

## Rapid Route-Finding for Bifurcating Reactions Cartesian Coordinates

1a			
H	0.32533	2.41860	2.84563
H	-0.67198	2.38228	-2.79712
C	2.81316	0.22608	0.25276
C	3.43887	-0.86835	1.18494
H	3.18780	1.22576	0.50282
C	1.32991	0.27142	0.21740
H	0.84288	3.11967	-3.41682
H	-0.13198	3.99336	-2.19323
C	3.48767	-2.41040	-0.75366
O	0.59456	-0.69762	0.36845
P	0.39466	1.85657	-0.15865
O	0.99972	2.35442	-1.53578
O	0.78392	3.00009	0.88016
O	-1.08209	1.51372	-0.15308
C	0.18529	3.01261	-2.55510
C	0.06461	3.20660	2.13704
H	-1.01056	3.20309	1.95513
H	0.40156	4.17883	2.49559
C	4.39381	-1.63740	0.18925
H	3.28393	0.65072	-1.92943
C	4.15684	-0.27525	2.40256
C	4.85217	-0.49401	-0.74459
H	5.36119	0.33111	-0.23266
H	2.65347	-1.54514	1.53383
H	5.17061	-2.21423	0.69764
C	2.89495	-1.52510	-1.57260
H	5.47127	-0.84492	-1.57575
H	3.27002	-3.47082	-0.67397
C	3.41562	-0.15093	-1.20164
H	2.09719	-1.71438	-2.28266
H	4.59344	-1.07379	3.01375
H	4.96702	0.40503	2.11194
H	3.46213	0.28385	3.04131
Cl	-2.01575	-2.87814	0.34557
Sn	-1.88379	-0.53360	0.04845
Cl	-4.08153	0.21179	-0.31890
Cl	-1.13631	-0.69245	-2.25016
Cl	-1.68230	-0.05260	2.40261
1b			
H	-0.53371	2.89671	-2.38872
H	0.98761	2.18932	2.95710
C	-2.75904	0.97840	-0.73877
C	-3.62978	-0.14130	-1.24738
H	-3.07149	2.01115	-0.86673
C	-1.58408	0.72672	-0.14783
H	-0.41009	2.90637	3.82261
H	0.43098	3.85785	2.55940
C	-1.85731	-1.72590	-0.20166
O	-1.04050	-0.50691	0.07956
P	-0.43049	1.98028	0.42774
O	-0.82836	2.30442	1.92545

O	-0.66900	3.35335	-0.34279
O	1.00120	1.47425	0.25826
C	0.12767	2.85667	2.87637
C	-0.10801	3.59665	-1.66664
H	0.97702	3.48572	-1.63364
H	-0.38764	4.62182	-1.90892
C	-3.35466	-1.43205	-0.44762
H	-3.26441	-2.91047	2.64690
C	-5.11790	0.24165	-1.28148
C	-4.00774	-1.55816	0.95581
H	-4.10290	-0.58689	1.46341
H	-3.32030	-0.33511	-2.28762
H	-3.71548	-2.28091	-1.04272
C	-1.85836	-2.55132	1.05655
H	-5.01669	-1.98469	0.90052
H	-1.35440	-2.18002	-1.05743
C	-3.03112	-2.44454	1.69316
H	-0.97963	-3.08923	1.39415
H	-5.72138	-0.58234	-1.67972
H	-5.49598	0.48809	-0.28305
H	-5.27756	1.11416	-1.92617
Cl	1.58716	-2.83567	-0.58269
Sn	1.71514	-0.48593	-0.16659
Cl	3.96646	0.12995	-0.34272
Cl	1.50510	-0.79722	2.20205
Cl	0.96081	0.01405	-2.40740

2a

C	-3.91803	1.40068	-0.18077
C	-2.81589	0.67300	0.62424
H	-4.24791	2.29310	0.36110
H	-2.57921	1.13832	1.58101
C	-3.56882	-1.43972	-0.49814
C	-3.41059	-0.77802	0.86053
H	-2.91533	-2.21375	-0.88567
H	-2.87305	-1.33310	1.63042
C	-4.55018	-0.79246	-1.14833
C	-5.05605	0.31723	-0.24067
H	-4.85987	-0.94108	-2.17795
H	-6.03991	0.72854	-0.47515
C	-4.87341	-0.35279	1.14398
H	-4.97906	0.33948	1.98879
H	-5.52476	-1.21843	1.29399
H	-3.57491	1.70576	-1.17099
O	-1.39211	0.67666	-1.27511
N	-1.48550	0.58642	-0.06970
O	-0.51382	0.35711	0.69538
Sn	1.80761	-0.02810	0.02086
Cl	1.93706	-0.22925	2.33800
Cl	0.80207	-1.84178	-1.06022
Cl	4.04717	-0.41650	-0.59385
Cl	1.56767	2.15595	-0.76791

2b

C	-3.27170	1.81665	-0.05891
C	-2.09494	1.27079	0.68051
H	-3.79471	2.55028	0.56019
H	-1.70700	1.64023	1.62148

C	-3.70583	-1.67770	-0.13453
C	-4.61461	-1.34277	0.78836
H	-3.23034	-2.64602	-0.25185
H	-5.00698	-2.01698	1.54502
C	-3.37949	-0.52346	-1.03419
C	-4.22126	0.67300	-0.49842
H	-3.53152	-0.72822	-2.09682
H	-4.86988	1.05769	-1.29046
C	-5.07615	0.08796	0.66714
H	-4.94589	0.63890	1.60890
H	-6.14751	0.13991	0.43207
H	-2.89998	2.34375	-0.94964
O	-1.92562	-0.22420	-1.04993
N	-1.47390	0.25975	0.17002
O	-0.45380	-0.34974	0.67380
Sn	1.67880	-0.05873	0.03960
Cl	1.99425	-1.01662	2.15431
Cl	1.22251	-1.48584	-1.76056
Cl	3.97260	0.33924	-0.43961
Cl	1.03008	2.21636	-0.17766

3a

H	-4.40682	-1.94644	1.06612
H	-3.06420	2.33318	-1.38562
C	1.05616	0.38653	0.31419
C	2.35132	-0.02464	1.08260
H	0.76352	1.41756	0.55282
C	-0.15244	-0.47970	0.56674
H	-2.68839	3.44671	-0.03415
H	-3.86817	2.12300	0.20664
C	3.01059	-1.35443	-0.90205
O	-0.15161	-1.53449	1.17296
P	-1.78781	0.03235	-0.21794
O	-1.84526	1.60217	0.15179
O	-2.94284	-0.56863	0.73605
O	-1.90152	-0.33668	-1.65821
C	-2.94650	2.42111	-0.30180
C	-3.45239	-1.90738	0.53799
H	-3.60157	-2.10476	-0.52689
H	-2.75338	-2.62980	0.96700
C	3.40415	-0.13041	-0.08740
H	0.81609	0.87962	-1.88607
C	2.74421	0.96896	2.18251
C	2.92157	0.99278	-1.03666
H	3.48228	1.02716	-1.97635
H	2.20853	-1.00889	1.53879
H	4.44261	-0.08990	0.25331
C	1.88282	-1.05650	-1.56721
H	2.90956	1.99039	-0.58126
H	3.49930	-2.32236	-0.84092
C	1.51469	0.37655	-1.21595
H	1.26246	-1.72241	-2.15815
H	3.66330	0.64504	2.68631
H	2.91852	1.97662	1.78447
H	1.95839	1.04385	2.94444

3b

H	3.69531	-2.11023	-1.82920
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H	3.56684	1.45101	1.91494
C	-0.63488	1.32951	-0.39405
C	-2.05324	1.29558	-0.90876
H	-0.18500	2.25412	-0.04854
C	0.07581	0.19369	-0.36775
H	3.55919	2.95701	0.94351
H	4.34714	1.48663	0.29944
C	-1.85548	-1.26361	-0.68381
O	-0.41324	-1.00647	-0.81535
P	1.77371	0.00164	0.24327
O	2.25941	1.53896	0.28335
O	2.62882	-0.58362	-1.00649
O	1.93466	-0.78586	1.49711
C	3.51804	1.86717	0.90463
C	2.85455	-2.00160	-1.14083
H	3.09779	-2.44454	-0.17140
H	1.96426	-2.48029	-1.55966
C	-2.73063	-0.00626	-0.42068
H	-2.99660	-1.89196	2.46003
C	-2.84967	2.55936	-0.55705
C	-3.08459	-0.06146	1.09373
H	-4.13841	0.18903	1.27161
H	-2.00740	1.23170	-2.00921
H	-3.66057	-0.14620	-0.98684
C	-2.09795	-2.13680	0.51973
H	-2.48956	0.64340	1.69071
H	-2.10061	-1.74661	-1.63426
C	-2.75264	-1.48072	1.48347
H	-1.71331	-3.15022	0.58242
H	-3.86880	2.50622	-0.95922
H	-2.92110	2.70456	0.52708
H	-2.36795	3.44855	-0.98111

4a

C	-0.47083	-0.88371	-1.15605
C	0.42364	0.30554	-0.73596
H	-0.61817	-0.88132	-2.24156
H	0.72783	0.93918	-1.57046
C	-0.73813	0.24597	1.47309
C	-0.48206	1.12737	0.25919
H	-0.25360	0.36690	2.43630
H	-0.10722	2.13466	0.44536
C	-1.53342	-0.76127	1.07837
C	-1.81584	-0.57428	-0.40431
H	-1.82947	-1.62761	1.66182
H	-2.67995	-1.10803	-0.80624
C	-1.82962	0.97279	-0.48906
H	-1.81237	1.35799	-1.51670
H	-2.65888	1.42806	0.06075
H	-0.03627	-1.84223	-0.86822
O	1.92732	-1.21888	0.29713
O	2.54361	0.85697	0.05516
N	1.73975	-0.06669	-0.08159

4b

C	-0.11681	1.79287	0.20451
C	-1.14495	1.07464	-0.61480
H	0.25518	2.65839	-0.35335

H	-1.55984	1.42905	-1.54979
C	1.01951	-1.54131	0.09058
C	1.84889	-0.98429	-0.79770
H	0.75245	-2.59186	0.15023
H	2.37968	-1.52636	-1.57659
C	0.44258	-0.52337	1.03504
C	1.04332	0.84271	0.57788
H	0.64828	-0.74958	2.08630
H	1.61517	1.29104	1.39696
C	1.98940	0.50654	-0.61424
H	1.71982	1.05014	-1.53089
H	3.02744	0.78610	-0.38792
H	-0.57495	2.17834	1.12736
O	-1.02019	-0.52333	1.04856
O	-2.43471	-0.84433	-0.69677
N	-1.58796	-0.08440	-0.20918

5a

H	3.16164	-0.16405	-0.79664
C	2.12332	0.18612	-0.84741
C	-0.26987	-0.54896	-0.11946
C	0.66462	1.72935	0.44174
C	-0.48087	0.98198	-0.17647
C	1.90252	1.34242	0.10825
C	1.16333	-1.00653	-0.58406
C	-1.59709	-0.99968	-0.72778
O	-2.57228	-0.08918	-0.18440
C	-1.91658	1.08631	0.32899
H	-0.45683	-1.26242	2.15494
C	1.28064	-1.62759	0.79939
H	1.97155	0.53173	-1.88279
C	0.08980	-1.18545	1.21830
H	0.48805	2.55662	1.12635
H	-0.50600	1.23290	-1.25171
H	2.77378	1.85089	0.51591
H	1.18639	-1.70740	-1.42856
H	-1.88725	-2.01741	-0.44757
H	2.08569	-2.18475	1.27234
H	-1.58601	-0.92957	-1.82716
H	-2.44905	1.97154	-0.03775
H	-1.96262	1.08744	1.42886

5b

H	-4.00260	-1.07433	-0.87103
C	-2.92566	-1.04884	-0.72853
C	0.76150	0.68039	-0.11834
C	-0.93077	-0.48862	0.73794
C	0.15914	-0.75517	-0.33729
C	-2.38720	-0.58018	0.39820
C	0.12907	1.81568	-0.88470
C	2.26155	0.46104	0.09808
O	2.51751	-0.90321	-0.24420
C	1.34370	-1.64954	0.06745
H	-0.08306	1.23060	2.00610
C	-0.82481	2.04147	0.03553
H	-2.32294	-1.42956	-1.54871
C	-0.33833	0.96051	0.97733
H	-0.74299	-1.09902	1.63250

H	-0.18668	-0.97025	-1.35080
H	-3.05482	-0.21763	1.18296
H	0.32266	2.21579	-1.87812
H	2.54852	0.66077	1.14382
H	-1.70300	2.68108	0.05503
H	2.88522	1.08311	-0.55195
H	1.39979	-2.59131	-0.48593
H	1.31063	-1.88409	1.14576

6a

H	3.19293	-0.21962	-0.77091
C	2.15996	0.14402	-0.84181
C	-0.26051	-0.54483	-0.12612
C	0.71238	1.73308	0.40302
C	-0.45617	0.98993	-0.18043
C	1.94682	1.32755	0.08018
C	1.17905	-1.02364	-0.55708
C	-1.56440	-1.03409	-0.77566
C	-1.87884	1.16436	0.37132
H	-0.48567	-1.23356	2.15869
C	1.27091	-1.61922	0.83856
H	2.02512	0.46416	-1.88789
C	0.07314	-1.16891	1.22735
H	0.54819	2.58287	1.06371
H	-0.49841	1.23528	-1.25777
H	2.82232	1.84179	0.47215
H	1.19938	-1.74687	-1.38310
H	-1.77487	-2.08871	-0.57019
H	2.06431	-2.17216	1.33645
H	-1.50525	-0.91852	-1.86564
H	-2.33737	2.11308	0.07197
H	-1.86207	1.14764	1.46836
C	-2.64858	-0.07639	-0.18749
H	-3.21700	-0.57005	0.60785
H	-3.37418	0.21351	-0.95468

6b

H	-4.00638	-1.16041	-0.85688
C	-2.93085	-1.11094	-0.70914
C	0.75654	0.70383	-0.09111
C	-0.95301	-0.46117	0.74314
C	0.15379	-0.74002	-0.31422
C	-2.40623	-0.59081	0.40163
C	0.13523	1.80994	-0.91197
C	2.25743	0.54066	0.19793
C	1.29771	-1.69982	0.07079
H	-0.17656	1.31084	1.98132
C	-0.85832	2.04507	-0.03808
H	-2.31561	-1.51215	-1.51018
C	-0.38976	1.00143	0.95361
H	-0.75760	-1.04346	1.65481
H	-0.20368	-0.92910	-1.33052
H	-3.08500	-0.21031	1.16860
H	0.35894	2.18763	-1.90859
H	2.45851	0.66257	1.27042
H	-1.74785	2.66900	-0.07168
H	2.86718	1.28541	-0.32542
H	1.24896	-2.65808	-0.45838

H	1.26419	-1.92458	1.14563
C	2.58041	-0.90456	-0.24731
H	3.47198	-1.31637	0.23919
H	2.76528	-0.92266	-1.32990

7a

H	3.44573	-0.27846	-0.75290
C	2.41918	0.09598	-0.85435
C	-0.02341	-0.53135	-0.08461
C	0.98925	1.75586	0.30673
C	-0.22181	1.00263	-0.18489
C	2.21715	1.33624	-0.01361
C	1.42279	-1.02914	-0.49361
C	-1.22061	-1.20528	-0.76224
O	-2.43308	-0.84707	-0.10488
C	-1.55936	1.37739	0.47173
H	-0.27709	-1.16146	2.20700
C	1.50553	-1.56735	0.92534
H	2.29579	0.34795	-1.91998
C	0.30134	-1.11294	1.28854
H	0.84039	2.65256	0.90697
H	-0.32726	1.21916	-1.26472
H	3.09541	1.88479	0.32116
H	1.42606	-1.79767	-1.27941
H	-1.15161	-2.29554	-0.69650
H	2.29059	-2.11438	1.44247
H	-1.26986	-0.92248	-1.82960
H	-3.63586	0.70313	0.36900
H	-1.77132	2.44768	0.34297
H	-1.51654	1.18146	1.55092
C	-2.68837	0.55213	-0.15747
H	-2.82996	0.86479	-1.20782

7b

H	4.17557	-1.39985	0.71878
C	3.10109	-1.26633	0.62624
C	-0.43247	0.81127	0.18080
C	1.10545	-0.49516	-0.74041
C	0.02820	-0.68925	0.37296
C	2.56017	-0.73185	-0.46962
C	0.39353	1.82204	0.95341
C	-1.92444	1.08034	0.06548
O	-2.66561	-0.00071	-0.48264
C	-1.05903	-1.73697	0.04211
H	0.38541	1.29682	-1.97733
C	1.29372	2.00061	-0.02627
H	2.50064	-1.59637	1.46998
C	0.64475	1.00095	-0.95693
H	0.82218	-1.07434	-1.62951
H	0.43063	-0.87037	1.37385
H	3.22418	-0.42688	-1.28191
H	0.31229	2.18817	1.97563
H	-2.11510	1.94803	-0.57556
H	2.22295	2.56107	-0.09055
H	-2.32011	1.31550	1.07129
H	-3.22457	-1.90221	-0.07083
H	-0.90705	-2.65145	0.62982
H	-0.99545	-2.02556	-1.01400

C	-2.46733	-1.18988	0.27194
H	-2.64851	-0.99147	1.34322

8a

H	3.47112	-0.30000	-0.74357
C	2.44534	0.07430	-0.85621
C	-0.01264	-0.54525	-0.08726
C	1.01267	1.74798	0.27673
C	-0.20693	0.99173	-0.19278
C	2.24135	1.32969	-0.04066
C	1.44512	-1.03828	-0.47499
C	-1.18537	-1.24763	-0.79110
C	-1.52303	1.41116	0.48434
H	-0.25758	-1.14087	2.22512
C	1.52505	-1.54899	0.95289
H	2.32672	0.30491	-1.92738
C	0.31322	-1.10383	1.30005
H	0.86593	2.65658	0.86000
H	-0.32580	1.20261	-1.27187
H	3.11796	1.88957	0.27990
H	1.44802	-1.82403	-1.24311
H	-1.05492	-2.33623	-0.73892
H	2.31466	-2.07177	1.48845
H	-1.18514	-0.97601	-1.85762
H	-3.64693	0.94364	0.38310
H	-1.65541	2.49844	0.40208
H	-1.46947	1.18505	1.55918
C	-2.72160	0.68372	-0.14677
H	-2.84553	1.03807	-1.18095
C	-2.52930	-0.84239	-0.15936
H	-3.35818	-1.32191	-0.69567
H	-2.56885	-1.22136	0.87198

