	-0.0340054
H	-15.4628474	3.1694517	0.9617402
N	-16.6029912	2.1509370	-0.5801144
H	-17.4248597	1.7837641	-0.0693107
C	-16.3830177	2.0466382	-1.9013787
H	-17.1162370	1.6374254	-2.5905615
N	-15.1911724	2.5657692	-2.2165639
C	-14.6095144	3.0165515	-1.0290081
C	-13.2733813	3.6766694	-0.8042749
H	-12.4712326	3.1458713	-1.3399508
H	-13.0610640	3.6312470	0.2781466
C	-13.3132436	5.1582344	-1.2242630
N	-13.8664529	5.2416911	-2.6020626
H	-13.2423227	4.2767447	-3.1517821
H	-11.2672967	4.5090866	-3.5098833
H	-13.9804715	5.7187133	-0.5543322
C	-11.9616782	5.8609267	-1.3305095
O	-11.0518483	5.4481236	-2.0776160
N	-11.9098639	7.0227212	-0.6473630
H	-12.7141551	7.3163965	-0.0795653
C	-10.7687768	7.9101638	-0.6392992
H	-10.4225554	8.0871540	0.3911769
H	-9.9878240	7.3924399	-1.1869741
C	-10.9771819	9.2690631	-1.2870278
O	-10.1745917	10.1725865	-1.0335313
N	-12.0241159	9.3819562	-2.1430218
H	-12.7443434	8.6558946	-2.0629273
C	-12.5716951	10.7260046	-2.3838052
H	-11.6971758	11.3732796	-2.5362200
C	-13.3672581	10.7844586	-3.7000796
H	-13.4900489	11.8378585	-3.9929884
H	-12.7685281	10.3298004	-4.5142835
C	-14.7992877	10.2105527	-3.7371839
H	-15.3368144	10.4427630	-2.7995431
H	-15.3327630	10.6844660	-4.5802408
C	-14.8418733	8.7142707	-3.9545398

O	-15.1183143	8.3003161	-5.1223922
O	-14.6161417	7.9467480	-2.9498070
H	-13.1317085	11.0148316	-1.4578719
H	-16.2957414	-0.2771392	-5.4845214
C	-16.5575380	0.3786230	-4.6393834
H	-17.2665371	-0.1893824	-4.0152945
H	-15.6443151	0.5675030	-4.0434712
C	-17.1929407	1.6434922	-5.1033152
N	-16.6311042	2.8748839	-4.8302411
C	-17.4372571	3.8121287	-5.3429136
H	-17.2626399	4.8880096	-5.3849096
N	-18.4966549	3.2135711	-5.9249619
H	-19.2663215	3.6761758	-6.4393791
C	-18.3658603	1.8525515	-5.7998855
H	-19.1034408	1.1704908	-6.2093802
H	-12.2939365	3.7585961	-9.0913200
C	-11.9862521	4.5183200	-8.3360640
H	-10.9919593	4.2554387	-7.9386610
H	-11.8871401	5.5101473	-8.8216149
C	-12.9743249	4.6082928	-7.2534929
N	-13.5877498	5.7777820	-6.8401278
H	-13.5177661	6.6978729	-7.2940893
C	-14.3607208	5.4952512	-5.7636077
H	-14.9363164	6.2486762	-5.2294211
N	-14.2630902	4.1939686	-5.5026729
C	-13.4049065	3.6278761	-6.4042535
H	-13.0992602	2.5855403	-6.3414662
Cu	-14.7815150	3.0566230	-4.0592300
O	-12.6855840	3.2753438	-3.5225993
H	-15.8446068	6.8251256	-3.1201037
O	-11.5919931	3.8939227	-4.2507425
H	-13.7722000	6.2014842	-2.9917506
O	-13.3761221	0.6786123	-3.5215779
H	-12.8501067	1.5146655	-3.4452817
H	-13.4695069	0.5389231	-4.5095929
O	-17.1999755	6.8719698	-6.0252129
H	-18.0531740	7.1974456	-5.6320903
H	-16.4964486	7.5350711	-5.7575370
O	-15.2375826	7.1156810	-0.1628360
H	-16.1406201	6.6994328	0.0443481
H	-15.2442754	7.6269956	-1.0057731
O	-16.5041849	6.0939345	-3.3092781
H	-16.8428747	6.2968829	-4.2176964
H	-14.8937305	5.0832522	-2.6093623

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Energy = -4249.3804038105

C	-15.3845990	2.7037847	-0.1172124
H	-15.2402864	2.9954596	0.9011818
N	-16.5504748	2.1496668	-0.6048968
H	-17.3486356	1.7935597	-0.0473335
C	-16.4593759	2.1240999	-1.9436537
H	-17.2735429	1.8086336	-2.5923345
N	-15.2675137	2.6102517	-2.3362952
C	-14.5649308	2.9565516	-1.1824921
C	-13.1919528	3.5655492	-1.1553565

H	-12.4686255	2.9754436	-1.7508353
H	-12.8389661	3.5774997	-0.1095279
C	-13.2483619	5.0027217	-1.6955152
N	-13.5858457	4.9519520	-3.1301305
H	-11.5023940	2.2553105	-4.0172624
H	-10.8019713	4.5880143	-3.5881482
H	-14.0555675	5.5478923	-1.1780775
C	-11.9334341	5.7870858	-1.5498440
O	-10.8925758	5.4391825	-2.1364499
N	-12.0223034	6.9121117	-0.8051010
H	-12.9004787	7.1320731	-0.3204733
C	-10.8969228	7.8132698	-0.6217851
H	-10.6912619	7.9655085	0.4493261
H	-10.0364601	7.3134839	-1.0642465
C	-11.0346175	9.1919239	-1.2558698
O	-10.2287023	10.0789126	-0.9562909
N	-12.0497225	9.3474893	-2.1451098
H	-12.7718755	8.6197861	-2.1182569
C	-12.5713102	10.7037025	-2.3777549
H	-11.6896343	11.3393493	-2.5441598
C	-13.3959558	10.7518845	-3.6729549
H	-13.5348275	11.8057173	-3.9657270
H	-12.8208846	10.2971943	-4.5040423
C	-14.8227768	10.1565861	-3.6457833
H	-15.3080542	10.3294814	-2.6688340
H	-15.4077364	10.6692642	-4.4291780
C	-14.9032931	8.6774903	-3.9663858
O	-15.2292943	8.3937459	-5.1640470
O	-14.6842936	7.8064989	-3.0516591
H	-13.1288797	11.0080894	-1.4547395
H	-16.2798575	-0.2547645	-5.4785678
C	-16.5073254	0.4336458	-4.6312607
H	-17.1937870	-0.1185149	-3.9663058
H	-15.5825649	0.6381413	-4.0702174
C	-17.1668570	1.6866757	-5.1140569
N	-16.7373656	2.9830552	-4.8637984
C	-17.6208681	3.8057790	-5.4424853
H	-17.5397990	4.8899125	-5.5349680
N	-18.5929319	3.0884579	-6.0313828
H	-19.3890208	3.4782272	-6.5665965
C	-18.3333766	1.7585309	-5.8495426
H	-18.9893137	0.9880629	-6.2407263
H	-12.2937584	3.7352138	-9.0796641
C	-11.9822780	4.4554320	-8.3003007
H	-11.0442956	4.1167507	-7.8449852
H	-11.7770380	5.4433803	-8.7591822
C	-13.0163147	4.6341446	-7.2706754
N	-13.5542535	5.8761730	-7.0032563
H	-13.3950949	6.7416963	-7.5367393
C	-14.4013329	5.7614288	-5.9611147
H	-14.9144822	6.6179409	-5.5221914
N	-14.4344076	4.4935431	-5.5665066
C	-13.5730100	3.7717351	-6.3587389
H	-13.3575407	2.7201419	-6.1898608
Cu	-15.2007371	3.8739881	-3.8762502
O	-10.6158491	2.7318680	-4.0505774
H	-15.7217305	6.5224541	-3.2594688