8b

H	-4.17512	-1.46046	-0.67372
C	-3.10251	-1.30597	-0.59175
C	0.41588	0.83713	-0.18873
C	-1.10940	-0.48079	0.74598
C	-0.03507	-0.67018	-0.37223
C	-2.56218	-0.74719	0.49225
C	-0.43830	1.81603	-0.97567
C	1.90328	1.16177	-0.07454
C	1.03140	-1.74592	-0.05986
H	-0.42684	1.33785	1.96437
C	-1.33970	1.99675	0.00098
H	-2.50228	-1.63525	-1.43596
C	-0.67307	1.02280	0.94569
H	-0.80948	-1.04688	1.63876
H	-0.44864	-0.84519	-1.37018
H	-3.22509	-0.44372	1.30623
H	-0.36262	2.16690	-2.00413
H	2.03493	2.06539	0.53602
H	-2.27786	2.54316	0.05955
H	2.26785	1.42186	-1.08051
H	3.16996	-2.07665	-0.04576
H	0.80930	-2.66033	-0.62442
H	0.97312	-2.02549	1.00135
C	2.46908	-1.28163	-0.33042



H	2.61975	-1.10051	-1.40520
C	2.76661	0.00566	0.44962
H	3.82722	0.27467	0.36725
H	2.56968	-0.16619	1.51835

9a

C	0.64598	0.05749	0.09634
C	-0.26470	1.05529	-0.62728
C	-0.85476	1.91492	0.48231
C	-0.21536	1.52702	1.74815
C	0.61182	0.50703	1.53483
O	-1.70718	2.75335	0.33030
C	2.06596	0.08646	-0.43367
O	2.42341	0.62998	-1.44235
O	2.88868	-0.60764	0.34916
C	4.24065	-0.67494	-0.07871
C	-1.37179	0.39953	-1.44290
C	-2.10495	-0.63240	-0.62667
C	-1.36847	-1.49339	0.08224
C	0.12895	-1.39679	-0.03583
H	0.62112	-2.01816	0.71029
C	-1.88119	-2.58515	0.96445
C	-3.59595	-0.57764	-0.68422
H	-2.05364	1.17822	-1.77926
H	0.33302	1.70187	-1.26882
H	1.20776	0.00839	2.28465
H	-0.42829	2.00860	2.68844
H	4.75665	-1.26626	0.66761
H	4.30654	-1.14914	-1.05339
H	4.66872	0.32114	-0.13926
H	0.44162	-1.78130	-1.01129
H	-0.94017	-0.05458	-2.33851
H	-4.08022	-1.35373	-0.10082
H	-3.95036	0.38978	-0.32653
H	-3.93726	-0.67358	-1.71617
H	-1.50801	-3.55597	0.63359
H	-1.52964	-2.44672	1.98836
H	-2.96431	-2.63870	0.99006

9b

C	-1.04974	0.41083	-0.09610
C	-0.20003	1.33974	0.72032
C	0.63228	1.89178	-0.43078
C	1.05116	0.54066	-1.01805
C	-0.31488	-0.05973	-1.11465
O	0.89716	3.00433	-0.76248
C	-2.43899	0.08587	0.23973
O	-3.01381	0.51613	1.20685
O	-2.99909	-0.73999	-0.64107
C	-4.34460	-1.09757	-0.37434
C	0.88625	0.48339	1.41100
C	1.78001	-0.04301	0.24704
C	1.92658	-1.55139	0.17020
C	1.75814	-2.35441	1.21636
H	1.93158	-3.41715	1.12929
C	2.36476	-2.11249	-1.15068
C	3.17734	0.58004	0.34062
H	1.46977	1.09190	2.09954

H	-0.72432	2.04655	1.35046
H	-0.64607	-0.75865	-1.86516
H	1.65149	0.56611	-1.92000
H	-4.63548	-1.76583	-1.17555
H	-4.42226	-1.59825	0.58638
H	-4.97815	-0.21541	-0.36567
H	1.45833	-1.99743	2.18915
H	0.41849	-0.31197	1.98047
H	3.80637	0.28354	-0.49620
H	3.12416	1.66789	0.34219
H	3.66561	0.26094	1.25890
H	2.56137	-3.17807	-1.07377
H	1.60314	-1.96958	-1.91690
H	3.27218	-1.63061	-1.51346

10a

C	-0.65823	2.24895	0.62453
C	-0.69290	1.32856	-0.59110
C	-0.47110	-0.09287	-0.01542
C	-0.38968	0.13917	1.46850
C	-0.47642	1.41951	1.81848
C	0.36100	1.75290	-1.61748
C	1.72359	1.45813	-1.09150
C	1.96008	0.25473	-0.55253
H	-0.24356	-0.68475	2.15073
O	-0.76134	3.44848	0.57330
H	2.49052	2.21960	-1.11136
H	0.22881	2.81092	-1.82931
H	0.18217	1.20841	-2.54960
C	-1.65088	-0.96534	-0.40281
H	-1.68338	1.42385	-1.03710
H	-0.41984	1.82649	2.81445
O	-2.65977	-0.85313	0.45130
O	-1.69632	-1.64767	-1.39109
C	-3.83800	-1.57365	0.11948
H	-4.54075	-1.36884	0.91740
H	-4.23313	-1.23456	-0.83347
H	-3.62738	-2.63706	0.05826
C	3.22345	-0.10998	0.05030
C	3.40848	-1.30871	0.62160
C	2.34129	-2.29419	0.64480
C	1.14832	-2.04200	0.10306
C	0.83008	-0.74536	-0.57117
H	4.01533	0.62583	0.03904
H	4.35702	-1.55755	1.07357
H	2.53508	-3.25484	1.10013
H	0.37782	-2.80083	0.10046
H	0.58623	-0.97713	-1.61368

10b

C	0.86172	2.38777	-0.34253
C	1.31950	1.44436	0.76834
C	1.58228	0.24866	-0.09720
C	0.69852	0.24472	-1.10814
C	-0.17576	1.44698	-0.96595
C	-0.04798	1.22161	1.46168
C	-1.07968	1.28475	0.30370

C	-2.08017	0.16606	0.20615
H	0.61977	-0.49945	-1.88328
O	1.16975	3.50362	-0.61843
H	-1.64167	2.21502	0.38904
H	-0.24152	2.00497	2.19132
H	-0.06483	0.27176	1.98818
C	2.62709	-0.73848	0.19078
H	2.13221	1.76996	1.40450
H	-0.69720	1.79409	-1.84967
O	2.68500	-1.70417	-0.72359
O	3.35355	-0.68675	1.15019
C	3.68176	-2.68975	-0.51094
H	3.58696	-3.38598	-1.33515
H	4.66905	-2.23716	-0.50682
H	3.52122	-3.19622	0.43639
C	-3.38460	0.45785	-0.18468
C	-4.33341	-0.54248	-0.32531
C	-3.99228	-1.86248	-0.07489
C	-2.69857	-2.16786	0.31839
C	-1.75268	-1.16369	0.45948
H	-3.66151	1.48534	-0.37853
H	-5.33947	-0.28902	-0.62560
H	-4.72880	-2.64518	-0.17945
H	-2.42264	-3.19227	0.52140
H	-0.75234	-1.42560	0.76909

11a

C	-0.51231	2.38113	0.71601
C	-0.68258	1.53085	-0.53715
C	-0.59145	0.07130	-0.03164
C	-0.48788	0.21440	1.46004
C	-0.42464	1.47936	1.87023
C	0.37544	1.89104	-1.58300
C	1.71602	1.45572	-1.08505
C	1.85549	0.23543	-0.56919
C	0.64095	-0.66011	-0.65103
C	0.82738	-2.09786	-0.13884
C	1.97722	-2.28970	0.83698
C	3.25397	-1.70841	0.25847
C	3.11129	-0.20201	0.13373
H	-0.45579	-0.64838	2.10756
O	-0.46279	3.58551	0.72814
H	4.10969	-1.94437	0.89020
H	1.76449	-1.80223	1.79183
H	2.09297	-3.35265	1.04842
H	1.01757	-2.73948	-0.99984
H	-0.10128	-2.46592	0.29997
H	3.09414	0.21347	1.14558
H	3.97599	0.23866	-0.36137
H	0.37366	-0.73107	-1.70677
H	3.44833	-2.15704	-0.71862
H	2.53466	2.16303	-1.06858
H	0.34276	2.96463	-1.75129
H	0.12047	1.40486	-2.52734
C	-1.82354	-0.69413	-0.47147
H	-1.67368	1.73989	-0.94068
H	-0.32431	1.83060	2.88413
O	-2.57118	-1.11583	0.54257

O	-2.10209	-0.89796	-1.62254
C	-3.75136	-1.82276	0.18898
H	-4.23177	-2.07855	1.12518
H	-4.40051	-1.19574	-0.41455
H	-3.50285	-2.71894	-0.37165

11b

C	1.11113	2.38618	-0.29669
C	1.55711	1.39601	0.77432
C	1.69383	0.19580	-0.11455
C	0.77292	0.27130	-1.08780
C	-0.00860	1.52769	-0.88868
C	0.21225	1.25887	1.52872
C	-0.86434	1.36780	0.41937
C	-1.90562	0.28896	0.30184
C	-1.92206	-0.82908	1.02598
C	-2.94690	-1.91261	0.88859
C	-3.78801	-1.76633	-0.36845
C	-4.19838	-0.31768	-0.55981
C	-2.97103	0.56243	-0.72775
H	0.60648	-0.45832	-1.86297
O	1.47370	3.48828	-0.56443
H	-4.85482	-0.20993	-1.42278
H	-3.20659	-2.09061	-1.23430
H	-4.66187	-2.41486	-0.31522
H	-3.59099	-1.90508	1.77307
H	-2.44715	-2.88259	0.90030
H	-2.55176	0.41789	-1.72830
H	-3.25456	1.61616	-0.67885
H	-1.16254	-0.99556	1.77674
H	-4.76526	0.01438	0.31252
H	-1.39620	2.31459	0.54377
H	0.09741	2.06299	2.25256
H	0.18291	0.32182	2.07355
C	2.66433	-0.87566	0.12491
H	2.41850	1.65546	1.37597
H	-0.53841	1.93312	-1.74187
O	2.62711	-1.82082	-0.81220
O	3.41513	-0.90409	1.06669
C	3.54303	-2.88860	-0.64021
H	3.37901	-3.55457	-1.47854
H	4.56416	-2.51850	-0.64258
H	3.35635	-3.40384	0.29763

12a

C	-1.26497	-1.96445	0.67070
C	-0.59803	-1.35594	-0.55640
C	0.35158	-0.28338	0.01265
C	0.19245	-0.40616	1.50604
C	-0.69300	-1.33103	1.86654
C	-1.66375	-0.85267	-1.53760
C	-2.33344	0.37934	-1.00801
C	-1.52157	1.29756	-0.51368
C	-0.02961	1.14480	-0.49240
C	0.35772	2.33514	0.33282
C	-0.74778	3.02068	0.59296
O	-1.88839	2.46746	0.09415
H	0.75921	0.21952	2.17717

O	-2.11890	-2.81333	0.64004
H	-0.89299	3.94407	1.12484
H	1.35607	2.60941	0.61962
H	0.36458	1.22722	-1.51169
H	-3.40631	0.48550	-0.99367
H	-2.38312	-1.65436	-1.68460
H	-1.19617	-0.66119	-2.50632
C	1.79086	-0.53187	-0.39915
H	-0.01326	-2.13657	-1.04020
H	-0.98402	-1.59624	2.86968
O	2.64190	0.16580	0.34841
O	2.13880	-1.23347	-1.30823
C	4.01572	0.02674	0.01375
H	4.55469	0.64559	0.72040
H	4.32292	-1.01067	0.10351
H	4.19409	0.36341	-1.00309

### 12b

C	0.37977	2.36659	-0.33471
C	0.95247	1.47710	0.76729
C	1.32274	0.31216	-0.10144
C	0.43374	0.21850	-1.10245
C	-0.56061	1.32178	-0.94501
C	-0.36993	1.11773	1.48576
C	-1.41135	1.03803	0.34108
C	-2.17731	-0.22797	0.27867
C	-2.06059	-1.44661	0.85940
C	-3.12431	-2.24454	0.33982
C	-3.80044	-1.44884	-0.51464
O	-3.23711	-0.22571	-0.56064
H	0.41957	-0.53287	-1.87449
O	0.56556	3.50838	-0.61316
H	-4.66588	-1.59430	-1.13207
H	-3.35061	-3.26766	0.57753
H	-1.31459	-1.75083	1.56974
H	-2.12639	1.85652	0.43274
H	-0.64289	1.89024	2.20091
H	-0.27004	0.18348	2.02927
C	2.45952	-0.56997	0.18008
H	1.73680	1.88724	1.38990
H	-1.13649	1.61173	-1.81473
O	2.62121	-1.50921	-0.74805
O	3.16937	-0.46021	1.14721
C	3.70427	-2.39930	-0.53674
H	3.68663	-3.08704	-1.37321
H	4.64395	-1.85533	-0.51085
H	3.57985	-2.93514	0.39981

### 13a

C	-1.02198	-0.07486	1.34209
C	-2.53216	1.31880	-0.26995
N	-1.90091	0.71933	0.44141
C	-3.35044	2.10461	-1.20010
C	0.36519	-0.17888	0.78046
C	1.34956	0.71479	1.16420
C	2.63665	0.62477	0.65801
C	2.94683	-0.38039	-0.25077
C	1.95672	-1.28957	-0.64045

C	0.68806	-1.18912	-0.12830
H	-1.06225	0.44284	2.28803
H	-1.52153	-1.02734	1.43401
H	-3.57781	3.05972	-0.74501
H	-4.26319	1.56071	-1.40210
H	-2.79188	2.25278	-2.11514
H	1.12864	1.49282	1.87464
H	3.37767	1.32778	0.98230
H	-0.05609	-1.90704	-0.42830
N	-6.05296	-1.70554	-0.08739
N	-5.29822	-0.94627	-0.21490
H	2.21953	-2.06569	-1.33354
O	4.14444	-0.56352	-0.79954
C	5.22902	0.26672	-0.45397
H	6.07122	-0.09833	-1.01879
H	5.03215	1.29699	-0.72572
H	5.44789	0.19906	0.60486

13b

C	-0.03651	-1.28768	-0.42622
C	-3.29531	0.95142	0.37689
N	-2.34593	0.37134	0.15150
C	-4.52400	1.70156	0.66839
C	1.23573	-0.88482	-0.21658
C	1.90244	-1.11844	1.04093
C	3.17110	-0.71396	1.24118
C	3.86831	-0.04024	0.19544
C	3.24449	0.21351	-1.05677
C	1.96895	-0.19795	-1.24530
H	-0.59965	-1.79982	0.32931
H	-0.53921	-1.11594	-1.35779
H	-4.56694	1.93173	1.72466
H	-5.38664	1.10865	0.39597
H	-4.52980	2.62332	0.10194
H	1.36734	-1.62494	1.82305
H	3.69144	-0.87558	2.16481
H	1.48292	-0.01108	-2.18542
N	-7.95947	-0.28729	-0.24497
N	-8.91620	-0.73695	-0.45692
H	3.77449	0.72237	-1.83579
O	5.07580	0.30774	0.47741
C	5.93109	0.99123	-0.44282
H	6.85584	1.13306	0.08822
H	6.09466	0.38174	-1.31946
H	5.50277	1.94704	-0.70689

14a

C	-0.57185	-0.13163	1.28782
C	-2.11824	1.27970	-0.26553
N	-1.46925	0.66909	0.41979
C	-2.95993	2.08033	-1.16146
C	0.82051	-0.16959	0.72015
C	1.75055	0.79588	1.08127
C	3.02987	0.75737	0.55881
C	3.41101	-0.24420	-0.32956
C	2.47018	-1.20740	-0.68275
C	1.18926	-1.17461	-0.16387
H	-0.62526	0.34557	2.25440

H	-1.03729	-1.10387	1.34175
H	-2.42215	2.24915	-2.08534
H	-3.18068	3.02514	-0.68218
H	-3.87482	1.53657	-1.35400
H	1.48537	1.57464	1.77573
H	3.74093	1.50896	0.85060
H	0.48454	-1.93868	-0.44434
N	-4.88162	-0.97881	-0.16199
N	-5.63646	-1.73565	-0.02133
H	2.74315	-1.99391	-1.36286
C	4.81959	-0.30465	-0.86882
H	5.25618	0.68404	-0.94068
H	5.45010	-0.89769	-0.21320
H	4.84555	-0.75947	-1.85154

14b

C	0.44470	-1.44004	0.02856
C	-2.65455	0.93335	-0.00294
N	-1.72353	0.28403	0.00494
C	-3.85976	1.77289	-0.01317
C	1.68910	-0.88542	0.01623
C	2.35969	-0.56686	1.23810
C	3.60674	-0.02232	1.21985
C	4.24706	0.23797	-0.00882
C	3.60093	-0.06362	-1.22494
C	2.35385	-0.60837	-1.21886
H	-0.06443	-1.66496	0.94517
H	-0.06876	-1.69575	-0.87751
H	-3.86812	2.40574	0.86428
H	-4.74058	1.14518	-0.01096
H	-3.86272	2.39199	-0.90040
H	1.86600	-0.76585	2.17178
H	4.11215	0.21225	2.13735
H	1.85575	-0.83874	-2.14293
N	-7.33340	-0.32481	-0.00474
N	-8.30582	-0.79047	-0.00347
H	4.10195	0.13979	-2.15223
C	5.60789	0.86763	-0.02270
H	5.49203	1.94895	-0.04089
H	6.17317	0.60955	0.86302
H	6.16909	0.57943	-0.90170

15a

C	-0.74704	-0.95112	-1.27788
C	-2.41165	-1.20843	0.70467
N	-1.70600	-1.10431	-0.16436
C	-3.32836	-1.34810	1.84144
C	0.65693	-0.80214	-0.74893
C	1.47503	-1.91478	-0.62222
C	2.76395	-1.76547	-0.13792
C	3.23620	-0.51455	0.22097
C	2.41116	0.59069	0.08868
C	1.12427	0.45708	-0.39744
Cl	2.99512	2.16116	0.52890
H	-0.87660	-1.83293	-1.88620
H	-1.08914	-0.08552	-1.82445
H	-3.76909	-2.33620	1.81573
H	-4.09802	-0.59259	1.75856

H	-2.76836	-1.21397	2.75790
H	1.12050	-2.88944	-0.90743
H	3.40503	-2.62193	-0.04462
H	4.23543	-0.39369	0.59320
H	0.50569	1.32912	-0.50676
N	-4.48520	1.47334	-0.33590
N	-5.04671	2.29360	-0.75337