O	-11.0358841	4.0867138	-4.4313304
H	-12.7728261	4.5869003	-3.6763934
O	-12.9491532	1.3641228	-3.8391177
H	-13.7525426	1.7723608	-3.4334717
H	-13.2666726	0.9760058	-4.7084208
O	-17.2500394	6.8671760	-6.0012791
H	-18.1061718	7.1808399	-5.5998835
H	-16.5672348	7.5623389	-5.7546297
O	-15.1737184	6.9215474	-0.2530290
H	-16.0862624	6.5675280	0.0246738
H	-15.2417999	7.4746529	-1.0675775
O	-16.3874296	5.7970517	-3.4966162
H	-16.7830122	6.1228370	-4.3537836
H	-13.7860270	5.9155118	-3.4536231

9a restrained

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Energy = -4249.4412791559

C	-15.5995603	3.1918520	-0.3744448
H	-15.9435015	4.1201309	0.0708213
N	-16.4210208	2.0958896	-0.5688252
H	-17.3848269	1.9657395	-0.2361752
C	-15.6626964	1.1217528	-1.1386795
H	-16.0559608	0.1477227	-1.4318464
N	-14.4120179	1.5264537	-1.3117601
C	-14.3500594	2.8282756	-0.8454098
C	-13.0732255	3.6210663	-0.8794043
H	-12.3924829	3.0796033	-1.5550868
H	-12.6269734	3.6755572	0.1351485
C	-13.2763051	5.0750696	-1.3651007
N	-13.8626051	5.2065744	-2.7336824
H	-13.1702649	4.7889396	-3.4124723
H	-11.4738039	3.7768988	-3.2212933
H	-13.9608969	5.5870068	-0.6718452
C	-11.9475016	5.8334142	-1.4011104
O	-10.9573823	5.4008917	-2.0064171
N	-11.9758303	7.0444290	-0.7679749
H	-12.8125838	7.3267343	-0.2454241
C	-10.8127313	7.8954969	-0.6453124
H	-10.5094984	8.0172969	0.4080038
H	-10.0185227	7.3715932	-1.1751733
C	-10.9618274	9.2918488	-1.2282059
O	-10.2144341	10.2080366	-0.8658131
N	-11.9415713	9.4350613	-2.1518792
H	-12.6024149	8.6526609	-2.1923135
C	-12.5420692	10.7526262	-2.3683686
H	-11.7121996	11.4492140	-2.5528694
C	-13.3850323	10.7739650	-3.6548140
H	-13.6518645	11.8214767	-3.8854636
H	-12.7754073	10.4338925	-4.5154849
C	-14.7341309	10.0127565	-3.6441629
H	-15.2059376	10.0528923	-2.6455623
H	-15.4044845	10.4896486	-4.3801996
C	-14.6087334	8.5715126	-4.0666417
O	-14.9929843	8.2099901	-5.1854992
O	-14.0447663	7.7999028	-3.1556178
H	-13.1157003	11.0283216	-1.4485866

H	-16.3038672	-0.2855405	-5.4776832
C	-16.5760578	0.3484588	-4.6169645
H	-17.3078555	-0.2234146	-4.0227981
H	-15.6560642	0.4553449	-4.0040196
C	-17.1642787	1.6620962	-4.9660746
N	-16.6907779	2.8011592	-4.3346146
C	-17.4656127	3.8067492	-4.7511188
H	-17.3723538	4.8434188	-4.4514781
N	-18.4026207	3.3610600	-5.6254521
H	-19.1177425	3.9026880	-6.1264552
C	-18.2304885	2.0010470	-5.7767461
H	-18.9062064	1.4119886	-6.3941587
H	-12.3005453	3.7500801	-9.0732543
C	-12.0055919	4.4915217	-8.2891075
H	-11.0058207	4.2215350	-7.9098855
H	-11.9075424	5.4935988	-8.7569763
C	-12.9967327	4.5562251	-7.1966249
N	-13.6750823	5.7175631	-6.8514842
H	-13.6146714	6.6231295	-7.3290057
C	-14.5016431	5.3999169	-5.8145372
H	-15.1900716	6.1110131	-5.3808710
N	-14.3717458	4.1274628	-5.4849304
C	-13.4306847	3.5890363	-6.3244056
H	-13.0786953	2.5658718	-6.1991978
Cu	-14.7400630	2.7450023	-3.8821768
O	-12.8496119	2.4173752	-3.5601370
H	-15.7468874	6.0180030	-3.1500091
O	-11.9950569	3.5639917	-4.0375479
H	-14.0051073	6.7933350	-3.2255182
O	-13.8222095	-0.1375516	-3.3334644
H	-13.7425710	0.5020427	-2.5677444
H	-13.5121822	0.4020050	-4.1056437
O	-17.2457931	6.9524801	-6.0849941
H	-18.0883174	7.2300315	-5.6381133
H	-16.5600925	7.6221908	-5.8368666
O	-15.2957691	7.1202502	-0.1653499
H	-16.1546433	6.6359937	0.1185118
H	-15.3222326	7.2053916	-1.1408049
O	-16.6032987	6.5111490	-3.1170033
H	-16.8622896	6.6102750	-4.0672382
H	-14.6340756	4.4964340	-2.7926949

9b

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Energy = -4249.4780874443

C	-15.6157066	3.1290644	-0.3663134
H	-15.9602481	4.0618680	0.0704500
N	-16.4525975	2.0583495	-0.6154150
H	-17.4275458	1.9454895	-0.3099071
C	-15.6947367	1.0732064	-1.1672126
H	-16.0982961	0.1124211	-1.4884142
N	-14.4272908	1.4474798	-1.2813409
C	-14.3565385	2.7364423	-0.7851138
C	-13.0609873	3.4983374	-0.7317427
H	-12.3466228	2.9570718	-1.3698649
H	-12.6731807	3.5388177	0.3057401
C	-13.2079898	4.9518150	-1.2061116

N	-13.7259163	5.0230192	-2.6107073
H	-13.0065019	4.5646493	-3.2886667
H	-11.3619398	3.5574199	-3.1327503
H	-13.9383261	5.4940220	-0.5863769
C	-11.8804335	5.7192183	-1.2551841
O	-10.8840812	5.2551593	-1.8239323
N	-11.9559987	6.9676484	-0.7162827
H	-12.8104364	7.2574048	-0.2270101
C	-10.8230285	7.8636552	-0.6378948
H	-10.5164032	8.0273293	0.4089698
H	-10.0136209	7.3511287	-1.1531187
C	-11.0029756	9.2397915	-1.2572217
O	-10.2227456	10.1484437	-0.9375806
N	-12.0123407	9.3809350	-2.1483305
H	-12.7113985	8.6268882	-2.1789777
C	-12.5589203	10.7258400	-2.3745072
H	-11.6900333	11.3796559	-2.5361281
C	-13.3837182	10.7857793	-3.6696054
H	-13.5598806	11.8452101	-3.9227362
H	-12.7908291	10.3823826	-4.5149214
C	-14.7841084	10.1415572	-3.6714122
H	-15.2917786	10.2924874	-2.7010038
H	-15.3799869	10.6306165	-4.4624032
C	-14.7762763	8.6574621	-3.9890394
O	-15.1490525	8.3351396	-5.1526305
O	-14.4243889	7.8336872	-3.0654752
H	-13.1239690	11.0165839	-1.4528288
H	-16.3141780	-0.2851080	-5.4823356
C	-16.6075885	0.3510381	-4.6306924
H	-17.3516967	-0.2197859	-4.0535459
H	-15.7015767	0.4629868	-4.0012745
C	-17.1776166	1.6663951	-5.0038896
N	-16.6115552	2.8120679	-4.4722956
C	-17.3424074	3.8408078	-4.9126261
H	-17.1639659	4.8855977	-4.6869593
N	-18.3521752	3.3950342	-5.6987126
H	-19.0484339	3.9518042	-6.2098312
C	-18.2670405	2.0198054	-5.7760690
H	-18.9999911	1.4384494	-6.3321440
H	-12.3045197	3.7504254	-9.0758997
C	-12.0147865	4.4945726	-8.2959855
H	-11.0209536	4.2159926	-7.9072761
H	-11.8988916	5.4904588	-8.7729527
C	-12.9986590	4.6024091	-7.1990228
N	-13.6389370	5.7906397	-6.8722582
H	-13.5924607	6.6747922	-7.3925903
C	-14.3900430	5.5549526	-5.7609756
H	-14.9924288	6.3307810	-5.2983327
N	-14.2502231	4.2994255	-5.3666568
C	-13.3898175	3.6908413	-6.2498503
H	-13.0638532	2.6587395	-6.1088518
Cu	-14.7275361	2.7199854	-3.9306316
O	-12.8826917	2.3655252	-3.4812440
H	-15.8332162	6.8489061	-3.1601333
O	-11.9819428	3.5093355	-3.9032908
H	-13.9275602	6.0078072	-2.9053880
O	-13.8617031	-0.2043928	-3.3477274

H	-13.7646177	0.4318219	-2.5830609
H	-13.5763263	0.3294599	-4.1325010
O	-17.2716587	7.0096280	-6.2145326
H	-18.1043993	7.2858388	-5.7553810
H	-16.5554726	7.6124059	-5.8720767
O	-15.2045511	7.0475772	-0.2159416
H	-16.1111056	6.6495786	-0.0028068
H	-15.2112668	7.4956078	-1.0933937
O	-16.7728255	6.5286294	-3.1882530
H	-17.0458282	6.6587204	-4.1254531
H	-14.5948700	4.4417377	-2.7216488

TS9b/c

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Energy = -4249.4764176096

C	-15.2945227	3.0762857	-0.0127353
H	-15.4004719	3.7373756	0.8352793
N	-16.2614508	2.1806626	-0.4290169
H	-17.1507297	1.9493670	0.0368500
C	-15.8152740	1.5959276	-1.5660253
H	-16.4030377	0.8725356	-2.1228203
N	-14.6089574	2.0577980	-1.8924248
C	-14.2494819	2.9726830	-0.9029289
C	-12.9246644	3.6841708	-0.8917582
H	-12.2161147	3.1630633	-1.5624552
H	-12.5290199	3.7159365	0.1407733
C	-13.0514142	5.1396061	-1.3831675
N	-13.4876236	5.1910081	-2.8092010
H	-12.6091711	4.9365100	-3.5386217
H	-10.8904725	4.8383406	-3.4317502
H	-13.8226845	5.6616420	-0.7929849
C	-11.7435768	5.9268601	-1.3270051
O	-10.7106540	5.5786896	-1.9247258
N	-11.8303702	7.0834604	-0.6335638
H	-12.7034728	7.3389419	-0.1571128
C	-10.7363988	8.0172620	-0.5321312
H	-10.5331128	8.2681388	0.5215409
H	-9.8535509	7.5262065	-0.9380652
C	-10.9348238	9.3323563	-1.2616994
O	-10.1460487	10.2552437	-1.0215936
N	-11.9708884	9.4115293	-2.1298238
H	-12.6610875	8.6511758	-2.0843708
C	-12.5647812	10.7323036	-2.3836409
H	-11.7180212	11.4120369	-2.5575943
C	-13.3887885	10.7551869	-3.6842583
H	-13.5979457	11.8109514	-3.9371296
H	-12.7720861	10.3738115	-4.5225825
C	-14.7656810	10.0556535	-3.7070720
H	-15.3042038	10.2296269	-2.7568342
H	-15.3527079	10.4995990	-4.5322780
C	-14.6875009	8.5555728	-3.9589831
O	-14.9284922	8.1366655	-5.1233667
O	-14.3871195	7.8098651	-2.9518551
H	-13.1287760	11.0170950	-1.4577363
H	-16.2840621	-0.2550100	-5.4793058
C	-16.5154268	0.4281957	-4.6274779
H	-17.1742128	-0.1474959	-3.9495742