15b

C	-0.15286	0.85181	-1.41344
C	2.76409	0.29416	0.85853
N	1.85750	0.47100	0.19898
C	3.93791	0.06539	1.71137
C	-1.36881	0.78794	-0.77146
C	-1.95337	1.96294	-0.22968
C	-3.17232	1.89290	0.39205
C	-3.81951	0.66190	0.48779
C	-3.25980	-0.51057	-0.03299
C	-2.04575	-0.45768	-0.65672
Cl	-4.11041	-2.00434	0.12095
H	0.36617	1.78111	-1.54163
H	0.29403	-0.01346	-1.86178
H	4.10180	0.93050	2.33996
H	4.80928	-0.09971	1.09228
H	3.76860	-0.80318	2.33373
H	-1.43359	2.89942	-0.31367
H	-3.63369	2.76887	0.80503
H	-4.77558	0.60389	0.97434
H	-1.60120	-1.34811	-1.05999
N	7.33294	-0.57055	-0.36656
N	8.29580	-0.74877	-0.81772

16a

C	-1.92529	-1.98728	-0.00018
C	-3.70096	-0.09053	0.00010
N	-2.94245	-0.92085	-0.00003
C	-4.69623	0.98751	0.00024
C	-0.53633	-1.39419	-0.00012
C	0.10072	-1.12903	1.20456
C	1.37420	-0.58842	1.21135
C	1.98410	-0.32495	0.00002
C	1.37430	-0.58834	-1.21137
C	0.10081	-1.12894	-1.20471
N	3.33033	0.25134	0.00009
O	3.82753	0.46705	-1.05961
O	3.82751	0.46683	1.05985
H	-2.13010	-2.57714	0.88018
H	-2.13011	-2.57691	-0.88070
H	-4.17522	1.93555	-0.00058
H	-5.30881	0.89614	0.88789
H	-5.31003	0.89525	-0.88646
H	-0.38182	-1.35007	2.13970
H	1.88710	-0.38055	2.12832
H	1.88726	-0.38041	-2.12828
H	-0.38165	-1.34990	-2.13992
N	-1.33654	2.53478	-0.00011
N	-0.42974	3.11788	-0.00016



## 16b

C	-1.38725	-2.30867	0.00005
C	-4.16334	-0.07993	-0.00003
N	-3.26545	-0.77367	-0.00002
C	-5.32388	0.82059	0.00004
C	-0.19420	-1.58820	0.00006
C	0.41571	-1.23273	1.22384
C	1.60621	-0.54667	1.22689
C	2.16734	-0.22159	0.00008
C	1.60625	-0.54672	-1.22674
C	0.41575	-1.23278	-1.22371
N	3.44293	0.51877	0.00008
O	3.90342	0.78644	-1.06134
O	3.90336	0.78653	1.06151
H	-1.83390	-2.65044	0.91254
H	-1.83387	-2.65049	-0.91243
H	-5.92126	0.63834	0.88331
H	-5.92157	0.63807	-0.88296
H	-4.98211	1.84699	-0.00018
H	-0.05248	-1.50073	2.15284
H	2.09664	-0.26406	2.13542
H	2.09672	-0.26415	-2.13527
H	-0.05240	-1.50082	-2.15271
N	-1.80616	2.78414	-0.00034
N	-0.78639	2.43415	-0.00041

## 17a

C	2.63362	1.45865	-0.48131
C	1.66599	1.03561	0.62648
O	2.02331	1.24184	1.78985
H	2.32015	1.16086	-1.47944
H	3.60494	1.00413	-0.27116
C	0.25387	0.64849	0.33244
C	-0.52955	0.12152	1.36497
C	-1.87492	-0.18533	1.17423
C	-2.49401	0.03322	-0.07163
C	-1.70834	0.57666	-1.10694
C	-0.36494	0.87559	-0.90629
H	-0.06126	-0.05439	2.32816
H	-2.43751	-0.60054	2.00395
H	-2.14070	0.72662	-2.09250
H	0.20911	1.27154	-1.73781
O	2.72541	2.90252	-0.47740
Br	2.38552	-1.77220	-0.33014
H	2.91402	3.15055	0.44338
N	-3.85001	-0.31421	-0.31960
C	-4.69516	0.71815	-0.90817
H	-4.18124	1.22002	-1.72887
H	-5.60665	0.25801	-1.30906
H	-4.99212	1.48842	-0.16913
C	-4.54432	-1.06828	0.70771
H	-3.95121	-1.93920	1.00065
H	-4.76725	-0.47473	1.61656
H	-5.49659	-1.42546	0.29860

## 17b

C	2.65585	0.51463	-0.53247
C	1.66095	1.30452	0.37635

O	2.03483	1.43816	1.61398
H	2.46062	0.61549	-1.60085
H	3.67163	0.82249	-0.28668
C	0.21098	0.80245	0.16794
C	-0.49652	0.31072	1.26254
C	-1.82475	-0.11898	1.14561
C	-2.48260	-0.08192	-0.09354
C	-1.76626	0.40248	-1.20407
C	-0.44865	0.83651	-1.06915
H	0.01698	0.29908	2.22025
H	-2.33926	-0.48074	2.03166
H	-2.24107	0.41447	-2.18354
H	0.07200	1.22150	-1.94275
O	1.71972	2.64961	-0.37880
Br	2.62281	-1.46763	-0.21744
H	2.07086	3.19615	0.34523
N	-3.82979	-0.54112	-0.27650
C	-4.76369	0.46333	-0.77528
H	-4.33194	0.99928	-1.62245
H	-5.68542	-0.02843	-1.11311
H	-5.03301	1.21015	-0.00097
C	-4.40798	-1.30791	0.81122
H	-3.73010	-2.11623	1.10122
H	-4.63094	-0.70179	1.71291
H	-5.35040	-1.75352	0.46868

18a

C	1.29930	1.70648	-0.45103
C	0.41069	1.03477	0.59835
O	0.63664	1.29495	1.78337
H	1.14056	1.33474	-1.46111
H	2.34144	1.53378	-0.17153
C	-0.88157	0.37028	0.22059
C	-1.53966	-0.41171	1.18306
C	-2.79655	-0.95044	0.92169
C	-3.42519	-0.70897	-0.30750
C	-2.78349	0.07966	-1.26558
C	-1.51745	0.61215	-1.00439
H	-1.03796	-0.59198	2.12815
H	-3.28565	-1.57137	1.66990
H	-4.40620	-1.13268	-0.51442
H	-3.26463	0.27768	-2.22147
H	-1.02948	1.22236	-1.75808
O	0.99645	3.12176	-0.46788
Br	1.79487	-1.43478	-0.22921
H	1.06030	3.41768	0.45567

18b

C	1.48843	0.78005	-0.58678
C	0.29031	1.35385	0.23417
O	0.57630	1.70761	1.45134
H	1.30006	0.70375	-1.65842
H	2.36775	1.39067	-0.38460
C	-0.96776	0.46015	0.07657
C	-1.53131	-0.10751	1.22353
C	-2.69255	-0.88297	1.14637
C	-3.30691	-1.11085	-0.09016
C	-2.75209	-0.54534	-1.24430

C	-1.58872	0.22584	-1.15787
H	-1.04113	0.10342	2.17006
H	-3.11842	-1.31480	2.05171
H	-4.21191	-1.71368	-0.15399
H	-3.22702	-0.70585	-2.21178
H	-1.17732	0.68082	-2.05558
O	0.00459	2.58072	-0.65719
Br	2.01860	-1.07892	-0.04932
H	0.17329	3.27175	0.00633

19a

C	2.27100	1.45101	-0.55913
C	1.34945	0.97906	0.56697
O	1.69860	1.21368	1.72737
H	1.97905	1.08981	-1.54307
H	3.28145	1.09699	-0.33979
C	-0.07177	0.57704	0.29366
C	-0.80814	-0.01886	1.32901
C	-2.16200	-0.30346	1.17794
C	-2.79080	0.02768	-0.02461
C	-2.09131	0.62984	-1.06673
C	-0.73037	0.90077	-0.89877
H	-0.29367	-0.26444	2.25203
H	-2.72363	-0.78194	1.97466
H	-2.59747	0.88407	-1.99302
H	-0.18739	1.37251	-1.71135
O	2.22819	2.89620	-0.60970
Br	2.10610	-1.69855	-0.25544
H	2.41430	3.20110	0.29414
Cl	-4.51746	-0.32273	-0.22616

19b

C	-2.24364	0.43770	0.60518
C	-1.11419	1.25224	-0.13131
O	-1.43484	1.87427	-1.17893
H	-1.93721	0.26654	1.67226
H	-3.11525	1.12089	0.63791
C	0.30272	0.68120	-0.06988
C	1.20987	1.02616	-1.08087
C	2.53365	0.57672	-1.06403
C	2.95120	-0.24063	-0.01651
C	2.07238	-0.62039	0.99851
C	0.75257	-0.16050	0.95533
H	0.85261	1.66837	-1.88087
H	3.23143	0.85907	-1.85016
H	2.41335	-1.25528	1.80823
H	0.08174	-0.44130	1.76008
O	-1.03467	2.39963	1.43700
Br	-2.79972	-1.24436	-0.20173
H	-1.37399	3.18928	0.97598
Cl	4.63567	-0.80947	0.04082

20a

C	-2.40876	1.31315	-0.08795
C	-1.13474	0.79746	-0.75982
O	-1.11137	0.76916	-1.99343
H	-2.41529	1.18703	0.99266
H	-3.25701	0.76943	-0.51135

C	0.15863	0.68867	0.00151
C	1.24252	0.06571	-0.63818
C	2.48610	0.06567	-0.02555
C	2.70110	0.67003	1.21615
C	1.62254	1.30243	1.83794
C	0.36098	1.31376	1.23815
H	1.08431	-0.40413	-1.60186
H	3.68438	0.64872	1.67585
H	1.76956	1.78789	2.80027
H	-0.46329	1.81252	1.73671
O	-2.52119	2.73138	-0.34853
Br	-1.84504	-1.75853	0.35446
H	-2.43119	2.83392	-1.31083
Cl	3.85267	-0.72898	-0.83208

20b

C	-2.28979	0.61700	0.01434
C	-1.03182	1.17213	-0.72310
O	-0.99128	0.93880	-1.99923
H	-2.42997	1.01622	1.01959
H	-3.16428	0.80480	-0.60757
C	0.26551	0.81363	0.05649
C	1.25935	0.10964	-0.63003
C	2.46354	-0.17049	0.00707
C	2.71574	0.21157	1.32425
C	1.71696	0.91705	2.00513
C	0.50209	1.20699	1.37963
H	1.05936	-0.16426	-1.66140
H	3.66534	-0.02201	1.79673
H	1.89556	1.23753	3.03046
H	-0.25465	1.77724	1.91134
O	-1.24585	2.66484	-0.42364
Br	-2.24769	-1.36784	0.27420
H	-1.31999	2.98281	-1.34002
Cl	3.73561	-1.05014	-0.88035

21a

C	2.87528	1.41166	-0.57412
C	1.96023	0.94885	0.56093
O	2.31963	1.18547	1.71786
H	2.56461	1.06097	-1.55609
H	3.88219	1.03814	-0.36999
C	0.52752	0.56750	0.30310
C	-0.21253	0.00684	1.35680
C	-1.57289	-0.23687	1.22195
C	-2.22582	0.08643	0.02179
C	-1.50315	0.65985	-1.02976
C	-0.13651	0.89681	-0.88620
H	0.30764	-0.23915	2.27612
H	-2.12953	-0.68804	2.03824
H	-2.00374	0.91779	-1.95829
H	0.41072	1.34226	-1.71017
O	2.85831	2.85637	-0.61637
Br	2.58998	-1.70606	-0.26259
H	3.05734	3.15316	0.28750
C	-3.70326	-0.11095	-0.10331
F	-4.16264	-1.16749	0.62233
F	-4.42051	0.97415	0.33665

F	-4.10744	-0.31651	-1.38738
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21b

C	2.89698	0.38468	-0.61377
C	1.95276	1.33260	0.19035
O	2.34826	1.61896	1.39361
H	2.69088	0.35329	-1.68438
H	3.92745	0.68055	-0.42042
C	0.47868	0.85520	0.08100
C	-0.20619	0.54175	1.25907
C	-1.54488	0.15217	1.23262
C	-2.22157	0.06473	0.00803
C	-1.54916	0.38005	-1.18101
C	-0.20968	0.76532	-1.13627
H	0.34594	0.63540	2.18980
H	-2.06326	-0.09059	2.15662
H	-2.07108	0.32183	-2.13250
H	0.30051	1.02633	-2.05930
O	2.02293	2.55321	-0.73887
Br	2.77816	-1.52766	-0.03203
H	2.38272	3.19521	-0.10272
C	-3.67179	-0.29309	-0.02422
F	-4.04163	-1.12673	0.98957
F	-4.49746	0.79933	0.08662
F	-4.04636	-0.90945	-1.18271

22a

C	2.59322	1.38593	-0.51630
C	1.65909	0.90294	0.59513
O	2.01241	1.09614	1.76133
H	2.27232	1.09536	-1.51453
H	3.58420	0.96216	-0.33064
C	0.22766	0.53593	0.31432
C	-0.52949	-0.03424	1.35604
C	-1.89045	-0.24858	1.21543
C	-2.51639	0.12666	0.01685
C	-1.79352	0.71235	-1.02759
C	-0.42741	0.91516	-0.87021
H	-0.01748	-0.30782	2.27181
H	-2.47658	-0.70137	2.00630
H	-2.30464	1.00194	-1.93795
H	0.13193	1.37452	-1.67789
O	2.63365	2.82796	-0.48797
Br	2.14064	-1.72244	-0.33438
H	2.83623	3.07332	0.43053
N	-3.94542	-0.08729	-0.14020
O	-4.57145	-0.60406	0.79728
O	-4.48294	0.25764	-1.20375

22b

C	2.56415	0.38862	-0.60493
C	1.61397	1.32696	0.20249
O	2.00051	1.60754	1.40922
H	2.37031	0.37349	-1.67810
H	3.59273	0.68036	-0.39571
C	0.14325	0.83807	0.08824
C	-0.54079	0.51523	1.26735
C	-1.87274	0.11358	1.24101

C	-2.52883	0.03225	0.00624
C	-1.87334	0.35406	-1.18943
C	-0.54040	0.74750	-1.13536
H	0.01098	0.61247	2.19767
H	-2.40768	-0.14028	2.14914
H	-2.40978	0.29053	-2.12920
H	-0.02842	1.01967	-2.05363
O	1.66591	2.55301	-0.71611
Br	2.42916	-1.52823	-0.04761
H	1.99987	3.20205	-0.07296
N	-3.92159	-0.39007	-0.03729
O	-4.49419	-0.65701	1.02924
O	-4.48334	-0.46818	-1.14025

23a

Rh	-0.64125	-0.14431	-0.36892
C	2.54788	0.34290	0.60564
C	2.52817	1.86571	0.63539
O	2.67101	2.44801	-0.57633
C	2.67281	3.88682	-0.56767
H	1.71955	4.26169	-0.18721
H	2.81581	4.18400	-1.60692
H	3.48379	4.26573	0.05908
O	2.47227	2.49769	1.66834
C	1.86652	-0.39442	-0.52119
C	1.36439	0.06988	-1.69637
H	1.05350	-0.62950	-2.46631
H	1.38728	1.11940	-1.96082
H	1.89593	-1.47375	-0.38027
O	-0.15991	-0.88876	1.51870
C	-1.09228	-1.10639	2.35267
O	-2.33194	-0.92879	2.19575
Rh	-2.96384	-0.18610	0.38302
O	-3.08207	-2.11106	-0.36174
C	-2.05215	-2.61163	-0.89655
O	-0.90893	-2.07963	-1.05124
H	-2.15331	-3.63700	-1.27757
O	-2.68937	1.73751	1.08462
C	-1.55917	2.27815	0.91702
O	-0.53109	1.78937	0.35326
H	-1.44658	3.29950	1.30450
O	-3.53465	0.55893	-1.44816
C	-2.62672	0.77298	-2.30006
O	-1.37757	0.59100	-2.17509
H	-2.95467	1.16588	-3.27221
H	-0.77513	-1.49770	3.32886
C	4.04685	-0.15823	0.76893
C	4.07854	-1.58660	1.25680
C	4.76290	-2.56570	0.65928
C	5.59390	-2.36297	-0.57863
C	5.55307	-0.94440	-1.07910
C	4.86902	0.03506	-0.48178
H	4.88490	1.03754	-0.90291
H	6.12692	-0.72578	-1.97836
H	5.26080	-3.05185	-1.37234
H	6.63715	-2.66034	-0.37916
H	4.74500	-3.56895	1.08220
H	3.50710	-1.79805	2.15996

H	2.04495	0.05351	1.53434
H	4.45157	0.48298	1.56942

23b

Rh	-0.52987	-0.05869	0.15124
C	1.74456	0.56812	0.92448
C	2.05828	1.99536	0.62909
O	2.18068	2.29487	-0.68212
C	2.45970	3.67473	-0.96611
H	1.65997	4.31230	-0.58088
H	2.51472	3.74228	-2.05300
H	3.40674	3.97744	-0.51128
O	2.19963	2.81390	1.51469
C	1.95214	-0.54547	0.15724
C	2.50008	-0.64761	-1.23465
H	1.94121	-1.42976	-1.76317
H	2.35853	0.28912	-1.77362
H	1.81872	-1.49378	0.67257
O	-0.80009	-0.71111	2.09761
C	-1.98096	-0.97570	2.48300
O	-3.05412	-0.89448	1.82038
Rh	-2.94343	-0.25463	-0.14018
O	-2.67761	-2.20103	-0.75739
C	-1.49786	-2.65076	-0.78285
O	-0.42378	-2.04716	-0.47854
H	-1.38230	-3.69368	-1.10842
O	-3.14195	1.69410	0.48685
C	-2.08417	2.32153	0.77948
O	-0.88974	1.89811	0.73990
H	-2.20887	3.36167	1.10900
O	-2.69799	0.39570	-2.08140
C	-1.52327	0.65128	-2.47500
O	-0.43879	0.56382	-1.82258
H	-1.42592	0.99213	-3.51487
H	-2.07607	-1.31759	3.52238
C	5.39427	-0.04015	0.53699
C	5.15994	-1.22600	1.36541
C	4.63092	-2.34031	0.83203
C	4.32698	-2.41665	-0.64531
C	4.01891	-1.04280	-1.28785
C	4.88756	0.04973	-0.70532
H	5.03329	0.94914	-1.29948
H	4.23493	-1.12434	-2.36097
H	3.49863	-3.11107	-0.83774
H	5.20413	-2.85478	-1.14983
H	4.47383	-3.22919	1.43918
H	5.42972	-1.18630	2.41797
H	1.50911	0.43240	1.97562
H	5.97569	0.77783	0.95596