H	-15.5692982	0.6402361	-4.0911069
C	-17.1786369	1.7173569	-4.9911995
N	-16.9869858	2.8370777	-4.2074300
C	-17.8023271	3.7602421	-4.6975099
H	-17.9065008	4.7737371	-4.3172266
N	-18.5063537	3.2909204	-5.7647856
H	-19.2246926	3.7729534	-6.3227212
C	-18.1291587	1.9821038	-5.9626031
H	-18.6199092	1.3651799	-6.7121883
H	-12.3331666	3.7562847	-9.0441161
C	-12.1042589	4.5002714	-8.2227241
H	-11.0636899	4.3334439	-7.8858899
H	-12.1419835	5.5201187	-8.6564068
C	-13.0410353	4.3921695	-7.0678769
N	-13.8565727	5.4009313	-6.5693201
H	-13.9500801	6.3563589	-6.9213133
C	-14.5351709	4.9003911	-5.4951412
H	-15.2774095	5.4724127	-4.9456596
N	-14.1743625	3.6359416	-5.2651955
C	-13.2562968	3.3248675	-6.2341046
H	-12.7610783	2.3673833	-6.2324937
Cu	-13.8917981	2.4658770	-3.6576560
O	-11.7542118	3.1362374	-3.6069330
H	-15.8392256	6.8016429	-3.0783336
O	-11.4910379	4.4970376	-4.1640208
H	-13.8624074	6.1499894	-3.0277742
O	-12.3641145	0.8390366	-4.0996082
H	-11.8483862	1.7133646	-4.2306683
H	-12.8746053	0.6650667	-4.9457774
O	-17.1439094	6.9537907	-6.1461441
H	-17.9739772	7.2587189	-5.7021924
H	-16.4061584	7.5322085	-5.8048235
O	-15.1837178	7.0693181	-0.2057469
H	-16.0810013	6.6383788	-0.0413237
H	-15.1455552	7.4951630	-1.0953388
O	-16.7836162	6.5290388	-3.1873519
H	-16.9359059	6.5311251	-4.1616753
H	-14.2319215	4.4737942	-2.9750458

9c

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Energy = -4249.5227510416

C	-15.3832998	2.8311993	-0.0176628
H	-15.2848741	3.3400708	0.9255130
N	-16.5203787	2.1690945	-0.4366558
H	-17.3275480	1.8765022	0.1360689
C	-16.3763699	1.8837785	-1.7442726
H	-17.1492223	1.4078543	-2.3437239
N	-15.1842601	2.3066255	-2.1677176
C	-14.5262716	2.8772718	-1.0881698
C	-13.1623677	3.4978793	-1.1469490
H	-12.5256637	2.9496030	-1.8694329
H	-12.6966068	3.4384944	-0.1462288
C	-13.2710829	4.9718255	-1.5840242
N	-13.7321659	5.0229718	-2.9782342
H	-11.7081933	3.4214240	-4.3760951
H	-10.8824677	4.5453574	-3.6598856

H	-14.0351152	5.4715600	-0.9666147
C	-11.9479647	5.7331756	-1.4612434
O	-10.8991208	5.3312993	-1.9921743
N	-12.0383004	6.9237681	-0.8043357
H	-12.9139555	7.1725543	-0.3296091
C	-10.9004380	7.8060118	-0.6474198
H	-10.6474984	7.9507740	0.4161545
H	-10.0685523	7.2887109	-1.1265685
C	-11.0363306	9.1922489	-1.2601726
O	-10.2389107	10.0870265	-0.9424394
N	-12.0465961	9.3517922	-2.1518404
H	-12.7549971	8.6085470	-2.1486131
C	-12.5763018	10.7024810	-2.3827574
H	-11.6964783	11.3441876	-2.5430335
C	-13.3932252	10.7580049	-3.6856105
H	-13.5362856	11.8166158	-3.9638515
H	-12.8046270	10.3184097	-4.5154908
C	-14.8125849	10.1508483	-3.6903722
H	-15.3279391	10.3541272	-2.7336292
H	-15.3747854	10.6385955	-4.5077172
C	-14.8738238	8.6531827	-3.9629908
O	-15.1006503	8.3028929	-5.1557373
O	-14.7465277	7.8427762	-2.9734916
H	-13.1332723	11.0055161	-1.4580588
H	-16.2958233	-0.2599286	-5.4866186
C	-16.5531030	0.4180573	-4.6473496
H	-17.2780514	-0.1401639	-4.0293060
H	-15.6273181	0.5476305	-4.0557597
C	-17.1647372	1.7142592	-5.0736035
N	-16.6917127	2.9363079	-4.6233830
C	-17.4978048	3.8823823	-5.1085179
H	-17.3776114	4.9532230	-4.9356691
N	-18.4781931	3.3108817	-5.8439112
H	-19.2280874	3.7836734	-6.3704249
C	-18.2910968	1.9465689	-5.8408273
H	-18.9877078	1.2787026	-6.3426702
H	-12.2982349	3.7556899	-9.0821801
C	-12.0011574	4.5084990	-8.3114385
H	-11.0168494	4.2436663	-7.8924625
H	-11.8948449	5.5055351	-8.7864824
C	-13.0087160	4.5809156	-7.2417054
N	-13.6651899	5.7358268	-6.8535207
H	-13.6067105	6.6561271	-7.3047131
C	-14.4622449	5.4327710	-5.7983459
H	-15.0901620	6.1673946	-5.2976592
N	-14.3264556	4.1391883	-5.5165903
C	-13.4296772	3.5939483	-6.3910586
H	-13.1038950	2.5586096	-6.3083961
Cu	-14.7593677	3.1238534	-3.9120377
O	-13.0010331	2.3212399	-3.8800309
H	-16.0790839	6.8484954	-3.2510315
O	-11.0952546	4.1963878	-4.5641161
H	-14.0989337	5.9685257	-3.1836542
O	-13.8011849	-0.1266409	-2.9277426
H	-14.4079092	0.1893675	-2.2309101
H	-13.4757940	0.7303336	-3.3466288
O	-17.2768805	7.3250830	-6.5733982

H	-18.0535422	7.2424298	-5.9774890
H	-16.5336687	7.6447906	-5.9974851
O	-15.1805162	7.0899647	-0.2277660
H	-16.0604687	6.6347624	-0.0542347
H	-15.1561302	7.4703213	-1.1432440
O	-16.9324538	6.3436885	-3.4000778
H	-17.5998017	6.9768471	-3.7460532
H	-12.9264284	4.8574213	-3.6102651