24a

C	0.52099	-1.16346	0.48159
C	-0.23031	-0.14968	-0.39243
H	-0.08528	-0.41028	-1.44931
C	-1.73777	-0.18197	-0.12589
O	-2.35078	-1.18886	-0.40729
C	2.01681	-1.13473	0.13940
C	2.48104	0.28851	-0.02535

C	1.62340	1.30402	-0.14143
O	0.26025	1.18358	-0.19068
C	-2.39073	1.03154	0.48590
H	2.58710	-1.62534	0.93527
H	1.92310	2.34275	-0.20392
H	0.08503	-2.15127	0.32508
H	3.54083	0.51325	-0.01953
H	2.21079	-1.71388	-0.77228
H	0.37395	-0.89507	1.53330
H	-3.44935	0.83062	0.64359
H	-1.90388	1.28946	1.43068
H	-2.25870	1.89661	-0.16976

24b

C	-0.54985	1.94982	-0.07898
C	-1.69062	0.96560	-0.09929
H	-2.70509	1.34148	-0.15651
C	-1.51529	-0.35839	-0.01227
O	-0.27087	-0.95047	0.03714
C	0.74202	1.25819	0.37245
C	0.83848	-0.11370	-0.30223
C	2.09114	-0.87628	0.09197
O	3.20405	-0.45952	-0.10481
C	-2.59689	-1.38897	0.05614
H	1.63071	1.84051	0.12189
H	1.90496	-1.85362	0.58249
H	-0.78177	2.77592	0.60172
H	0.85661	0.02065	-1.39376
H	0.73215	1.11343	1.45770
H	-0.41165	2.40487	-1.06836
H	-2.52487	-2.08120	-0.78827
H	-2.49980	-1.98081	0.97163
H	-3.58052	-0.91890	0.04616

25a

C	-1.19951	-1.11374	-0.28668
C	-0.54355	0.07605	0.01367
C	-1.11759	1.36259	-0.02075
C	-0.09487	2.35549	-0.02259
C	1.12995	1.73578	0.05163
C	0.93579	0.30255	0.03779
C	1.93646	-0.61169	-0.00543
C	1.77390	-2.08847	0.01248
C	-2.62095	-1.26522	0.10293
H	2.09226	2.22269	0.13930
H	-0.26586	3.42331	-0.05017
H	-2.17431	1.56591	-0.12515
H	2.95039	-0.22229	-0.08699
H	1.82516	-2.46707	1.04147
H	2.56887	-2.58330	-0.55187
H	0.77818	-2.35542	-0.37066
H	-2.62863	-2.01454	0.90951
H	-3.13372	-0.37002	0.49663
H	-3.21019	-1.71933	-0.70033

25b

C	-1.18864	-1.08284	0.13315
C	-0.52372	0.07978	-0.02335



C	-1.11137	1.41806	-0.17274
C	-0.11132	2.33097	-0.08824
C	1.15585	1.63520	0.08871
C	0.94679	0.28451	0.09781
C	2.00850	-0.70714	0.17611
C	2.00459	-1.97222	-0.26981
C	-2.66824	-1.28050	0.06666
H	2.12071	2.11925	0.16972
H	-0.22266	3.40601	-0.13537
H	-2.16520	1.62858	-0.27604
H	2.92996	-0.33652	0.62229
H	2.88153	-2.59851	-0.15643
H	1.15989	-2.41044	-0.78656
H	-0.60859	-1.97442	0.35141
H	-3.04391	-1.66531	1.02201
H	-3.21078	-0.36674	-0.17385
H	-2.91559	-2.03687	-0.68706

26a

C	-2.42265	0.38737	-0.15561
C	-3.08381	-0.01695	1.14919
C	-3.45868	-1.28894	1.02660
C	-3.01372	-1.70899	-0.35319
C	-3.25770	-0.43842	-1.15051
O	-1.56063	-1.73898	-0.32962
C	-1.15749	-0.44891	-0.19207
C	0.12332	-0.06418	-0.09063
H	-2.29047	1.44522	-0.33377
H	-3.12183	0.60445	2.02936
H	-3.87108	-1.93879	1.78064
H	-3.35294	-2.66005	-0.74235
H	-4.29927	-0.13507	-1.17873
H	-2.83476	-0.48181	-2.15211
C	1.27191	-0.99216	-0.06782
C	1.16756	-2.31309	0.37866
C	2.52789	-0.54448	-0.48749
C	2.27327	-3.14637	0.39729
H	0.21413	-2.68619	0.71247
C	3.63081	-1.38198	-0.47470
H	2.64019	0.47320	-0.83036
C	3.51085	-2.68974	-0.03129
H	2.16551	-4.16116	0.75242
H	4.58694	-1.00853	-0.81171
H	4.37026	-3.34374	-0.01702
C	0.41750	1.39150	-0.00468
C	0.97810	1.92692	1.15427
C	0.16799	2.24795	-1.07405
C	1.25688	3.28043	1.24953
H	1.19337	1.27004	1.98485
C	0.44469	3.60486	-0.98175
H	-0.23763	1.84030	-1.98940
C	0.98802	4.12587	0.18184
H	1.68429	3.67692	2.15902
H	0.24334	4.25191	-1.82318
H	1.20668	5.18098	0.25529

26b

C	-0.66889	-2.45633	0.05624
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C	-0.63817	-1.35968	-1.03703
C	-2.09481	-1.19227	-1.34565
C	-2.85230	-2.10732	-0.74851
C	-2.06317	-3.07576	0.08456
O	-0.56225	-1.28331	2.24562
C	-0.42748	-1.34725	1.05967
C	-0.04209	-0.32558	-0.02032
H	0.15318	-3.16880	0.04099
H	-0.03891	-1.54474	-1.92440
H	-2.46954	-0.40939	-1.98709
H	-3.92593	-2.17009	-0.84895
H	-2.07774	-4.07781	-0.34722
H	-2.44143	-3.16206	1.10333
C	-0.67293	1.04670	0.02457
C	-1.28168	1.54135	1.17104
C	-0.63855	1.84628	-1.11553
C	-1.84923	2.80893	1.17313
H	-1.31072	0.93685	2.06418
C	-1.20838	3.10743	-1.11461
H	-0.15663	1.48030	-2.01153
C	-1.81752	3.59475	0.03375
H	-2.31900	3.17888	2.07275
H	-1.17388	3.71236	-2.00894
H	-2.26060	4.57961	0.03802
C	1.47547	-0.21064	-0.07010
C	2.18522	-0.27239	-1.26404
C	2.17763	0.02014	1.11075
C	3.56279	-0.10768	-1.27923
H	1.67040	-0.44160	-2.19781
C	3.55320	0.17981	1.09703
H	1.63967	0.07389	2.04603
C	4.25252	0.11628	-0.09906
H	4.09513	-0.15620	-2.21787
H	4.07917	0.35408	2.02411
H	5.32512	0.24067	-0.11066

27a

C	1.12278	1.02457	0.29610
C	1.90400	0.96704	-1.00347
C	2.56222	-0.19059	-1.01688
C	2.18963	-0.88850	0.26779
C	2.09442	0.28162	1.23330
O	0.78267	-1.25566	0.15185
C	0.10886	-0.08688	0.14744
C	-1.21151	-0.01549	0.02202
Cl	-2.04301	1.49176	0.03153
Cl	-2.19198	-1.40966	-0.14890
H	0.72519	1.98223	0.60338
H	1.82430	1.69480	-1.79449
H	3.14024	-0.61793	-1.81913
H	2.73247	-1.77925	0.55358
H	3.03027	0.81376	1.36837
H	1.65871	0.00538	2.19099

27b

C	-1.13710	-1.04612	-0.33433
C	-0.47522	0.16808	-1.04360
C	-1.44036	1.27258	-0.74263

C	-2.55620	0.82818	-0.17344
C	-2.56762	-0.65764	0.03171
O	-0.05554	-1.20857	1.91815
C	-0.12249	-0.86664	0.78544
C	0.73549	0.07395	-0.08488
Cl	2.05234	-0.87305	-0.81085
Cl	1.34708	1.53644	0.65705
H	-1.03048	-2.00746	-0.83013
H	-0.20526	0.08718	-2.09305
H	-1.23303	2.30296	-0.98452
H	-3.38814	1.45698	0.10678
H	-3.29932	-1.14274	-0.61542
H	-2.80854	-0.94035	1.05612

28a

C	1.77274	-0.97848	0.48374
C	1.31072	-0.69981	-0.95696
C	0.81133	-1.34220	1.55322
C	0.33689	-1.71946	-1.50132
C	-0.52489	-1.46401	1.47418
C	-0.86641	-1.94499	-0.97485
C	-1.39831	-1.24074	0.26086
O	2.95972	-0.87271	0.75863
H	0.64757	-2.26828	-2.38793
H	-1.52781	-2.67055	-1.44360
H	-2.38133	-1.67206	0.48193
H	-1.05276	-1.71257	2.39385
C	-0.00028	2.17889	0.62161
H	1.30544	-1.50865	2.50788
C	0.73690	0.75549	-1.06538
H	2.22957	-0.72382	-1.54935
C	-0.38411	1.08912	-0.08372
C	1.77229	1.81452	-0.78728
H	0.36920	0.86276	-2.09703
C	1.32539	2.62808	0.18719
H	-0.57203	2.66650	1.40287
H	2.72621	1.85953	-1.29920
H	1.84607	3.48464	0.60243
C	-1.67762	0.31532	0.03712
C	-2.50511	0.82431	1.23348
C	-2.52325	0.48501	-1.24603
H	-1.98068	0.15308	-2.13496
H	-2.79195	1.53816	-1.38176
H	-3.45020	-0.09862	-1.17659
H	-1.94905	0.74232	2.17288
H	-3.43245	0.24792	1.33020
H	-2.78120	1.87491	1.09426

28b

C	-1.90132	0.27535	-0.00000
C	-1.10495	0.14317	-1.30052
C	-1.10495	0.14317	1.30052
C	-0.35774	1.41439	-1.60983
C	-0.35774	1.41439	1.60983
C	0.16106	2.29809	-0.73392
C	0.16106	2.29809	0.73391
O	-3.09804	0.48001	-0.00000
H	-0.20432	1.61134	-2.66954

H	0.67988	3.15140	-1.16857
H	0.67988	3.15140	1.16857
H	-0.20432	1.61134	2.66954
C	-0.13470	-1.11543	1.18135
H	-1.83741	-0.04671	2.09220
C	-0.13470	-1.11543	-1.18135
H	-1.83741	-0.04672	-2.09220
C	0.78560	-0.86599	0.00000
C	-0.94776	-2.29377	-0.67033
H	0.36103	-1.28311	-2.13999
C	-0.94776	-2.29377	0.67034
H	0.36103	-1.28310	2.13999
H	-1.51798	-2.95664	-1.31351
H	-1.51798	-2.95664	1.31351
C	2.06819	-0.48451	0.00000
C	2.85451	-0.23147	1.26364
C	2.85451	-0.23147	-1.26364
H	2.29066	-0.44313	-2.17445
H	3.77081	-0.83752	-1.28056
H	3.16959	0.81997	-1.30773
H	2.29065	-0.44312	2.17445
H	3.16960	0.81996	1.30772
H	3.77081	-0.83753	1.28057

29a

C	-1.85108	-0.22813	0.35603
C	-0.92680	0.26857	1.48068
C	-1.41753	-1.23019	-0.66688
C	-0.17951	-0.82396	2.20822
C	-0.19739	-1.79928	-0.74187
C	0.69829	-1.62870	1.61203
C	1.01662	-1.57196	0.12970
O	-2.97898	0.24205	0.28711
H	-0.36435	-0.91849	3.27622
H	1.23235	-2.37241	2.19964
H	1.71683	-2.38886	-0.07975
H	-0.03747	-2.49064	-1.56876
C	0.63587	1.83722	-1.27124
C	0.04602	1.36864	0.93055
H	-1.60332	0.76822	2.17950
C	0.87992	0.95116	-0.27746
C	-0.67684	2.59999	0.44821
H	0.71025	1.63514	1.76638
C	-0.31950	2.85504	-0.82405
H	1.06927	1.81636	-2.26464
H	-1.38555	3.14820	1.05748
H	-0.67040	3.67594	-1.44077
C	1.79694	-0.24972	-0.30716
C	2.35081	-0.47396	-1.72760
C	2.99044	-0.03676	0.65197
H	2.65841	0.14492	1.67744
H	3.58541	0.82358	0.32682
H	3.64147	-0.92042	0.65797
H	1.54624	-0.62027	-2.45527
H	3.00051	-1.35654	-1.75007
H	2.94794	0.38550	-2.05059
C	-2.49251	-1.56311	-1.67470
H	-3.38625	-1.95513	-1.17697

H	-2.81144	-0.66048	-2.20723
H	-2.14058	-2.29998	-2.40300

29b

C	-1.65464	0.37718	-0.55667
C	-0.56554	0.32127	-1.63335
C	-1.23149	0.08086	0.89504
C	0.25277	1.58523	-1.64571
C	-0.50635	1.28120	1.46391
C	0.56383	2.36592	-0.59268
C	0.21964	2.22027	0.82540
O	-2.80240	0.65081	-0.84543
H	0.65045	1.86916	-2.61855
H	1.18231	3.23663	-0.80587
H	0.64807	2.99664	1.45797
H	-0.58651	1.37293	2.54680
C	-0.26360	-1.19574	0.86478
C	0.32645	-0.97545	-1.41106
H	-1.09436	0.22841	-2.58796
C	0.92516	-0.87211	-0.02039
C	-0.59954	-2.16798	-1.23803
H	1.04297	-1.06967	-2.23016
C	-0.93131	-2.29649	0.05450
H	-0.02278	-1.47338	1.89383
H	-0.99261	-2.75137	-2.06475
H	-1.63731	-3.00932	0.46735
C	2.17387	-0.54744	0.33411
C	2.62225	-0.44254	1.77173
C	3.25579	-0.21257	-0.66405
H	2.93242	-0.30982	-1.70248
H	4.13406	-0.85651	-0.51794
H	3.59492	0.82236	-0.52022
H	1.84677	-0.72053	2.48846
H	2.92501	0.58905	1.99772
H	3.49993	-1.07778	1.95435
C	-2.47676	-0.21773	1.74319
H	-3.15245	0.64103	1.75007
H	-3.03021	-1.06869	1.33615
H	-2.18473	-0.44878	2.77440

30a

C	-1.61630	-1.43827	-0.45476
C	-1.32390	-0.95039	0.97060
C	-0.55077	-1.46568	-1.48451
C	-0.10970	-1.60384	1.58400
C	0.75135	-1.15652	-1.36659
C	1.12759	-1.47810	1.10679
C	1.53431	-0.70429	-0.14480
O	-2.75054	-1.78277	-0.75500
H	-0.27267	-2.18745	2.48773
H	1.94345	-1.95393	1.64847
H	1.34220	-1.21731	-2.28060
C	-0.81881	2.10054	-0.73716
H	-0.93118	-1.77207	-2.45655
C	-1.20853	0.61045	1.00449
H	-2.21359	-1.21962	1.54668
C	-0.17273	1.21659	0.05961
C	-2.49264	1.29082	0.60430

H	-0.95790	0.87539	2.04269
C	-2.24507	2.14630	-0.40410
H	-0.37150	2.70027	-1.52106
H	-3.44867	1.06913	1.06371
H	-2.96899	2.77918	-0.90683
C	1.30869	0.88695	0.06718
C	2.01999	1.67100	-1.05432
C	1.91711	1.33627	1.41837
H	1.44588	0.83139	2.26491
H	1.77450	2.41524	1.54216
H	2.99339	1.13531	1.45873
H	1.67060	1.36955	-2.04749
H	3.10321	1.53178	-1.01074
H	1.82976	2.74285	-0.94012
C	3.02375	-1.03456	-0.40809
H	3.66618	-0.67088	0.39974
H	3.15087	-2.12145	-0.46918
H	3.38272	-0.60883	-1.34840

30b

C	-1.41037	-1.38460	0.05589
C	-1.15584	-0.54329	1.30709
C	-0.69757	-0.92919	-1.21722
C	0.18869	-0.87308	1.89938
C	0.75365	-1.33344	-1.22280
C	1.31050	-1.24781	1.25488
C	1.60104	-1.45672	-0.17880
O	-2.13020	-2.36234	0.07589
H	0.25276	-0.76497	2.98095
H	2.17748	-1.41992	1.89268
H	1.16374	-1.50305	-2.21725
C	-0.87807	0.64767	-1.36871
H	-1.20939	-1.42555	-2.04848
C	-1.28975	0.99939	0.92943
H	-1.94152	-0.80429	2.02381
C	-0.25517	1.28923	-0.14270
C	-2.57952	1.18409	0.14624
H	-1.21398	1.60279	1.83669
C	-2.34551	0.98386	-1.15847
H	-0.46852	0.96733	-2.32947
H	-3.54770	1.34720	0.60904
H	-3.08947	0.95535	-1.94836
C	0.92896	1.90145	-0.02460
C	1.89118	2.06607	-1.17608
C	1.44630	2.45441	1.28139
H	0.73498	2.35845	2.10430
H	1.70848	3.51647	1.17885
H	2.36462	1.92867	1.57672
H	1.50007	1.69120	-2.12396
H	2.82421	1.52403	-0.96776
H	2.16295	3.12205	-1.31124
C	3.04700	-1.82883	-0.44432
H	3.72392	-1.03964	-0.08876
H	3.32381	-2.74705	0.09064
H	3.24202	-1.98561	-1.50910

31a

C	0.21209	1.36540	-0.21227
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C	1.70419	1.25042	-0.02062
C	2.35446	0.08490	0.06691
C	1.66122	-1.24979	-0.02440
C	0.26942	-1.12792	-0.65986
C	-0.52231	0.01991	0.00818
O	-0.64452	-0.24464	1.39649
C	-1.89895	0.10383	-0.62560
O	-2.92503	-0.02855	0.01274
H	2.25443	2.18638	0.05373
H	0.00241	1.75237	-1.22152
H	3.43017	0.08181	0.23126
H	2.26950	-1.95375	-0.60554
H	1.56259	-1.67788	0.98213
H	0.36901	-0.91703	-1.73269
H	-0.28744	-2.06452	-0.54825
H	-0.20768	2.09115	0.49432
H	-1.92196	0.28950	-1.71872
H	-1.59539	-0.28301	1.59742