TS9b/d

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Energy = -4249.4716884635

C	-15.6076451	3.1194894	-0.3186584
H	-15.9657361	4.0369095	0.1389275
N	-16.4277765	2.0467951	-0.6134880
H	-17.4048398	1.9148467	-0.3218281
C	-15.6478114	1.0897123	-1.1847016
H	-16.0307601	0.1317740	-1.5385358
N	-14.3825272	1.4831602	-1.2653628
C	-14.3367987	2.7541039	-0.7247943
C	-13.0604410	3.5424445	-0.6292817
H	-12.3029861	3.0091094	-1.2195545
H	-12.7279680	3.6275347	0.4245424
C	-13.2197824	4.9757841	-1.1588931
N	-13.7861227	4.9909650	-2.5488907
H	-13.1769556	4.3715040	-3.1975617
H	-11.3666170	3.7347441	-3.1788482
H	-13.9354662	5.5426239	-0.5449672
C	-11.8951631	5.7394100	-1.2564133
O	-10.9091923	5.2705032	-1.8402771
N	-11.9528972	6.9873434	-0.7161489
H	-12.7982205	7.2874337	-0.2173458
C	-10.8119211	7.8726898	-0.6511508
H	-10.4863437	8.0282973	0.3911277
H	-10.0177342	7.3563800	-1.1853619
C	-10.9969168	9.2511569	-1.2610742
O	-10.2221929	10.1620277	-0.9350191
N	-12.0054783	9.3903063	-2.1527734
H	-12.6983553	8.6306214	-2.1924420
C	-12.5587019	10.7318295	-2.3757069
H	-11.6943380	11.3909675	-2.5397601
C	-13.3877254	10.7880167	-3.6680236
H	-13.5755010	11.8471097	-3.9160166
H	-12.7934709	10.3943280	-4.5169556
C	-14.7811388	10.1287505	-3.6662180
H	-15.2831132	10.2653590	-2.6906661
H	-15.3874733	10.6196537	-4.4480232
C	-14.7637738	8.6475095	-4.0002545
O	-15.1504198	8.3375157	-5.1632118
O	-14.3941451	7.8144515	-3.0927698
H	-13.1235349	11.0190791	-1.4529293
H	-16.3130946	-0.2845853	-5.4813906
C	-16.6044690	0.3525830	-4.6288769
H	-17.3358383	-0.2234734	-4.0404233
H	-15.6961114	0.4836468	-4.0072869
C	-17.1950615	1.6565288	-5.0104256
N	-16.6509163	2.8156211	-4.4865283

C	-17.3943906	3.8288948	-4.9424673
H	-17.2260361	4.8800781	-4.7410966
N	-18.3915734	3.3593893	-5.7299516
H	-19.0968245	3.9001115	-6.2475312
C	-18.2849863	1.9854980	-5.7923816
H	-19.0053926	1.3871157	-6.3461168
H	-12.3040592	3.7506777	-9.0761757
C	-12.0138813	4.4952122	-8.2966570
H	-11.0225408	4.2143804	-7.9032799
H	-11.8935087	5.4902030	-8.7743366
C	-13.0039651	4.6062153	-7.2061605
N	-13.6277886	5.7999574	-6.8691728
H	-13.5680718	6.6882957	-7.3807891
C	-14.3934105	5.5619368	-5.7687208
H	-14.9881648	6.3402013	-5.3017774
N	-14.2804369	4.2988835	-5.3930638
C	-13.4198921	3.6889007	-6.2738987
H	-13.1071605	2.6516569	-6.1458871
Cu	-14.7716603	2.7880936	-3.9439020
O	-12.9423595	2.5881852	-3.3303072
H	-15.8012746	6.8317001	-3.1731514
O	-11.9623315	3.5707455	-3.9557979
H	-13.8823702	5.9667512	-2.9188249
O	-13.8323751	-0.1530524	-3.3518332
H	-13.7102369	0.5090493	-2.6139318
H	-13.6028419	0.3577288	-4.1682165
O	-17.2688402	6.9926761	-6.1990919
H	-18.1011183	7.2724780	-5.7406543
H	-16.5536301	7.6039384	-5.8688604
O	-15.2184794	7.0671734	-0.2063119
H	-16.1201828	6.6558594	0.0076629
H	-15.2226749	7.4860616	-1.0972884
O	-16.7369230	6.4979533	-3.1995156
H	-17.0092648	6.6207068	-4.1386121
H	-14.7276888	4.5385479	-2.5575541

9d

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Energy = -4249.5428185574

C	-15.3984398	2.8774406	-0.2620245
H	-15.6550255	3.7008096	0.4000946
N	-16.2650584	1.8405239	-0.5458260
H	-17.1997791	1.6836430	-0.1381337
C	-15.6296464	1.0055831	-1.4106797
H	-16.0840053	0.0905019	-1.7885899
N	-14.4038129	1.4426540	-1.6940322
C	-14.2375449	2.6169682	-0.9711582
C	-12.9619274	3.4156292	-0.9854322
H	-12.2284678	2.9308190	-1.6541579
H	-12.5268151	3.4612253	0.0313005
C	-13.2110530	4.8483867	-1.4895925
N	-13.7088022	4.7680833	-2.8803221
H	-11.3124764	2.0327600	-3.8905754
H	-10.8272998	4.4180153	-3.4880360
H	-13.9952530	5.3378587	-0.8897017
C	-11.9434568	5.7096463	-1.4687391
O	-10.9074959	5.3721784	-2.0725417

N	-12.0434689	6.8888088	-0.8003725
H	-12.9129582	7.1181345	-0.3059115
C	-10.9125561	7.7865971	-0.6550425
H	-10.6560538	7.9245467	0.4082029
H	-10.0807717	7.2783786	-1.1432967
C	-11.0509933	9.1798798	-1.2525987
O	-10.2592155	10.0715175	-0.9093260
N	-12.0464331	9.3505208	-2.1546713
H	-12.7514155	8.6021659	-2.2054866
C	-12.5712930	10.7042503	-2.3788329
H	-11.6936198	11.3482157	-2.5424851
C	-13.4007664	10.7619690	-3.6717774
H	-13.5898796	11.8225651	-3.9182080
H	-12.8053639	10.3697788	-4.5206242
C	-14.7921916	10.0929471	-3.6691995
H	-15.2899708	10.2293796	-2.6911945
H	-15.4004983	10.5872696	-4.4479474
C	-14.7864536	8.6067597	-4.0069097
O	-15.1397883	8.3027280	-5.1854067
O	-14.4616693	7.7655312	-3.0956798
H	-13.1301488	11.0070702	-1.4558400
H	-16.2782213	-0.2507493	-5.4691196
C	-16.4960445	0.4348667	-4.6050564
H	-17.1553472	-0.1336286	-3.9231430
H	-15.5550097	0.6433233	-4.0689115
C	-17.1662122	1.7165236	-4.9728452
N	-16.9429498	2.8984427	-4.2733334
C	-17.8097446	3.7913700	-4.7683023
H	-17.8887300	4.8260443	-4.4510656
N	-18.5580019	3.2391580	-5.7481980
H	-19.3023404	3.6918434	-6.2998041
C	-18.1786287	1.9259091	-5.8884399
H	-18.7071309	1.2542349	-6.5610938
H	-12.3075092	3.7442703	-9.0594264
C	-12.0255985	4.4725404	-8.2555042
H	-11.0388815	4.1919522	-7.8560381
H	-11.9114456	5.4783364	-8.7101157
C	-13.0278461	4.5460564	-7.1668836
N	-13.6988176	5.7160850	-6.8473735
H	-13.6204174	6.6195498	-7.3278312
C	-14.5302637	5.4435561	-5.8075722
H	-15.1726650	6.1988208	-5.3680827
N	-14.4226468	4.1688489	-5.4464480
C	-13.4777498	3.6039976	-6.2680884
H	-13.1284091	2.5835670	-6.1365818
Cu	-15.2766248	3.6525107	-3.5393680
O	-10.4527284	2.5720478	-3.8736032
H	-15.7986005	6.7067924	-3.2365942
O	-10.9305986	3.8840878	-4.3322113
H	-12.9396166	4.4097908	-3.4793065
O	-12.6288706	1.0396750	-3.8061288
H	-13.3000687	1.1285979	-3.0560343
H	-13.1328455	0.8717772	-4.6481779
O	-17.2837481	7.0778021	-6.2737980
H	-18.1072618	7.3308598	-5.7872103
H	-16.5591507	7.6614159	-5.9101612
O	-15.1660832	7.0265211	-0.2511809

H	-16.0632400	6.6097319	-0.0617281
H	-15.1332401	7.3888127	-1.1696953
O	-16.7233460	6.3477858	-3.3383767
H	-16.9637779	6.5516445	-4.2721803
H	-13.9058890	5.7310679	-3.2116244

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82

Energy = -4213.6357995950

C	-15.4146970	2.8220752	-0.0105789
H	-15.3181672	3.3217365	0.9360527
N	-16.5461795	2.1602188	-0.4398914
H	-17.3517498	1.8594621	0.1295434
C	-16.3947023	1.8894745	-1.7495951
H	-17.1688617	1.4256402	-2.3569629
N	-15.2022004	2.3209942	-2.1618652
C	-14.5511112	2.8826227	-1.0721559
C	-13.1912397	3.5135770	-1.0906355
H	-12.5236605	2.9548260	-1.7730570
H	-12.7693471	3.4662013	-0.0700853
C	-13.2941084	4.9821576	-1.5411991
N	-13.7407315	5.0100835	-2.9418260
H	-14.0620756	5.9626868	-3.1863788
H	-12.9271125	4.7806309	-3.5335592
H	-14.0615388	5.4936774	-0.9386327
C	-11.9678903	5.7464820	-1.4440091
O	-10.9427527	5.3526801	-2.0103449
N	-12.0466683	6.9426848	-0.7842660
H	-12.9083146	7.1973652	-0.2888497
C	-10.8976841	7.8120678	-0.6481697
H	-10.6208193	7.9580829	0.4095773
H	-10.0827969	7.2812972	-1.1437492
C	-11.0295074	9.1970034	-1.2637362
O	-10.2281787	10.0924141	-0.9568985
N	-12.0451201	9.3536121	-2.1513219
H	-12.7536902	8.6107112	-2.1280887
C	-12.5775132	10.7025889	-2.3826135
H	-11.6981547	11.3455481	-2.5434796
C	-13.3958729	10.7565987	-3.6851861
H	-13.5427573	11.8150323	-3.9634738
H	-12.8060511	10.3187950	-4.5152457
C	-14.8134122	10.1432770	-3.6892118
H	-15.3265667	10.3416111	-2.7303961
H	-15.3790823	10.6324896	-4.5035780
C	-14.8670629	8.6458119	-3.9681872
O	-15.0764451	8.2978969	-5.1660633
O	-14.7484464	7.8330529	-2.9811973
H	-13.1339474	11.0055378	-1.4578953
H	-16.2890650	-0.2584150	-5.4838595
C	-16.5339627	0.4223828	-4.6410471
H	-17.2478631	-0.1327821	-4.0076599
H	-15.6091359	0.5896184	-4.0589959
C	-17.1536996	1.7152286	-5.0730475
N	-16.6751161	2.9388611	-4.6373718
C	-17.4874263	3.8798333	-5.1200635
H	-17.3720365	4.9513823	-4.9454997
N	-18.4751327	3.3030413	-5.8430857

H	-19.2317149	3.7718714	-6.3640330
C	-18.2876740	1.9389582	-5.8319385
H	-18.9888433	1.2685320	-6.3238764
H	-12.2918566	3.7581049	-9.0845584
C	-11.9793316	4.5146232	-8.3198242
H	-10.9693302	4.2580732	-7.9577408
H	-11.9003624	5.5116439	-8.8003871
C	-12.9433506	4.5874271	-7.2105608
N	-13.6639521	5.7239246	-6.8722852
H	-13.6336028	6.6361385	-7.3432321
C	-14.4646890	5.4126907	-5.8212110
H	-15.1266985	6.1343700	-5.3446815
N	-14.2697728	4.1385029	-5.4931806
C	-13.3240382	3.6111225	-6.3270073
H	-12.9677520	2.5883401	-6.2106513
Cu	-14.7448990	3.1211860	-3.8917818
O	-12.9681874	2.3776203	-3.8253412
C	-9.4581443	3.0246634	-3.8549058
H	-9.6859471	3.7402466	-3.0449873
H	-8.9226634	3.5656420	-4.6612634
H	-8.8386276	2.1781513	-3.4970418
H	-10.4341312	2.6442182	-4.2150571
O	-13.2931971	0.1802364	-2.2699066
H	-14.2271581	0.2839027	-2.0067731
H	-13.1543211	0.9567918	-2.9013954
O	-17.2508087	7.3494776	-6.5812150
H	-18.0183411	7.2522044	-5.9761594
H	-16.5044438	7.6772885	-6.0123431
O	-15.1962551	7.1163216	-0.2078314
H	-16.0689399	6.6443356	-0.0372477
H	-15.1593113	7.4670306	-1.1338019
O	-16.9322297	6.3337811	-3.4165995
H	-17.5976759	6.9780845	-3.7454853
H	-16.0752472	6.8320501	-3.2614293