31b

C	-0.01212	-1.49631	-0.42034
C	1.42946	-1.48009	0.02396
C	2.20878	-0.39055	0.06089
C	1.76383	0.99899	-0.33217
C	0.55401	1.53836	0.48208
C	-0.75614	0.87790	0.11328
O	-1.64541	1.49675	-0.45570
C	-0.97415	-0.60599	0.41950
O	-2.30951	-0.96875	0.14799
H	1.85312	-2.42949	0.34527
H	-0.41937	-2.50826	-0.35419
H	3.23547	-0.49772	0.40573
H	2.59221	1.70030	-0.19530
H	1.50728	1.03218	-1.40051
H	0.74935	1.38292	1.54995
H	0.42938	2.60930	0.29944
H	-0.10473	-1.19181	-1.47233
H	-0.76225	-0.77518	1.48537
H	-2.72312	-0.20011	-0.28482

32a

C	0.12268	1.31642	-0.32563
C	1.61140	1.30879	-0.07153
C	2.33224	0.18823	0.06555
C	1.73791	-1.19417	-0.03170
C	0.32352	-1.17644	-0.62902
C	-0.52930	-0.05933	0.02055
C	-1.90842	-0.04680	-0.61569
O	-2.95060	0.05396	-0.00231
H	2.09977	2.27858	0.00354
H	-0.06569	1.58071	-1.37787
H	3.39935	0.26038	0.26783
H	2.38905	-1.83743	-0.63679
H	1.70870	-1.65242	0.96718
H	0.38617	-0.99718	-1.71061
H	-0.16585	-2.14297	-0.47214
H	-0.36506	2.09289	0.27722
H	-1.90671	-0.10478	-1.72628

H	-1.52773	0.09072	1.80447
N	-0.65804	-0.30310	1.45423
H	0.11896	0.10128	1.96711

32b

C	0.03691	-1.50381	-0.42477
C	1.48337	-1.44503	0.00063
C	2.23062	-0.33370	0.04663
C	1.74173	1.04955	-0.31643
C	0.51269	1.53085	0.50121
C	-0.78319	0.84799	0.12258
C	-0.94441	-0.64043	0.41669
O	-2.26513	-1.06654	0.15711
H	1.94444	-2.38555	0.29651
H	-0.33574	-2.52863	-0.35138
H	3.26587	-0.41693	0.37246
H	2.54946	1.77190	-0.16220
H	1.48770	1.09433	-1.38537
H	0.71122	1.36172	1.56678
H	0.38676	2.61049	0.35695
H	-0.07618	-1.20501	-1.47649
H	-0.71886	-0.80444	1.48157
H	-2.71894	-0.30469	-0.25192
N	-1.77539	1.41429	-0.45029
H	-1.61322	2.40665	-0.63098

33a

C	0.60050	1.36712	-0.23549
C	2.08580	1.24904	-0.00030
C	2.73452	0.08406	0.10129
C	2.04474	-1.25031	-0.01036
C	0.66649	-1.12971	-0.67407
C	-0.14509	0.01882	-0.01808
O	-0.23929	-0.24198	1.37122
C	-1.48842	0.10881	-0.69268
H	2.63304	2.18537	0.09170
H	0.42011	1.74584	-1.25224
H	3.80541	0.08133	0.29458
H	2.66493	-1.95045	-0.58394
H	1.92721	-1.68321	0.99182
H	0.78604	-0.91653	-1.74377
H	0.10614	-2.06468	-0.57334
H	0.16018	2.09679	0.45378
H	-1.43380	0.27255	-1.77257
H	-1.18417	-0.24932	1.61053
S	-2.93513	-0.01681	0.04324

33b

C	0.05790	-1.39959	0.48411
C	-1.37068	-1.71355	0.09718
C	-2.38463	-0.84777	-0.05081
C	-2.33284	0.65059	0.13993
C	-1.19930	1.37780	-0.63490
C	0.15837	1.05472	-0.04333
O	0.68506	1.80548	0.75967
C	0.75839	-0.31236	-0.39093
H	-1.58553	-2.76667	-0.07570
H	0.65728	-2.30972	0.40833



H	-3.35411	-1.25706	-0.32980
H	-3.28484	1.08520	-0.18008
H	-2.22788	0.89531	1.20651
H	-1.24059	1.09037	-1.69109
H	-1.33963	2.45883	-0.54908
H	0.11987	-1.07834	1.53333
H	0.56010	-0.53753	-1.44298
H	2.62371	0.52628	0.82389
S	2.59174	-0.33810	-0.21176

35a

C	-0.84792	0.85064	-0.17320
C	-1.25015	1.82512	1.03749
C	-1.85715	1.02451	2.15694
C	-2.85558	0.19207	1.85679
C	-3.27216	0.10142	0.41303
C	-2.02446	-0.18711	-0.49624
C	-4.42061	-0.88903	0.16710
C	-3.95755	-2.34180	0.28368
C	-1.60935	-1.68162	-0.50027
C	-2.83184	-2.59768	-0.71813
C	-0.57816	-1.98764	-1.59824
C	-0.73641	1.77212	-1.38789
C	0.47068	0.19046	0.29021
C	1.68152	1.38120	-1.46242
O	-1.69904	2.34747	-1.87214
O	0.46225	-0.53953	1.27378
N	0.52648	1.97711	-1.91918
C	1.72652	0.51145	-0.42256
C	3.00765	-0.12538	-0.03483
C	3.37471	-0.27552	1.31370
C	3.89812	-0.57766	-1.02344
C	4.60266	-0.83979	1.65412
C	5.12877	-1.13689	-0.68093
C	5.48675	-1.26885	0.66139
C	-0.10111	2.72962	1.50283
H	-3.62796	1.09478	0.10102
H	-2.35198	0.04046	-1.51754
H	-4.82668	-0.72528	-0.84098
H	-5.23440	-0.67448	0.87201
H	-3.59671	-2.54110	1.30277
H	-4.79539	-3.02737	0.10464
H	-1.17824	-1.92608	0.47602
H	-2.49864	-3.64242	-0.66646
H	-3.21988	-2.44554	-1.73774
H	0.36224	-1.44359	-1.47767
H	-0.98395	-1.73372	-2.58685
H	-1.45902	1.13306	3.16248
H	-3.34150	-0.42804	2.60702
H	2.58055	1.66989	-1.99714
H	2.69114	0.04462	2.09018
H	3.61082	-0.51273	-2.07015
H	4.87046	-0.94416	2.70228
H	5.79966	-1.48275	-1.46297
H	6.44169	-1.71113	0.93232
H	0.56214	2.62005	-2.70084
H	0.68560	2.15600	2.00304
H	0.35126	3.28083	0.67108

H	-0.48368	3.46404	2.21989
H	-2.02724	2.46925	0.60461
H	-0.33083	-3.05556	-1.60464

35b

C	-0.82480	-1.27581	-0.47567
C	-0.51396	3.55988	-0.93741
C	-0.27242	2.80451	0.13646
C	-0.84783	1.44554	0.45236
C	-1.95531	0.92373	-0.47294
C	-2.15250	-0.59992	-0.27372
C	-3.28434	1.68386	-0.27605
C	-3.98469	1.33908	1.04675
C	-2.82545	-0.93507	1.08843
C	-4.15845	-0.17566	1.20729
C	-3.03195	-2.44185	1.28180
C	-0.78159	-2.56758	-1.12394
C	0.33233	-0.63757	-0.09412
C	1.65924	-2.46964	-0.85568
O	-1.74684	-3.20675	-1.54791
O	0.33353	0.57685	0.49521
N	0.51632	-3.09818	-1.25160
C	1.63872	-1.23252	-0.27299
C	2.90146	-0.56851	0.13181
C	3.15105	0.78244	-0.16827
C	3.90208	-1.30020	0.79220
C	4.36547	1.37261	0.17502
C	5.12071	-0.70993	1.12816
C	5.35741	0.63041	0.82138
C	0.13421	4.88790	-1.20575
H	-1.61688	1.06565	-1.50723
H	-2.82694	-0.96335	-1.06004
H	-3.94739	1.40518	-1.10657
H	-3.12419	2.76494	-0.34874
H	-3.40604	1.73176	1.89451
H	-4.95897	1.84227	1.08540
H	-2.15985	-0.58206	1.89162
H	-4.62677	-0.40275	2.17397
H	-4.84509	-0.54912	0.43221
H	-2.07781	-2.97579	1.31813
H	-3.60975	-2.86835	0.45568
H	0.45263	3.14974	0.87410
H	-1.21447	1.45372	1.48529
H	2.58796	-2.99353	-1.05208
H	2.38788	1.36595	-0.67082
H	3.71143	-2.33564	1.06279
H	4.54057	2.41744	-0.06883
H	5.87891	-1.29549	1.64167
H	6.30298	1.09482	1.08820
H	0.55716	-4.00064	-1.70908
H	0.84279	5.16012	-0.41628
H	0.67539	4.87346	-2.16128
H	-0.61612	5.68625	-1.28229
H	-1.22672	3.22349	-1.68901
H	-3.56480	-2.63582	2.22077

36a

C	1.11902	0.00001	0.02351
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C	0.33391	1.28862	0.05381
C	0.33393	-1.28864	0.05329
C	-0.22428	1.60282	-1.30987
C	-0.22411	-1.60224	-1.31060
C	-0.61011	0.73463	-2.25723
C	-0.60996	-0.73364	-2.25759
H	-0.33067	2.66395	-1.52292
H	-0.99506	1.17215	-3.17591
H	-0.99465	-1.17080	-3.17656
H	-0.33020	-2.66328	-1.52426
C	-0.79606	-1.17510	1.15223
H	1.00313	-2.10527	0.34252
C	-0.79611	1.17459	1.15273
H	1.00309	2.10516	0.34337
C	-1.67162	-0.00020	0.77699
C	-0.16325	0.66708	2.43491
H	-1.30283	2.13675	1.24484
C	-0.16313	-0.66812	2.43459
H	-1.30274	-2.13733	1.24393
H	0.29678	1.31065	3.17681
H	0.29698	-1.31197	3.17620
C	-2.87915	-0.00008	0.20997
C	-3.61461	-1.26204	-0.15810
C	-3.61458	1.26204	-0.15752
H	-3.08539	2.17111	0.13407
H	-4.60827	1.28085	0.30730
H	-3.76820	1.30269	-1.24323
H	-3.08545	-2.17126	0.13309
H	-3.76827	-1.30222	-1.24381
H	-4.60829	-1.28102	0.30674
C	2.47011	0.00003	-0.05456
C	3.22638	1.21998	-0.10523
N	3.82310	2.21314	-0.14079
C	3.22639	-1.21989	-0.10564
N	3.82311	-2.21304	-0.14152

36b

C	-1.15684	-0.65543	0.25233
C	-0.44766	0.18648	1.29575
C	-0.46834	-1.67358	-0.53346
C	0.43765	-0.62197	2.21728
C	0.83120	-2.00834	-0.49436
C	1.50414	-1.29692	1.80479
C	1.92066	-1.40946	0.35445
H	0.18890	-0.59573	3.27482
H	2.12109	-1.81565	2.53410
H	2.77653	-2.09195	0.31324
H	1.14465	-2.78804	-1.18493
C	0.97952	1.58506	-1.59483
H	-1.09552	-2.21547	-1.23592
C	0.34821	1.35223	0.62528
H	-1.21402	0.66468	1.91061
C	1.31415	0.92625	-0.46788
C	-0.54647	2.34369	-0.06665
H	0.89392	1.85118	1.43865
C	-0.16725	2.46307	-1.34728
H	1.47307	1.49755	-2.55572
H	-1.36905	2.84788	0.42634

H	-0.61833	3.10578	-2.09452
C	2.44551	-0.05470	-0.27135
C	3.11333	-0.38092	-1.61511
C	3.50791	0.54436	0.66895
H	3.08738	0.80408	1.64423
H	3.93081	1.45172	0.22624
H	4.32415	-0.17029	0.83067
H	2.39693	-0.79044	-2.33463
H	3.91737	-1.11178	-1.47431
H	3.55734	0.51834	-2.05383
C	-2.48551	-0.43344	0.01579
C	-3.23684	0.55253	0.73562
N	-3.83780	1.35264	1.32244
C	-3.22120	-1.15610	-0.98103
N	-3.81196	-1.74389	-1.78741

36c

C	1.42164	0.44211	0.25041
C	-0.02143	0.80690	0.47861
C	2.43085	1.32732	0.20936
C	-0.45054	1.58181	-0.74196
C	2.24479	2.75974	0.20282
C	0.06829	2.79067	-1.02443
C	1.18470	3.41083	-0.34376
H	-1.21274	1.15912	-1.38857
H	-0.35828	3.35291	-1.85279
H	1.24176	4.49622	-0.39571
H	3.08237	3.35847	0.55271
C	-1.76454	-1.52142	-1.16400
H	3.45506	0.96166	0.15431
C	-0.76493	-0.53043	0.76146
H	-0.09307	1.47262	1.34973
C	-2.07955	-0.70051	0.01282
C	0.13985	-1.65800	0.19794
H	-0.88820	-0.64129	1.84141
C	-0.51788	-2.00382	-1.11434
H	-2.45533	-1.70753	-1.97848
H	0.14454	-2.54417	0.84253
H	-0.04938	-2.63475	-1.86131
C	-3.25925	-0.15573	0.34973
C	-4.52165	-0.35822	-0.44521
C	-3.42430	0.73524	1.55190
H	-2.50874	0.84263	2.13769
H	-4.21095	0.35333	2.21485
H	-3.73704	1.73945	1.23739
H	-4.39145	-1.01611	-1.30649
H	-4.90593	0.60400	-0.80730
H	-5.30551	-0.79022	0.18975
C	1.59761	-1.07955	0.14832
C	2.35391	-1.55390	1.32423
N	2.91596	-1.91209	2.27009
C	2.31815	-1.47824	-1.07215
N	2.86382	-1.78720	-2.04440

37a

C	-1.77485	4.20711	0.15769
C	-2.28048	2.90405	0.09710
C	-1.39391	1.83997	0.03387

C	-0.00799	2.10372	0.03264
C	0.50535	3.38663	0.09329
C	-0.40352	4.44849	0.15508
C	-1.62871	0.39630	-0.04016
Au	-3.48134	-0.50025	-0.06087
P	-5.65197	-1.49829	-0.07981
C	0.66619	0.79167	-0.03465
C	1.90633	0.44554	-0.03374
Au	3.78335	-0.21337	-0.05564
P	6.02814	-1.01093	-0.08428
C	-0.44942	-0.26516	-0.08608
C	-0.14245	-1.72304	-0.13933
C	0.41828	-2.27381	1.16906
H	6.36967	-1.89605	-1.11981
H	6.46806	-1.71804	1.04654
H	7.02873	-0.03322	-0.21058
H	-1.07669	-2.24390	-0.38706
H	0.55381	-1.92986	-0.96718
H	-6.47266	-1.25692	-1.19716
H	-6.53969	-1.15223	0.95562
H	-5.73522	-2.90142	-0.01407
H	0.61803	-3.34776	1.09213
H	1.35964	-1.77930	1.44813
H	-0.28929	-2.11279	1.99068
H	1.57625	3.57596	0.09139
H	-0.03336	5.46915	0.20039
H	-3.35396	2.72500	0.10045
H	-2.46406	5.04645	0.20697

### 37b

C	-2.42477	4.00800	0.14034
C	-2.39638	2.63564	0.06728
C	-1.19413	1.88581	0.01769
C	0.02510	2.71482	0.05230
C	-0.01622	4.11900	0.12348
C	-1.23180	4.75575	0.16748
C	-1.14975	0.45754	-0.06454
Au	-2.92857	-0.63256	-0.06549
P	-4.96292	-1.87857	-0.05797
C	1.01946	1.79291	-0.00217
C	1.32390	0.54994	-0.07429
Au	3.27119	-0.18045	-0.06079
P	5.49057	-0.99535	-0.04787
C	0.05506	-0.21784	-0.11982
C	0.19916	-1.71776	-0.16692
C	0.51451	-2.31138	1.20087
H	5.91732	-1.70365	-1.18402
H	5.83613	-1.89453	0.97515
H	6.51482	-0.04122	0.07506
H	-0.73520	-2.14682	-0.55263
H	0.98589	-1.98224	-0.88796
H	-6.16767	-1.16640	-0.20520
H	-5.26615	-2.63659	1.08830
H	-5.13610	-2.85892	-1.05267
H	0.62760	-3.39927	1.14487
H	1.44742	-1.89743	1.60970
H	-0.28509	-2.08387	1.91638
H	0.91572	4.67523	0.14328

H	-1.27079	5.83997	0.22336
H	-3.32943	2.07546	0.04412
H	-3.38131	4.52217	0.17576

38a

C	-0.30563	1.71526	0.42720
C	-1.33974	-0.40057	0.07312
C	-0.55168	-1.56682	-0.50493
C	0.88393	-1.01812	-0.73950
C	0.88046	0.36579	-1.47750
C	0.86659	1.63451	-0.58222
H	-1.22062	2.06951	-0.05091
H	-0.06772	2.40649	1.24317
H	1.42777	-1.73164	-1.36876
H	1.78477	0.42256	-2.09503
H	0.03496	0.39694	-2.17712
H	1.81695	1.69088	-0.03736
H	0.84222	2.52165	-1.22740
H	-1.04802	-1.87420	-1.42853
O	-2.42337	-0.04431	-0.36311
C	1.55400	-0.92270	0.63957
H	1.82923	-1.92475	0.98972
H	2.47994	-0.34009	0.58950
C	0.53336	-0.28992	1.63518
N	-0.60437	0.38162	0.98521
H	0.12152	-1.06558	2.28823
H	1.01183	0.44221	2.29180
H	-0.52304	-2.43540	0.16571

38b

C	-1.53335	0.86331	0.72153
C	-1.35510	-0.53917	0.15428
C	0.64569	-1.21619	-0.92757
C	1.39191	0.13300	-0.85515
C	0.43307	1.35306	-1.02732
C	-0.40740	1.81567	0.19881
H	-2.51673	1.19421	0.38237
H	-1.55542	0.86713	1.81631
H	2.18041	0.19702	-1.61423
H	1.04928	2.21499	-1.31165
H	-0.23451	1.16541	-1.87885
H	0.27618	2.06124	1.01798
H	-0.88055	2.76404	-0.07819
H	-0.03833	-1.32883	-1.76905
O	-2.18918	-1.02138	-0.59813
C	1.97372	0.04646	0.57153
H	2.89459	-0.54597	0.56919
H	2.21691	1.02239	1.00185
C	0.84936	-0.69840	1.35839
N	-0.11662	-1.18332	0.34559
H	1.24983	-1.56959	1.88719
H	0.35445	-0.07393	2.10329
H	1.34627	-2.06014	-0.92734

39a

C	1.83032	0.68180	0.57062
C	-0.42146	1.21967	0.05837
C	-1.33199	0.20732	-0.65162

C	-0.47562	-1.05988	-0.83664
C	0.92034	-0.70188	-1.46377
C	2.08487	-0.43841	-0.47093
H	2.01067	1.67078	0.14645
H	2.48938	0.56433	1.43687
H	-1.00012	-1.73057	-1.52613
H	1.22321	-1.54320	-2.09666
H	0.80837	0.15551	-2.14046
H	2.31934	-1.37276	0.05229
H	2.98351	-0.18735	-1.04762
H	-1.66286	0.65080	-1.59321
O	-0.27584	2.35031	-0.37989
C	-0.33022	-1.72645	0.54144
H	-1.25835	-2.23821	0.80857
H	0.45775	-2.48528	0.51033
C	-0.02380	-0.62641	1.60046
N	0.42252	0.65345	1.01777
H	-0.92179	-0.41989	2.18686
H	0.74922	-0.94670	2.30405
F	-2.49599	-0.09207	0.08732

#### 39b

C	2.10735	-0.05965	0.43073
C	1.12432	1.08192	0.20742
C	-1.03354	0.63072	-0.59929
C	-0.99072	-0.89855	-0.72165
C	0.42107	-1.36366	-1.19550
C	1.57442	-1.41059	-0.15207
H	3.02638	0.24912	-0.07128
H	2.35342	-0.17887	1.49144
H	-1.74512	-1.26035	-1.42746
H	0.31167	-2.38653	-1.57423
H	0.72959	-0.75673	-2.05776
H	1.27676	-2.07334	0.66649
H	2.41960	-1.91142	-0.63618
H	-0.65105	1.19578	-1.44843
O	1.43275	2.07226	-0.43284
C	-1.29236	-1.31181	0.73313
H	-2.36984	-1.31021	0.91326
H	-0.91612	-2.30913	0.97706
C	-0.59764	-0.18972	1.56129
N	-0.22592	0.86739	0.58592
H	-1.28328	0.25124	2.28925
H	0.28067	-0.53295	2.10925
F	-2.35451	1.05572	-0.38384

#### 40a

C	-1.55012	1.26802	0.19970
C	0.69933	0.93749	-0.48858
C	1.37415	-0.43227	-0.33905
C	0.32077	-1.32610	0.35561
C	-0.36641	-0.62024	1.57359
C	-1.67502	0.16103	1.27571
H	-1.12864	2.18426	0.61620
H	-2.52941	1.51383	-0.22424
H	0.84249	-2.21765	0.71900
H	-0.61431	-1.39313	2.30990
H	0.36354	0.03642	2.06216

H	-2.45231	-0.55144	0.97376
H	-2.03380	0.61282	2.20857
O	1.20252	1.96870	-0.08812
C	-0.68624	-1.70355	-0.74251
H	-0.24827	-2.45181	-1.41342
H	-1.58163	-2.15546	-0.30526
C	-1.03109	-0.41690	-1.55670
N	-0.64494	0.83608	-0.88709
H	-0.52084	-0.44050	-2.52490
H	-2.10041	-0.35288	-1.77443
H	1.68236	-0.87100	-1.29662
F	2.52260	-0.30228	0.43303

40b

C	-1.23684	1.49271	0.09356
C	-1.48161	0.00382	0.38123
C	0.39951	-1.31679	-0.40236
C	1.52836	-0.28657	-0.54979
C	1.03964	1.04833	-1.16439
C	0.18903	1.96743	-0.25969
H	-1.92056	1.70762	-0.73432
H	-1.62299	2.07206	0.94246
H	2.33225	-0.69080	-1.17526
H	1.93336	1.61472	-1.45348
H	0.49707	0.83518	-2.09318
H	0.75126	2.19737	0.65174
H	0.08201	2.92860	-0.77645
O	-2.58838	-0.46529	0.23803
C	1.95646	-0.15965	0.92490
H	2.64916	-0.96395	1.19351
H	2.46253	0.78619	1.13789
C	0.61674	-0.31520	1.71070
N	-0.38450	-0.85472	0.75955
H	0.72342	-1.01832	2.54318
H	0.26175	0.62765	2.13612
H	0.78649	-2.32538	-0.21231
F	-0.40056	-1.40779	-1.53177

41a

C	1.21191	-0.85910	0.50480
C	0.30931	1.35684	0.00213
C	-1.07096	1.40603	-0.64164
C	-1.59435	-0.04505	-0.74408
C	-0.54873	-0.98528	-1.42932
C	0.41427	-1.73482	-0.48008
H	1.50386	-1.43975	1.38797
H	-2.50068	-0.04509	-1.35973
H	-1.08686	-1.74926	-2.00231
H	0.02872	-0.40958	-2.16363
H	-0.15685	-2.45971	0.11190
H	1.13367	-2.32103	-1.06253
H	-0.95786	1.88772	-1.61651
O	1.23197	2.06793	-0.33453
C	-1.94249	-0.50453	0.68303
H	-2.87948	-0.03431	1.00347
H	-2.10813	-1.58639	0.72018
C	-0.79638	-0.06716	1.64679
N	0.45988	0.31357	0.97018



H	-1.11183	0.79946	2.23472
H	-0.55586	-0.85334	2.36924
H	-1.76067	2.02507	-0.05156
F	2.38684	-0.43932	-0.10400

41b

C	-1.44310	0.36229	0.61134
C	-0.84805	-0.95360	0.09296
C	1.33223	-1.06691	-0.83024
C	1.64052	0.44509	-0.80980
C	0.37518	1.30612	-1.11834
C	-0.64323	1.56285	0.02909
H	-1.47235	0.40517	1.70392
H	2.42579	0.70552	-1.52852
H	0.71955	2.29807	-1.43433
H	-0.14916	0.87888	-1.98232
H	-0.13714	2.07987	0.85079
H	-1.40144	2.25989	-0.34180
H	0.77362	-1.41946	-1.69734
O	-1.45914	-1.64884	-0.69512
C	2.11837	0.60991	0.64883
H	3.17379	0.33302	0.73585
H	2.02044	1.63242	1.02495
C	1.22505	-0.40934	1.42501
N	0.50217	-1.19505	0.39491
H	1.83776	-1.10643	2.00535
H	0.53528	0.06066	2.12704
H	2.24527	-1.66552	-0.72997
F	-2.77282	0.43951	0.19664

42a

C	-1.20574	0.22918	0.71176
C	-0.16683	0.66080	-0.35673
C	-0.35530	-0.24899	-1.60707
C	0.12818	-1.65859	-1.14146
C	0.52349	-1.41192	0.33221
C	-0.79038	-1.20751	1.12884
H	-1.38133	-0.25099	-2.00272
H	-1.21854	0.92720	1.55132
H	-0.64468	-2.42873	-1.23309
H	0.97826	-2.00085	-1.73523
H	-1.54432	-1.96003	0.86543
H	-0.64591	-1.26922	2.20970
H	0.24750	0.13740	-2.43200
C	-0.16225	2.15735	-0.65215
H	-1.09197	2.48954	-1.13489
H	-0.02472	2.75372	0.25600
H	0.64518	2.41213	-1.34421
H	1.16802	-2.18332	0.75951
C	1.13192	0.02773	0.29813
C	2.39030	0.15675	-0.58031
H	3.19866	-0.44433	-0.15160
H	2.25526	-0.16940	-1.61248
H	2.73934	1.19404	-0.60335
C	1.50263	0.59059	1.68602
H	2.36297	0.04329	2.08363
H	1.79939	1.64178	1.61173
H	0.71356	0.52349	2.43934

N	-2.64946	0.27760	0.19375
H	-2.90223	1.22442	-0.10917
H	-2.77179	-0.34689	-0.61010
H	-3.31256	-0.00875	0.92047

42b

C	0.58796	0.49300	-0.85191
C	-0.62100	0.93146	-0.22630
C	1.21265	0.15310	0.66405
C	0.65333	-1.24759	0.97369
C	-0.43011	-1.41360	-0.11743
C	0.34536	-0.93455	-1.36262
H	2.29606	0.20704	0.44182
H	1.20958	1.20508	-1.39025
H	1.42954	-2.00755	0.84919
H	0.26909	-1.33260	1.99109
H	1.27904	-1.47866	-1.52036
H	-0.22280	-0.94832	-2.29496
H	1.00142	0.90691	1.42843
C	-0.96776	2.33605	0.07461
H	-0.12380	3.01641	-0.05242
H	-1.74035	2.62793	-0.65497
H	-1.41802	2.45849	1.06339
H	-0.88222	-2.40486	-0.17888
C	-1.47975	-0.26462	0.09091
C	-2.16134	-0.22807	1.47116
H	-2.64470	-1.19091	1.66149
H	-1.45983	-0.03834	2.28706
H	-2.93845	0.54035	1.50921
C	-2.59678	-0.31733	-1.00639
H	-3.14153	-1.25763	-0.88351
H	-3.30443	0.50459	-0.87136
H	-2.21587	-0.27775	-2.02840
N	4.41909	0.24050	0.04618
H	4.74946	-0.02514	-0.87962
H	4.80664	1.16266	0.23728
H	4.86217	-0.39837	0.70398

43a

C	-0.24261	2.22580	-0.29161
C	-1.37603	1.73217	0.35597
C	-2.58414	2.40260	0.24080
C	-2.61932	3.56647	-0.54167
C	-1.46924	4.04634	-1.17582
C	-0.24311	3.37865	-1.05929
C	0.48218	0.31425	0.71679
C	-0.98803	0.50128	1.15694
H	-3.48220	2.03550	0.72837
H	-3.55547	4.10332	-0.65551
H	-1.52316	4.95174	-1.77159
H	0.65091	3.74857	-1.55113
H	1.77639	1.43826	-0.40884
N	0.84256	1.34470	-0.01558
S	1.45466	-1.00270	1.21887
O	-0.98265	-0.83404	-1.22289
C	2.99136	-0.69078	0.32943
C	3.08757	-1.05864	-1.02056
C	4.08689	-0.16431	1.02533

C	4.30212	-0.87407	-1.68202
H	2.23397	-1.48667	-1.53781
C	5.29583	0.00532	0.34865
H	4.00098	0.09613	2.07575
C	5.40172	-0.34673	-0.99902
H	4.39092	-1.15631	-2.72655
H	6.15414	0.40706	0.87815
H	6.34684	-0.21719	-1.51748
C	-1.08481	0.71334	2.67379
H	-0.47672	1.56803	2.98177
H	-2.12735	0.91366	2.93426
H	-0.75283	-0.18122	3.20819
C	-1.74133	-1.18432	-0.35723
O	-1.79886	-0.66389	0.88593
C	-2.78997	-2.31163	-0.50511
F	-4.01805	-1.79704	-0.35063
F	-2.68716	-2.86335	-1.70927
F	-2.58493	-3.24424	0.43469

43b

C	-2.34531	-0.04985	-0.83737
C	-2.59803	-1.06284	0.16740
C	-3.92289	-1.58371	0.32896
C	-4.91348	-1.10278	-0.48131
C	-4.63497	-0.09233	-1.46006
C	-3.37989	0.44997	-1.64881
C	-0.34112	-0.42202	0.23678
C	-1.41768	-1.33515	0.82815
H	-4.12441	-2.34599	1.07384
H	-5.92727	-1.47765	-0.39223
H	-5.45418	0.26083	-2.08001
H	-3.19620	1.21442	-2.39590
H	-0.59747	1.00380	-1.35570
N	-1.04680	0.28045	-0.80772
S	0.14195	0.73294	1.62574
O	1.63839	-2.13705	1.37572
C	0.59946	2.22229	0.74367
C	1.75481	2.26199	-0.05525
C	-0.17397	3.37669	0.93809
C	2.11562	3.45920	-0.67323
H	2.36797	1.37652	-0.18490
C	0.21246	4.57224	0.33228
H	-1.05900	3.33820	1.56560
C	1.35053	4.61248	-0.47676
H	3.00735	3.49478	-1.29175
H	-0.37658	5.47038	0.49148
H	1.64727	5.54470	-0.94789
C	-1.21801	-2.28913	1.94605
H	-2.17569	-2.59773	2.37064
H	-0.68334	-3.18274	1.60037
H	-0.58980	-1.85882	2.73277
C	1.70700	-1.74992	0.24591
O	0.77383	-1.02609	-0.42936
C	2.92397	-1.97008	-0.68476
F	2.52987	-2.41609	-1.88308
F	3.55574	-0.78947	-0.84989
F	3.75983	-2.83979	-0.13517

## 44a

C	-0.26584	2.23503	-0.30496
C	-1.39136	1.73134	0.34739
C	-2.60355	2.39649	0.24725
C	-2.64908	3.56643	-0.52568
C	-1.50551	4.05795	-1.16303
C	-0.27592	3.39428	-1.06175
C	0.48477	0.33101	0.69375
C	-0.98569	0.50371	1.14218
H	-3.49482	2.02297	0.74169
H	-3.58811	4.10072	-0.62656
H	-1.56757	4.96904	-1.74908
H	0.61738	3.76793	-1.55061
H	1.75638	1.48266	-0.44145
N	0.82750	1.36163	-0.04470
S	1.46208	-0.97971	1.20117
O	-1.05270	-0.80517	-1.27151
C	3.00694	-0.67412	0.32472
C	3.12461	-1.06970	-1.01498
C	4.09120	-0.13194	1.02596
C	4.34790	-0.89595	-1.66257
H	2.27983	-1.50822	-1.53664
C	5.30945	0.02678	0.36368
H	3.98834	0.15046	2.06870
C	5.43609	-0.35214	-0.97489
H	4.45158	-1.19783	-2.70004
H	6.15862	0.44211	0.89720
H	6.38822	-0.23045	-1.48217
C	-1.07967	0.70888	2.65912
H	-0.47795	1.56715	2.96875
H	-2.12336	0.89845	2.92197
H	-0.73626	-0.18485	3.18685
C	-1.76194	-1.17634	-0.37355
O	-1.78595	-0.67230	0.87330
C	-2.77976	-2.33507	-0.48528
F	-4.01225	-1.88810	-0.20267
F	-2.76456	-2.83086	-1.72045
F	-2.46149	-3.30508	0.38504

## 44b

C	-2.36504	0.09698	-0.83081
C	-2.67552	-0.89075	0.18405
C	-4.02818	-1.33462	0.35108
C	-4.98717	-0.81118	-0.46910
C	-4.64976	0.16705	-1.46354
C	-3.36761	0.63818	-1.65561
C	-0.38858	-0.37510	0.25017
C	-1.51489	-1.22708	0.84474
H	-4.27167	-2.07071	1.10919
H	-6.02075	-1.12552	-0.37718
H	-5.44673	0.55427	-2.09154
H	-3.13888	1.38036	-2.41189
H	-0.56312	1.03323	-1.37523
N	-1.05272	0.36099	-0.79764
S	0.16534	0.74954	1.63323
O	1.49702	-2.22919	1.36995
C	0.77251	2.18235	0.74559
C	2.00525	2.13991	0.07436

C	0.03631	3.37481	0.81030
C	2.48569	3.29360	-0.54514
H	2.58151	1.22190	0.03595
C	0.53642	4.52515	0.20033
H	-0.91045	3.39880	1.34058
C	1.75627	4.48382	-0.47947
H	3.43772	3.26478	-1.06636
H	-0.02671	5.45185	0.25652
H	2.14217	5.38141	-0.95335
C	-1.37024	-2.18426	1.96755
H	-2.34585	-2.43882	2.38601
H	-0.88387	-3.10609	1.62698
H	-0.72604	-1.78315	2.75671
C	1.56898	-1.83977	0.23991
O	0.69058	-1.04669	-0.41836
C	2.75467	-2.14787	-0.70583
F	2.32259	-2.51593	-1.91850
F	3.50565	-1.03573	-0.83714
F	3.50296	-3.11747	-0.18977

45a

C	-0.18871	2.22387	-0.31118
C	-1.32832	1.75391	0.34330
C	-2.51759	2.46073	0.25663
C	-2.52855	3.63605	-0.50953
C	-1.37293	4.09146	-1.15200
C	-0.16476	3.38773	-1.06120
C	0.50022	0.28780	0.66619
C	-0.95805	0.50872	1.12818
H	-3.41741	2.11483	0.75501
H	-3.44993	4.20176	-0.60175
H	-1.40750	5.00705	-1.73338
H	0.73653	3.73536	-1.55403
H	1.81056	1.40910	-0.45210
N	0.87423	1.31105	-0.06484
S	1.43498	-1.06348	1.14590
O	-1.17375	-0.75353	-1.31632
C	3.00326	-0.75679	0.31296
C	3.19147	-1.23958	-0.98862
C	4.03167	-0.10934	1.00909
C	4.42927	-1.05128	-1.60428
H	2.38755	-1.75142	-1.50738
C	5.26384	0.06827	0.37843
H	3.87259	0.24602	2.02187
C	5.46104	-0.40058	-0.92275
H	4.58593	-1.41855	-2.61364
H	6.06814	0.56993	0.90728
H	6.42331	-0.26172	-1.40609
C	-1.02818	0.71313	2.64604
H	-0.39077	1.54770	2.94731
H	-2.06137	0.94168	2.91927
H	-0.70953	-0.19293	3.16810
C	-1.84039	-1.12417	-0.38591
O	-1.79920	-0.64330	0.86598
C	-2.88151	-2.26402	-0.46666
F	-4.10013	-1.79966	-0.14920
F	-2.91419	-2.76058	-1.70384
F	-2.56061	-3.24545	0.39076

## 45b

C	-2.35800	0.04416	-0.82529
C	-2.64656	-0.96187	0.17965
C	-3.98861	-1.44189	0.33797
C	-4.95728	-0.92953	-0.47666
C	-4.64183	0.07108	-1.45749
C	-3.37165	0.57384	-1.64390
C	-0.37627	-0.38539	0.25495
C	-1.48133	-1.27197	0.84071
H	-4.21518	-2.19423	1.08498
H	-5.98342	-1.26897	-0.39181
H	-5.44760	0.44875	-2.07963
H	-3.15789	1.33182	-2.38825
H	-0.58483	1.03132	-1.36146
N	-1.05265	0.33731	-0.79124
S	0.16078	0.74653	1.63746
O	1.59087	-2.15523	1.39003
C	0.71240	2.20344	0.75079
C	1.92677	2.19901	0.04641
C	-0.05435	3.37428	0.84137
C	2.35770	3.36805	-0.58106
H	2.52537	1.29678	-0.01498
C	0.39713	4.54137	0.22459
H	-0.99030	3.36815	1.39043
C	1.59810	4.53756	-0.48908
H	3.29343	3.36638	-1.13180
H	-0.19249	5.45015	0.29791
H	1.94433	5.44681	-0.97146
C	-1.30675	-2.23646	1.95257
H	-2.27418	-2.53886	2.35690
H	-0.77774	-3.13127	1.60346
H	-0.69239	-1.81432	2.75437
C	1.62439	-1.79095	0.24819
O	0.71844	-1.04178	-0.41211
C	2.80515	-2.08775	-0.70704
F	2.37582	-2.47653	-1.91393
F	3.54019	-0.96706	-0.85518
F	3.57739	-3.04131	-0.18786