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Energy = -4213.6118609380

C	-15.4181790	2.8432425	0.0034419
H	-15.3370320	3.3514743	0.9464781
N	-16.5375178	2.1671864	-0.4368686
H	-17.3494628	1.8640999	0.1221226
C	-16.3620569	1.8886288	-1.7417663
H	-17.1220376	1.4118721	-2.3564288
N	-15.1681741	2.3295553	-2.1401324
C	-14.5383541	2.9038590	-1.0439508
C	-13.1755600	3.5282095	-1.0375190
H	-12.5182847	2.9543157	-1.7098459
H	-12.7713172	3.4809811	-0.0100315
C	-13.2620791	4.9964290	-1.4896170
N	-13.7004814	5.0358270	-2.8948286
H	-14.0370738	5.9867935	-3.1267948
H	-12.8818171	4.8471848	-3.4900356
H	-14.0324661	5.5118425	-0.8946471
C	-11.9382833	5.7603890	-1.3754353
O	-10.8928980	5.3588010	-1.9019863
N	-12.0294630	6.9741974	-0.7544228

H	-12.8934366	7.2394859	-0.2680660
C	-10.8813080	7.8450830	-0.6253234
H	-10.6088659	8.0076049	0.4313806
H	-10.0614644	7.3101326	-1.1084399
C	-11.0176610	9.2184933	-1.2616341
O	-10.2196435	10.1199049	-0.9650857
N	-12.0338628	9.3620775	-2.1512904
H	-12.7391871	8.6163552	-2.1204622
C	-12.5757485	10.7073275	-2.3834610
H	-11.7015508	11.3558004	-2.5457268
C	-13.3961571	10.7592566	-3.6842728
H	-13.5440916	11.8177451	-3.9614359
H	-12.8073044	10.3223978	-4.5153218
C	-14.8131948	10.1459461	-3.6878844
H	-15.3272540	10.3425513	-2.7292147
H	-15.3783816	10.6342413	-4.5029205
C	-14.8666397	8.6491018	-3.9658082
O	-15.0840970	8.3019795	-5.1624353
O	-14.7399229	7.8370541	-2.9794348
H	-13.1329318	11.0073838	-1.4581894
H	-16.2867801	-0.2591783	-5.4827201
C	-16.5269754	0.4202986	-4.6376352
H	-17.2391412	-0.1337566	-4.0012447
H	-15.5983794	0.5894585	-4.0625946
C	-17.1384032	1.7175453	-5.0644985
N	-16.6427962	2.9357560	-4.6318136
C	-17.4495448	3.8847890	-5.1095711
H	-17.3252184	4.9552415	-4.9339196
N	-18.4494871	3.3183602	-5.8258318
H	-19.2016185	3.7941599	-6.3461703
C	-18.2750653	1.9522905	-5.8159791
H	-18.9835699	1.2878713	-6.3059630
H	-12.2949474	3.7561739	-9.0856501
C	-11.9882433	4.5105763	-8.3209776
H	-10.9825862	4.2489545	-7.9501017
H	-11.9021507	5.5080377	-8.7995958
C	-12.9587665	4.5847769	-7.2168034
N	-13.6531801	5.7336608	-6.8657350
H	-13.6232924	6.6426357	-7.3432045
C	-14.4311274	5.4386405	-5.7925701
H	-15.0703271	6.1739734	-5.3053302
N	-14.2442407	4.1647237	-5.4614364
C	-13.3374840	3.6147845	-6.3240165
H	-13.0056379	2.5835297	-6.1955265
Cu	-14.7116287	3.1212972	-3.8697901
O	-13.0340872	2.1246183	-3.8487496
C	-10.7360554	3.1145493	-4.1193445
H	-10.6239622	3.8188743	-3.2774766
H	-10.7033425	3.6118753	-5.1053087
H	-10.0910186	2.2195033	-4.0508462
H	-11.9463523	2.6047553	-4.0292842
O	-13.1823970	0.2143377	-2.0179052
H	-14.1467811	0.2588067	-1.8667615
H	-13.0399914	0.9479906	-2.7024364
O	-17.2589509	7.3430369	-6.5860756
H	-18.0266097	7.2421014	-5.9818786
H	-16.5139674	7.6686133	-6.0154383

O	-15.1996006	7.1218657	-0.2039772
H	-16.0686180	6.6420388	-0.0348396
H	-15.1597897	7.4632746	-1.1329765
O	-16.9297707	6.3414131	-3.4080918
H	-17.5938337	6.9853120	-3.7401275
H	-16.0720522	6.8375578	-3.2548279

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82

Energy = -4213.6260926030

C	-15.4143504	2.8476683	-0.0024291
H	-15.3380048	3.3620711	0.9384812
N	-16.5248839	2.1531550	-0.4371622
H	-17.3381884	1.8516332	0.1210215
C	-16.3401744	1.8588280	-1.7372328
H	-17.0934313	1.3652946	-2.3465626
N	-15.1508382	2.3093602	-2.1404140
C	-14.5321365	2.9088960	-1.0482234
C	-13.1804416	3.5596964	-1.0333358
H	-12.4790831	2.9706542	-1.6448735
H	-12.8218795	3.5792496	0.0118279
C	-13.2756963	4.9991592	-1.5679508
N	-13.6939419	4.9560354	-2.9740441
H	-13.9457817	5.9104788	-3.2797524
H	-12.8876466	4.6164274	-3.5249763
H	-14.0509504	5.5405069	-1.0030089
C	-11.9542785	5.7726929	-1.4852757
O	-10.9365120	5.4089257	-2.0858012
N	-12.0293680	6.9460551	-0.7858161
H	-12.8904198	7.1864512	-0.2825121
C	-10.8885358	7.8233093	-0.6443718
H	-10.6175853	7.9705922	0.4146894
H	-10.0670570	7.3021947	-1.1385467
C	-11.0272724	9.2062678	-1.2614441
O	-10.2311713	10.1061857	-0.9535335
N	-12.0412922	9.3572795	-2.1516482
H	-12.7478655	8.6119160	-2.1306932
C	-12.5781830	10.7038712	-2.3831156
H	-11.7028932	11.3512364	-2.5466998
C	-13.4011818	10.7566839	-3.6823862
H	-13.5645122	11.8165824	-3.9477347
H	-12.8083857	10.3370950	-4.5199833
C	-14.8099661	10.1227318	-3.6858167
H	-15.3173809	10.2979588	-2.7192939
H	-15.3897255	10.6167831	-4.4872844
C	-14.8480975	8.6284111	-3.9858853
O	-15.0786364	8.2949838	-5.1853072
O	-14.6969629	7.8034376	-3.0153663
H	-13.1340224	11.0060453	-1.4580947
H	-16.2887369	-0.2602647	-5.4839995
C	-16.5332272	0.4180734	-4.6403790
H	-17.2406281	-0.1400816	-4.0023081
H	-15.6073004	0.5964354	-4.0622950
C	-17.1533472	1.7116157	-5.0647011
N	-16.6747903	2.9254449	-4.6042569
C	-17.4827445	3.8760321	-5.0764791
H	-17.3651767	4.9441721	-4.8811555