## 46a

C	-0.18651	2.22356	-0.31231
C	-1.32634	1.75450	0.34254
C	-2.51533	2.46172	0.25606
C	-2.52603	3.63686	-0.51043
C	-1.37037	4.09135	-1.15351
C	-0.16245	3.38707	-1.06295
C	0.50126	0.28729	0.66493
C	-0.95654	0.50926	1.12744
H	-3.41505	2.11620	0.75486
H	-3.44716	4.20301	-0.60242
H	-1.40463	5.00673	-1.73525
H	0.73867	3.73395	-1.55654
H	1.81319	1.40937	-0.45091
N	0.87580	1.31002	-0.06632
S	1.43473	-1.06469	1.14490
O	-1.18270	-0.74859	-1.31991
C	3.00396	-0.75919	0.31340

C	3.19771	-1.25470	-0.98251
C	4.02741	-0.09908	1.00492
C	4.43590	-1.06655	-1.59740
H	2.39739	-1.77557	-1.49774
C	5.25989	0.07880	0.37491
H	3.86414	0.26629	2.01343
C	5.46256	-0.40280	-0.92076
H	4.59665	-1.44340	-2.60259
H	6.06008	0.59088	0.90002
H	6.42497	-0.26338	-1.40370
C	-1.02607	0.71373	2.64530
H	-0.38772	1.54767	2.94629
H	-2.05904	0.94305	2.91877
H	-0.70770	-0.19253	3.16714
C	-1.84413	-1.12129	-0.38654
O	-1.79845	-0.64273	0.86557
C	-2.88431	-2.26213	-0.46482
F	-4.10330	-1.79885	-0.14677
F	-2.91819	-2.76010	-1.70173
F	-2.56236	-3.24298	0.39290

46b

C	-2.35502	0.02079	-0.82514
C	-2.63440	-0.98958	0.17824
C	-3.97211	-1.48173	0.33614
C	-4.94551	-0.97595	-0.47683
C	-4.63931	0.02967	-1.45558
C	-3.37368	0.54368	-1.64191
C	-0.36999	-0.39210	0.25414
C	-1.46631	-1.29040	0.83815
H	-4.19173	-2.23754	1.08164
H	-5.96865	-1.32435	-0.39212
H	-5.44880	0.40191	-2.07613
H	-3.16685	1.30518	-2.38456
H	-0.59099	1.02426	-1.36069
N	-1.05214	0.32463	-0.79180
S	0.15572	0.74493	1.63749
O	1.62118	-2.13421	1.39311
C	0.68505	2.21076	0.75190
C	1.89534	2.22297	0.04072
C	-0.09590	3.37162	0.84889
C	2.30804	3.39841	-0.58705
H	2.50460	1.32826	-0.02600
C	0.33754	4.54549	0.23196
H	-1.02921	3.35240	1.40209
C	1.53442	4.55817	-0.48846
H	3.24030	3.40924	-1.14355
H	-0.26340	5.44645	0.30980
H	1.86626	5.47246	-0.97142
C	-1.28070	-2.25729	1.94613
H	-2.24448	-2.57308	2.34887
H	-0.74147	-3.14424	1.59246
H	-0.67176	-1.83113	2.74990
C	1.64716	-1.77377	0.24965
O	0.73157	-1.03856	-0.41161
C	2.82979	-2.05974	-0.70654
F	2.40408	-2.45921	-1.91116
F	3.55093	-0.93087	-0.86055

F	3.61511	-3.00156	-0.18452
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47a

C	-0.18460	2.22301	-0.31310
C	-1.32458	1.75487	0.34219
C	-2.51316	2.46280	0.25606
C	-2.52338	3.63786	-0.51056
C	-1.36765	4.09142	-1.15419
C	-0.16015	3.38635	-1.06404
C	0.50196	0.28630	0.66388
C	-0.95541	0.50942	1.12697
H	-3.41286	2.11783	0.75525
H	-3.44417	4.20463	-0.60223
H	-1.40150	5.00673	-1.73609
H	0.74093	3.73246	-1.55821
H	1.81499	1.40828	-0.45084
N	0.87705	1.30862	-0.06755
S	1.43447	-1.06629	1.14387
O	-1.18779	-0.74599	-1.32170
C	3.00438	-0.76126	0.31354
C	3.20183	-1.26442	-0.97880
C	4.02451	-0.09322	1.00235
C	4.44037	-1.07617	-1.59299
H	2.40391	-1.79091	-1.49197
C	5.25727	0.08506	0.37296
H	3.85841	0.27820	2.00817
C	5.46362	-0.40431	-0.91922
H	4.60389	-1.45884	-2.59552
H	6.05475	0.60358	0.89585
H	6.42621	-0.26444	-1.40171
C	-1.02415	0.71392	2.64485
H	-0.38472	1.54711	2.94560
H	-2.05679	0.94426	2.91871
H	-0.70636	-0.19268	3.16647
C	-1.84671	-1.11942	-0.38680
O	-1.79829	-0.64214	0.86545
C	-2.88718	-2.26005	-0.46383
F	-4.10609	-1.79630	-0.14600
F	-2.92162	-2.75906	-1.70047
F	-2.56570	-3.24061	0.39444

47b

C	-2.35358	0.00830	-0.82483
C	-2.62777	-1.00457	0.17756
C	-3.96306	-1.50330	0.33539
C	-4.93919	-1.00090	-0.47635
C	-4.63818	0.00752	-1.45389
C	-3.37507	0.52757	-1.64034
C	-0.36657	-0.39574	0.25350
C	-1.45801	-1.30049	0.83654
H	-4.17877	-2.26110	1.07996
H	-5.96067	-1.35408	-0.39154
H	-5.44977	0.37692	-2.07338
H	-3.17213	1.29097	-2.38208
H	-0.59491	1.02116	-1.35986
N	-1.05205	0.31788	-0.79216
S	0.15301	0.74377	1.63746
O	1.63740	-2.12259	1.39430



C	0.67028	2.21436	0.75264
C	1.87970	2.23632	0.04027
C	-0.11969	3.36899	0.85080
C	2.28261	3.41520	-0.58743
H	2.49568	1.34631	-0.02771
C	0.30395	4.54647	0.23390
H	-1.05256	3.34206	1.40441
C	1.50003	4.56883	-0.48764
H	3.21406	3.43342	-1.14511
H	-0.30414	5.44256	0.31238
H	1.82412	5.48582	-0.97075
C	-1.26612	-2.26906	1.94195
H	-2.22775	-2.59248	2.34375
H	-0.72113	-3.15138	1.58540
H	-0.66016	-1.84097	2.74693
C	1.65939	-1.76424	0.25000
O	0.73862	-1.03655	-0.41174
C	2.84313	-2.04416	-0.70658
F	2.41966	-2.44915	-1.91014
F	3.55672	-0.91094	-0.86339
F	3.63530	-2.97972	-0.18313

48a

C	0.33954	1.25265	-0.60765
C	2.10742	0.95234	0.93305
C	1.93774	-0.27306	1.46244
C	1.68228	-1.27253	0.40847
C	0.47815	-1.06736	-0.64091
C	-0.39000	0.12269	-0.56501
H	1.92605	-0.50424	2.52357
H	1.95826	-2.31369	0.55157
H	2.22378	1.87517	1.49407
H	-0.04516	2.26098	-0.48415
C	1.83407	0.92962	-0.57152
H	2.47423	1.57617	-1.17961
C	1.87411	-0.58805	-0.91354
H	2.50076	-0.98249	-1.70923
H	-1.46674	0.07202	-0.43348
N	-4.38857	-0.03891	0.07720
N	-5.44844	-0.00721	0.38934
H	0.10805	-1.99882	-1.06052

48b

C	-0.47904	-1.06831	-0.64061
C	-1.68244	-1.27191	0.40996
C	-1.93646	-0.27137	1.46326
C	-2.10590	0.95365	0.93294
C	-0.33914	1.25164	-0.60946
C	0.38982	0.12132	-0.56644
H	-1.92399	-0.50160	2.52459
H	-2.22127	1.87704	1.49325
H	-1.95886	-2.31280	0.55419
H	-0.10985	-2.00037	-1.05969
C	-1.87496	-0.58848	-0.91249
H	-2.50247	-0.98328	-1.70732
C	-1.83381	0.92946	-0.57183
H	-2.47411	1.57584	-1.17996
H	1.46663	0.07020	-0.43568

N	4.38828	-0.03898	0.07587
N	5.44735	-0.00685	0.39066
H	0.04622	2.25986	-0.48712

49a

C	2.41558	-1.48423	-0.66174
C	1.22131	-0.76825	-0.53095
C	1.25156	0.60389	-0.23719
C	2.48360	1.23299	-0.06430
C	3.69559	0.53661	-0.20132
C	3.64185	-0.82903	-0.50790
S	-0.33524	-1.60908	-0.86324
C	-1.27552	-1.16183	0.56806
Cl	-0.52014	-1.48222	2.14435
C	-2.50130	-0.61104	0.55985
C	-3.25731	-0.22131	-0.66550
O	-3.19566	-0.87821	-1.70009
C	-4.06813	1.04108	-0.53825
Cl	-1.30307	3.10841	0.35670
H	-4.65937	1.19783	-1.44293
H	-4.72263	0.99795	0.34133
H	-3.36735	1.88072	-0.37178
H	-2.94474	-0.34315	1.51403
H	0.33979	1.19731	-0.13368
H	2.48513	2.29451	0.17218
C	5.01745	1.24837	-0.01867
H	4.56553	-1.39457	-0.61447
H	2.38917	-2.54933	-0.87468
H	5.86246	0.57026	-0.17758
H	5.10781	1.66675	0.99129
H	5.11996	2.08402	-0.72161

49b

C	1.90106	-2.02203	0.56845
C	1.08081	-1.28962	-0.30161
C	1.52640	-0.06347	-0.81155
C	2.77231	0.43158	-0.42650
C	3.61460	-0.29575	0.42653
C	3.16216	-1.53090	0.91413
S	-0.48604	-2.01992	-0.78853
C	-1.74575	-0.93806	-0.13818
Cl	0.60220	3.23593	-1.11907
C	-1.59330	0.29979	0.36659
C	-2.64152	1.21884	0.88753
O	-3.82711	0.91530	0.99675
C	-2.12095	2.58236	1.28424
Cl	-3.30317	-1.73134	-0.32017
H	-2.95990	3.23975	1.52172
H	-1.47584	2.48203	2.16784
H	-1.48360	3.00635	0.49306
H	-0.59258	0.72079	0.34829
H	0.90930	0.55847	-1.45407
H	3.04876	1.41972	-0.78450
C	4.96908	0.25144	0.81580
H	3.79154	-2.10743	1.58909
H	1.54988	-2.96514	0.97692
H	5.44409	-0.36359	1.58724
H	4.88357	1.27445	1.19885

H	5.64525	0.28774	-0.04750
50a			
C	2.83849	-0.07399	-0.04192
C	1.53161	-0.13901	0.08675
C	0.75966	-1.35728	-0.35747
C	0.74702	1.00657	0.68131
C	-0.61953	1.09805	0.04166
C	-1.03286	2.21483	-0.55176
C	-1.37646	-0.16950	0.12704
C	-0.57440	-1.42565	0.38685
C	-2.69166	-0.24689	0.01116
F	-3.51698	0.75667	-0.19107
F	3.59374	0.95027	0.31244
H	1.28195	1.94681	0.57109
F	-3.38308	-1.36714	0.09939
F	3.59705	-1.03009	-0.54795
H	-0.39470	3.08816	-0.56624
H	-1.99380	2.29623	-1.03619
H	0.61812	0.83018	1.75513
H	-1.13685	-2.30425	0.07971
H	-0.38311	-1.52676	1.45904
H	0.56043	-1.29751	-1.43097
H	1.34021	-2.26299	-0.18843
50b			
C	1.05679	0.03171	0.44408
C	0.91047	1.28523	-0.36623
C	1.89208	1.72204	-1.13584
C	-0.45515	1.91430	-0.24504
C	-1.55282	0.90592	0.05087
C	-2.69051	1.26699	0.63332
C	-1.29929	-0.50172	-0.32858
C	-2.20350	-1.30835	-0.86851
C	0.09661	-1.04610	-0.09168
F	0.07131	-2.08290	0.77518
F	0.71367	0.27574	1.73690
H	-0.68117	2.43695	-1.17592
F	0.62622	-1.52443	-1.24420
F	2.30909	-0.45532	0.44539
H	-2.87778	2.29834	0.90291
H	-3.45560	0.54060	0.86988
H	-0.44272	2.65961	0.55188
H	-3.19826	-0.95307	-1.09941
H	-1.96443	-2.33742	-1.10236
H	1.76335	2.60160	-1.75284
H	2.84586	1.21539	-1.16792
51a			
C	0.83845	1.23125	1.08153
C	1.40205	-0.06620	0.57209
C	0.60685	-1.30624	0.91812
C	-0.74587	-0.93911	1.53972
C	-1.38477	0.12728	0.68511
C	-0.63290	1.40142	0.73239
C	-1.14780	2.61836	0.58804
C	-2.41565	-0.13882	-0.11973
H	-0.59941	-0.54084	2.54589

H	1.18057	-1.93806	1.60052
C	2.52897	-0.14658	-0.12401
H	1.40115	2.08584	0.71875
H	-1.36941	-1.82210	1.62593
H	0.43837	-1.89500	0.01444
H	-0.50962	3.48961	0.66132
H	-2.19918	2.78846	0.41897
H	0.93594	1.22657	2.17366
Cl	-3.10309	0.95652	-1.25301
Cl	-3.18850	-1.68513	-0.16812
Cl	3.50873	1.20434	-0.55848
Cl	3.16083	-1.65706	-0.66740

51b

C	-1.24961	1.63777	0.94053
C	0.20722	1.68667	0.52312
C	0.97209	2.73222	0.78939
C	-2.29933	-1.76528	-0.13194
C	-1.52861	-0.69642	0.02311
C	-2.06581	0.68231	0.11584
C	-3.17435	1.05600	-0.51249
C	-0.01903	-0.82150	0.20794
H	-3.37423	-1.65807	-0.15847
H	0.55106	3.59331	1.29132
C	0.71566	0.47880	-0.24648
H	-1.67389	2.63817	0.88904
H	-1.88912	-2.75989	-0.21818
H	2.01768	2.76748	0.52450
H	-3.54868	2.06661	-0.42105
H	-3.72590	0.37585	-1.14663
H	-1.28489	1.31580	1.98533
Cl	0.63111	-2.23195	-0.64300
Cl	0.31658	-1.02875	1.96367
Cl	0.32207	0.72526	-1.98269
Cl	2.47016	0.28352	-0.10268

TS1-1

H	-0.18402	2.80913	-2.67814
H	0.60176	2.20278	2.95215
C	-2.54689	0.60913	-0.95744
C	-3.09238	-0.51640	-1.61024
H	-3.11326	1.53047	-0.85372
C	-1.24749	0.54244	-0.44676
H	-0.89965	2.98428	3.55047
H	0.19216	3.88636	2.45467
C	-2.63062	-2.19190	0.60426
O	-0.55207	-0.52370	-0.44837
P	-0.31891	1.99370	0.22483
O	-0.99506	2.37568	1.60939
O	-0.53926	3.29776	-0.66758
O	1.12885	1.54395	0.29403
C	-0.20291	2.90169	2.71679
C	0.18874	3.49835	-1.91741
H	1.25556	3.33503	-1.75838
H	-0.01354	4.53150	-2.19947
C	-3.79232	-1.84005	-0.09173
H	-3.74788	0.20070	2.62457
C	-4.31999	-0.36406	-2.47590

C	-4.59043	-0.91718	0.81447
H	-5.05248	-0.05106	0.33073
H	-2.36444	-1.24491	-1.95659
H	-4.26732	-2.51207	-0.79934
C	-2.48940	-1.37070	1.76689
H	-5.41427	-1.49321	1.26802
H	-1.91177	-2.94372	0.29611
C	-3.58737	-0.56268	1.87068
H	-1.61576	-1.36542	2.40742
H	-4.77307	-1.32634	-2.73089
H	-5.08128	0.27418	-2.01492
H	-4.01909	0.11131	-3.41995
Cl	1.53444	-2.91662	-0.51240
Sn	1.65519	-0.57515	-0.07546
Cl	3.94767	-0.15825	0.34451
Cl	1.04409	-0.81207	2.28289
Cl	1.70669	0.10115	-2.40991

TS1-2

H	0.37554	2.55730	2.79709
H	-0.66532	2.44936	-2.79233
C	2.63262	0.39982	0.68499
C	3.23344	-0.82385	1.29129
H	3.18964	1.33297	0.68082
C	1.27825	0.43601	0.37520
H	0.84320	3.20442	-3.40587
H	-0.13522	4.05715	-2.17245
C	2.70989	-2.30891	-0.69531
O	0.52330	-0.59332	0.41741
P	0.37864	1.96292	-0.14479
O	1.00732	2.41520	-1.53433
O	0.69923	3.19309	0.82071
O	-1.08896	1.58188	-0.17056
C	0.18888	3.08152	-2.54320
C	0.03118	3.33489	2.11172
H	-1.04953	3.26255	1.98175
H	0.31930	4.32238	2.47182
C	3.83361	-1.76991	0.10319
H	3.20257	0.56014	-2.22827
C	4.33846	-0.51522	2.31278
C	4.49367	-0.78045	-0.88547
H	5.06823	0.02616	-0.42650
H	2.44580	-1.40670	1.77694
H	4.47982	-2.52454	0.55909
C	2.36877	-1.42413	-1.69684
H	5.16184	-1.32721	-1.56810
H	2.15281	-3.20500	-0.43959
C	3.27287	-0.34613	-1.63581
H	1.47352	-1.47100	-2.30558
H	4.75774	-1.44006	2.72417
H	5.15926	0.06347	1.87236
H	3.93042	0.06517	3.14723
Cl	-1.64714	-2.91428	0.34975
Sn	-1.67091	-0.54727	0.07782
Cl	-3.94717	-0.02556	-0.32232
Cl	-1.07177	-0.64243	-2.30687
Cl	-1.70220	-0.01089	2.44456