N	-18.4667411	3.3131790	-5.8170700
H	-19.2196609	3.7910152	-6.3348008
C	-18.2814922	1.9483403	-5.8281127
H	-18.9809591	1.2867614	-6.3349312
H	-12.2962348	3.7617821	-9.0835726
C	-11.9939061	4.5237991	-8.3181997
H	-10.9912583	4.2652212	-7.9359543
H	-11.9048601	5.5180542	-8.8023469
C	-12.9781975	4.5994010	-7.2250939
N	-13.6706219	5.7385588	-6.8425854
H	-13.6295746	6.6648557	-7.2842288
C	-14.4737491	5.4080398	-5.7979578
H	-15.1208528	6.1287372	-5.3003918
N	-14.3099467	4.1183427	-5.5118879
C	-13.3862601	3.6056152	-6.3767982
H	-13.0620199	2.5701871	-6.3360470
Cu	-14.7291084	3.1009635	-3.8852728
O	-12.8651804	2.3967548	-3.7760746
C	-9.4835623	2.9163896	-3.8025650
H	-9.9616704	3.8252942	-3.4081717
H	-8.4356551	2.9190039	-4.1408815
H	-10.0309742	1.9668160	-3.7406683
H	-12.6660874	1.8589746	-4.5691034
O	-12.9827158	0.3544787	-2.0519800
H	-13.9331972	0.3731104	-1.8263831
H	-12.9085765	1.1412541	-2.6911334
O	-17.2615097	7.3313151	-6.5809352
H	-18.0295653	7.2416197	-5.9754030
H	-16.5153394	7.6683759	-6.0176275
O	-15.1967805	7.1335844	-0.2086478
H	-16.0621847	6.6468729	-0.0480372
H	-15.1386653	7.4439899	-1.1472001
O	-16.9101591	6.3379222	-3.4021026
H	-17.5503041	7.0023271	-3.7384939
H	-16.0324772	6.8047590	-3.2622109

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Energy = -4213.7073487984

C	-15.5007277	2.8499072	-0.2897790
H	-15.8068040	3.6922346	0.3246172
N	-16.3288876	1.7877741	-0.5909061
H	-17.2733713	1.6193791	-0.2122386
C	-15.6220127	0.9382557	-1.3874920
H	-16.0341570	0.0021845	-1.7629227
N	-14.3903220	1.3897435	-1.6105074
C	-14.2942310	2.5878394	-0.9151446
C	-13.0303893	3.3973359	-0.8666876
H	-12.2800091	2.9057654	-1.5082681
H	-12.6343438	3.4283575	0.1669354
C	-13.2657836	4.8366696	-1.3443689
N	-13.7632212	4.8123079	-2.7466194
H	-14.0115437	5.7815865	-3.0200369
H	-12.9584253	4.5369965	-3.3456708
H	-14.0407867	5.3290500	-0.7357111
C	-11.9716109	5.6635958	-1.3071639
O	-10.9151944	5.2355168	-1.7853982

N	-12.0888969	6.9219317	-0.7831789
H	-12.9559077	7.1964862	-0.3070402
C	-10.9318419	7.7857694	-0.6513326
H	-10.6529502	7.9317734	0.4064170
H	-10.1191928	7.2430394	-1.1404641
C	-11.0483821	9.1727439	-1.2643503
O	-10.2409368	10.0602573	-0.9482657
N	-12.0560179	9.3441219	-2.1579631
H	-12.7700420	8.6046504	-2.1581150
C	-12.5763936	10.6997852	-2.3821519
H	-11.6939793	11.3381569	-2.5437627
C	-13.4029512	10.7595625	-3.6775871
H	-13.5722529	11.8195282	-3.9385616
H	-12.8147340	10.3448493	-4.5209885
C	-14.8071610	10.1169204	-3.6696092
H	-15.3073014	10.2808376	-2.6975780
H	-15.3984701	10.6103381	-4.4623434
C	-14.8340663	8.6263975	-3.9865788
O	-15.0872828	8.3147818	-5.1854513
O	-14.6531494	7.7841571	-3.0333342
H	-13.1325757	11.0049031	-1.4575175
H	-16.2783926	-0.2502404	-5.4668261
C	-16.4954609	0.4346836	-4.5995662
H	-17.1629678	-0.1312709	-3.9237624
H	-15.5509930	0.6309836	-4.0625988
C	-17.1541541	1.7239764	-4.9654468
N	-16.8881780	2.9159082	-4.3001877
C	-17.7267182	3.8279411	-4.8092663
H	-17.7265896	4.8820808	-4.5318426
N	-18.5120629	3.2717885	-5.7599330
H	-19.2532825	3.7277307	-6.3123214
C	-18.1754761	1.9425729	-5.8700931
H	-18.7329392	1.2694572	-6.5184919
H	-12.3169653	3.7469239	-9.0605928
C	-12.0529476	4.4813188	-8.2596546
H	-11.0592305	4.2115001	-7.8634254
H	-11.9457388	5.4851890	-8.7186788
C	-13.0675177	4.5548653	-7.1768273
N	-13.6762472	5.7398401	-6.7980208
H	-13.5831273	6.6540528	-7.2570901
C	-14.5105215	5.4645997	-5.7555509
H	-15.1222991	6.2370903	-5.2916264
N	-14.4599039	4.1765021	-5.4427448
C	-13.5704933	3.5949519	-6.3173901
H	-13.3402244	2.5313776	-6.2815967
Cu	-15.2555604	3.6322504	-3.4419327
O	-11.5235058	3.6888075	-4.3009834
C	-10.1244568	3.9341866	-4.3532016
H	-9.8767042	4.4167012	-3.3957511
H	-9.8609668	4.6227927	-5.1864884
H	-9.5512025	2.9854024	-4.4536200
H	-11.8973222	3.5192369	-5.1975536
O	-11.9012344	1.1160271	-3.0876827
H	-12.7936619	1.0721982	-2.6472680
H	-11.8860629	2.0067209	-3.5098638
O	-17.2620844	7.3752154	-6.6214134
H	-18.0073180	7.2106457	-6.0044110

H	-16.5183300	7.7113854	-6.0577605
O	-15.1950897	7.0865328	-0.2262427
H	-16.0742209	6.6315946	-0.0372441
H	-15.1566542	7.4018866	-1.1632598
O	-16.9156041	6.3955729	-3.3447242
H	-17.5404880	7.0376589	-3.7469961
H	-16.0204031	6.8401236	-3.2598062