TS2-1

C	-3.59638	1.77728	0.07455
C	-2.50588	1.32127	0.80427
H	-4.38196	2.28159	0.62848
H	-2.43029	1.25533	1.87946
C	-3.22561	-1.54826	-0.49982
C	-3.69553	-1.50418	0.78527
H	-2.40537	-2.15779	-0.85890
H	-3.32008	-2.08600	1.62017
C	-3.93735	-0.58942	-1.28487
C	-4.80325	0.14537	-0.46604
H	-3.78030	-0.42055	-2.34454
H	-5.63153	0.72818	-0.85843
C	-4.87869	-0.58681	0.86413
H	-4.90905	0.04148	1.75946
H	-5.80274	-1.18909	0.87495
H	-3.43077	2.12676	-0.93774
O	-1.35517	0.84474	-1.11348
N	-1.38044	0.89427	0.12018
O	-0.37091	0.54044	0.84451
Sn	1.64962	-0.03383	0.03122
Cl	2.08803	-0.19967	2.32465
Cl	0.52187	-1.89668	-0.88293
Cl	3.79560	-0.64765	-0.78885
Cl	1.64971	2.13689	-0.86924

TS2-2

C	-3.69779	1.55964	-0.00396
C	-2.56068	1.12259	0.82487
H	-4.37921	2.18502	0.57819
H	-2.46184	1.25681	1.89253
C	-3.07229	-1.53981	-0.44213
C	-3.52277	-1.28926	0.85749
H	-2.26152	-2.20362	-0.71626
H	-3.11741	-1.74519	1.75549
C	-3.69674	-0.63502	-1.28915
C	-4.55928	0.28254	-0.50556
H	-3.53525	-0.56000	-2.35875
H	-5.44122	0.65101	-1.03540
C	-4.80434	-0.51941	0.79758
H	-5.01822	0.09236	1.67748
H	-5.64338	-1.21703	0.65727
H	-3.36340	2.11002	-0.88658
O	-1.42812	0.65764	-1.07283
N	-1.42952	0.76349	0.17235
O	-0.38216	0.45098	0.88711
Sn	1.59609	-0.01041	0.03504
Cl	2.15597	-0.08891	2.31027
Cl	0.58829	-1.99844	-0.77861
Cl	3.74553	-0.52602	-0.85936
Cl	1.47427	2.13397	-0.93533

TS3-1

H	4.20059	-1.70386	-1.67413
H	3.12755	1.77290	1.96632
C	-0.89739	0.85252	-0.60951
C	-2.15561	0.65079	-1.22467
H	-0.66359	1.77278	-0.08383

C	0.10444	-0.15772	-0.72114
H	2.89894	3.25990	0.99357
H	3.97819	1.96382	0.39803
C	-2.60328	-1.65597	0.17991
O	-0.04912	-1.23817	-1.32109
P	1.73159	0.02593	0.17017
O	1.92094	1.63105	0.26214
O	2.86576	-0.36288	-0.92168
O	1.84016	-0.72821	1.45477
C	3.06040	2.18113	0.95342
C	3.27049	-1.73657	-1.10275
H	3.44009	-2.21445	-0.13376
H	2.50084	-2.27605	-1.66121
C	-3.24325	-0.39777	0.05702
H	-1.04305	-0.01089	2.59969
C	-3.02840	1.85546	-1.53306
C	-2.94420	0.34292	1.35719
H	-3.76050	0.12891	2.06843
H	-2.14644	-0.10085	-2.01170
H	-4.21479	-0.31454	-0.42516
C	-1.63828	-1.60026	1.20931
H	-2.86042	1.42901	1.28293
H	-2.75293	-2.49850	-0.48630
C	-1.70382	-0.36364	1.81602
H	-0.89380	-2.36015	1.41422
H	-4.05247	1.56824	-1.79559
H	-3.07241	2.56068	-0.69556
H	-2.60839	2.39432	-2.39208

TS3-2

H	4.04021	-1.80270	-1.76085
H	3.21827	1.77148	1.88224
C	-0.90796	0.91235	-0.54119
C	-2.23664	0.61893	-1.10929
H	-0.66759	1.87778	-0.10860
C	0.05977	-0.09131	-0.65430
H	3.01764	3.24909	0.88920
H	4.03295	1.90439	0.28931
C	-2.32609	-1.66413	0.09954
O	-0.19844	-1.21980	-1.16774
P	1.71440	0.04732	0.15575
O	1.96225	1.64544	0.21320
O	2.79800	-0.39852	-0.96771
O	1.84900	-0.69098	1.44791
C	3.13847	2.16450	0.86418
C	3.14594	-1.78870	-1.13408
H	3.35826	-2.24707	-0.16400
H	2.32770	-2.31794	-1.63041
C	-3.05420	-0.39039	-0.09652
H	-1.13993	0.04952	2.65275
C	-3.08869	1.85451	-1.42214
C	-2.98690	0.26236	1.30506
H	-3.83873	-0.08200	1.91291
H	-2.11408	0.01623	-2.01540
H	-4.05325	-0.51054	-0.52737
C	-1.53656	-1.59211	1.24565
H	-3.00289	1.35379	1.30472
H	-2.39679	-2.51565	-0.56614

C	-1.72260	-0.34557	1.82731
H	-0.78206	-2.31355	1.53443
H	-4.08575	1.57041	-1.77998
H	-3.21582	2.50791	-0.55135
H	-2.60783	2.44736	-2.20840

TS4-1

C	0.08364	1.65893	0.04008
C	-0.76202	0.81908	-0.68741
H	0.54454	2.47457	-0.51147
H	-0.87635	0.81031	-1.76136
C	0.85294	-1.43850	0.47381
C	0.99503	-1.12570	-0.86520
H	0.32439	-2.29753	0.87083
H	0.65916	-1.73367	-1.69801
C	1.38354	-0.38395	1.24885
C	1.79374	0.66161	0.39489
H	1.35068	-0.33131	2.33166
H	2.44755	1.46191	0.73265
C	1.93041	0.04252	-0.98962
H	1.74227	0.70979	-1.83420
H	2.96039	-0.33842	-1.09475
H	-0.20104	1.89539	1.05911
O	-1.70976	0.00608	1.23429
O	-2.58855	-0.55692	-0.69723
N	-1.74698	0.05024	-0.01192

TS4-2

C	0.22131	1.65395	0.08496
C	-0.74954	0.92465	-0.73425
H	0.67308	2.47742	-0.47593
H	-0.93362	1.06715	-1.78949
C	0.72537	-1.55170	0.28240
C	1.12840	-1.08317	-0.95652
H	0.20940	-2.48516	0.47381
H	0.98752	-1.60303	-1.89889
C	0.90260	-0.52889	1.22255
C	1.43770	0.67957	0.54770
H	0.73636	-0.61400	2.28879
H	2.12493	1.27253	1.15753
C	2.00626	0.11753	-0.77748
H	1.98821	0.82711	-1.60928
H	3.04881	-0.20567	-0.63469
H	-0.22910	2.03764	1.00418
O	-1.38229	-0.06556	1.17345
O	-2.53104	-0.52631	-0.66926
N	-1.61879	0.09848	-0.08082

TS5-1

H	-3.61215	-0.57364	-1.03424
C	-2.55782	-0.78845	-0.88719
C	0.48800	1.03388	-0.22004
C	-0.69904	-1.38061	0.65280
C	0.31215	-1.26453	-0.26674
C	-2.08578	-1.15111	0.32897
C	-0.61447	1.61541	-0.79575
C	1.92213	0.82981	-0.56957
O	2.49353	-0.22663	0.18627



C	1.77331	-1.46363	0.04062
H	0.15259	1.12870	2.20729
C	-1.21503	1.86330	0.56638
H	-1.93367	-0.74968	-1.77277
C	-0.16313	1.29290	1.18560
H	-0.45051	-1.59520	1.69006
H	0.05288	-1.24453	-1.32049
H	-2.78992	-1.21067	1.15763
H	-0.87460	1.91041	-1.80545
H	2.50845	1.71545	-0.28848
H	-2.15691	2.28723	0.89811
H	2.03896	0.67952	-1.65706
H	2.24139	-2.05661	-0.76068
H	1.91332	-1.99976	0.98536

TS5-2

H	-3.31175	-0.28762	-1.35081
C	-2.29800	-0.55836	-1.06743
C	0.36241	0.58986	-0.15034
C	-0.74505	-1.29857	0.65092
C	0.39203	-0.95875	-0.26763
C	-2.04734	-1.15253	0.15084
C	-0.83135	1.41207	-0.60867
C	1.80111	1.01883	-0.44342
O	2.61345	-0.15260	-0.29331
C	1.81802	-1.21812	0.22903
H	0.15573	0.69569	2.24506
C	-1.19842	1.69525	0.70538
H	-1.58622	-0.60132	-1.88271
C	-0.26349	0.80161	1.24991
H	-0.56437	-1.86513	1.56062
H	0.27771	-1.33542	-1.29170
H	-2.87730	-1.30605	0.84009
H	-1.08234	1.84821	-1.56896
H	2.13438	1.80839	0.24456
H	-2.01217	2.27530	1.13153
H	1.92088	1.38729	-1.47128
H	2.24474	-2.15840	-0.13329
H	1.85360	-1.22780	1.33170

TS6-1

H	-3.46406	-0.54830	-1.07038
C	-2.41972	-0.80133	-0.91099
C	0.35304	1.03685	-0.22488
C	-0.61676	-1.48381	0.63840
C	0.40646	-1.27295	-0.25649
C	-1.98685	-1.23817	0.30460
C	-0.84416	1.47210	-0.76015
C	1.78819	1.02106	-0.64921
C	1.87953	-1.42465	0.03286
H	0.10186	1.13364	2.21286
C	-1.38865	1.71604	0.62733
H	-1.79790	-0.82151	-1.79736
C	-0.25051	1.28152	1.19942
H	-0.37842	-1.74213	1.66866
H	0.15385	-1.22114	-1.31067
H	-2.70861	-1.30339	1.11722
H	-1.14696	1.78496	-1.75242

H	2.23453	2.01192	-0.46749
H	-2.35472	2.03881	1.00137
H	1.86037	0.83537	-1.72964
H	2.34775	-1.99475	-0.77998
H	2.03969	-1.99774	0.95404
C	2.56703	-0.03461	0.15138
H	2.57113	0.27214	1.20511
H	3.61587	-0.08018	-0.16491

TS6-2

H	-3.30061	-0.30274	-1.40895
C	-2.29160	-0.56643	-1.10232
C	0.34728	0.59933	-0.13499
C	-0.77149	-1.29748	0.64743
C	0.38999	-0.95400	-0.24276
C	-2.06405	-1.16315	0.11923
C	-0.86066	1.40275	-0.60576
C	1.77993	1.10825	-0.40081
C	1.80176	-1.26070	0.28555
H	0.08984	0.68730	2.25797
C	-1.25041	1.67788	0.70158
H	-1.56119	-0.60466	-1.90135
C	-0.31332	0.79059	1.25525
H	-0.60763	-1.87204	1.55579
H	0.28866	-1.33453	-1.26900
H	-2.90838	-1.32186	0.79013
H	-1.10025	1.84608	-1.56630
H	2.06016	1.86521	0.34080
H	-2.07899	2.24428	1.11840
H	1.85271	1.58943	-1.38336
H	2.14151	-2.27066	0.03094
H	1.81124	-1.18370	1.38126
C	2.68533	-0.15470	-0.33020
H	3.60402	0.01372	0.24170
H	2.99227	-0.44992	-1.34123

TS7-1

H	3.53184	0.56292	-1.38915
C	2.51247	0.82067	-1.11602
C	-0.03864	-1.13886	-0.12740
C	0.89681	1.55534	0.60640
C	-0.22917	1.36365	-0.14476
C	2.22211	1.29497	0.12692
C	1.18942	-1.43498	-0.67364
C	-1.43476	-1.41950	-0.58256
O	-2.46093	-0.72423	0.11608
C	-1.62923	1.59840	0.34803
H	0.22176	-1.12623	2.29277
C	1.78018	-1.56798	0.72742
H	1.79424	0.82912	-1.92679
C	0.59630	-1.26561	1.28601
H	0.78612	1.82259	1.65597
H	-0.13145	1.25632	-1.22234
H	3.03057	1.37976	0.85092
H	1.49437	-1.80160	-1.64736
H	-1.65924	-2.48019	-0.39544
H	2.77925	-1.76415	1.10113
H	-1.51964	-1.25182	-1.67001

H	-3.65553	0.88963	0.09438
H	-1.95331	2.61880	0.08178
H	-1.66856	1.52910	1.44210
C	-2.65135	0.62856	-0.25696
H	-2.64786	0.72162	-1.35728

TS7-2

H	-3.57645	-0.32019	-1.38779
C	-2.56309	-0.57939	-1.09173
C	0.09876	0.59560	-0.13413
C	-1.01473	-1.28346	0.64004
C	0.14938	-0.95546	-0.26534
C	-2.31640	-1.16715	0.12753
C	-1.14536	1.37779	-0.58532
C	1.41003	1.30373	-0.47626
O	2.55506	0.68785	0.09591
C	1.49397	-1.48399	0.26860
H	-0.12026	0.66557	2.25512
C	-1.49927	1.65454	0.72813
H	-1.83998	-0.60979	-1.89779
C	-0.54563	0.76541	1.26163
H	-0.83562	-1.87463	1.53490
H	0.01783	-1.30836	-1.29780
H	-3.14975	-1.32749	0.81157
H	-1.40464	1.82478	-1.53901
H	1.39698	2.33184	-0.10243
H	-2.31567	2.22285	1.16542
H	1.52130	1.33911	-1.57624
H	3.61975	-1.02984	0.12471
H	1.60498	-2.54752	0.01990
H	1.51834	-1.40470	1.36324
C	2.66688	-0.67777	-0.28274
H	2.71540	-0.76354	-1.38350

TS8-1

H	3.50091	0.51640	-1.40331
C	2.48557	0.79093	-1.13085
C	0.01871	-1.18604	-0.12903
C	0.88894	1.59617	0.57220
C	-0.24356	1.37619	-0.15896
C	2.21046	1.31535	0.09815
C	1.27590	-1.41561	-0.64142
C	-1.35732	-1.50256	-0.62984
C	-1.63736	1.63789	0.34303
H	0.22862	-1.10054	2.29856
C	1.83800	-1.49445	0.78061
H	1.76894	0.80583	-1.94273
C	0.62347	-1.25356	1.30042
H	0.78575	1.90312	1.61226
H	-0.15919	1.21227	-1.23003
H	3.02340	1.41649	0.81480
H	1.61340	-1.81299	-1.59228
H	-1.51424	-2.58692	-0.49594
H	2.83608	-1.62101	1.18549
H	-1.39955	-1.32807	-1.71476
H	-3.68668	1.03114	0.10381
H	-1.92031	2.67532	0.09914
H	-1.65855	1.56882	1.43965

C	-2.70243	0.70587	-0.25809
H	-2.72236	0.83801	-1.35048
C	-2.53308	-0.78590	0.06285
H	-3.45513	-1.30508	-0.22987
H	-2.44484	-0.91830	1.15115

TS8-2

H	-3.59530	-0.31835	-1.39197
C	-2.58084	-0.57265	-1.09484
C	0.08428	0.61111	-0.13651
C	-1.03076	-1.27353	0.63432
C	0.13702	-0.94062	-0.26866
C	-2.33270	-1.16851	0.12029
C	-1.17968	1.37643	-0.57773
C	1.37858	1.35407	-0.50004
C	1.46315	-1.50620	0.27565
H	-0.15104	0.65958	2.26004
C	-1.53191	1.64592	0.73566
H	-1.85621	-0.59622	-1.89986
C	-0.56879	0.76158	1.26263
H	-0.85023	-1.87478	1.52264
H	0.00737	-1.29268	-1.30217
H	-3.16630	-1.33864	0.80198
H	-1.44006	1.83049	-1.52812
H	1.30712	2.39378	-0.15749
H	-2.35512	2.20055	1.17818
H	1.44782	1.39299	-1.59860
H	3.61121	-1.25937	0.09184
H	1.49835	-2.58518	0.07667
H	1.48112	-1.39579	1.37015
C	2.69479	-0.79988	-0.29988
H	2.72279	-0.92538	-1.39279
C	2.65257	0.69372	0.04608
H	3.53525	1.21094	-0.35158
H	2.68894	0.80928	1.13926

TS9-1

C	-0.86454	-0.71390	0.19893
C	0.02594	-1.48503	-0.50592
C	1.14936	-1.82911	0.44645
C	0.92127	-0.98225	1.62979
C	-0.28590	-0.39954	1.49375
O	2.01290	-2.65134	0.26406
C	-2.18978	-0.35325	-0.28225
O	-2.57165	-0.51182	-1.41810
O	-2.95731	0.17397	0.67562
C	-4.26656	0.53899	0.27824
C	1.33961	-0.21937	-1.66164
C	1.90885	0.64463	-0.75602
C	1.14968	1.75357	-0.21941
C	-0.13066	1.97009	-0.58768
H	-0.70312	2.76271	-0.12864
C	1.78547	2.62196	0.82573
C	3.32965	0.43142	-0.33092
H	1.94476	-1.01388	-2.07394
H	-0.21943	-2.08573	-1.36575
H	-0.77863	0.22837	2.21788
H	1.58592	-0.94230	2.47491

H	-4.74542	0.93260	1.16678
H	-4.23364	1.29441	-0.50199
H	-4.80822	-0.32603	-0.09326
H	-0.61203	1.43999	-1.39183
H	0.48128	0.06493	-2.24851
H	3.48383	0.61247	0.72883
H	3.65073	-0.58251	-0.55216
H	3.98627	1.11389	-0.87466
H	1.11942	3.42982	1.11439
H	2.03124	2.05039	1.72009
H	2.71121	3.06507	0.46098

TS9-2

C	-0.83644	-0.58935	0.23003
C	0.15027	-1.37527	-0.53240
C	1.19581	-1.72133	0.52654
C	1.03655	-0.66788	1.51440
C	-0.27762	-0.21744	1.43737
O	2.03458	-2.58752	0.44963
C	-2.19150	-0.35084	-0.23653
O	-2.57629	-0.61009	-1.35397
O	-2.98078	0.19239	0.69491
C	-4.31186	0.45360	0.28984
C	1.09622	-0.50516	-1.45395
C	1.82392	0.47925	-0.61522
C	1.17268	1.69333	-0.27970
C	-0.10648	1.90223	-0.69298
H	-0.66321	2.75603	-0.33353
C	1.84033	2.67886	0.63448
C	3.29135	0.29104	-0.44139
H	1.79421	-1.20304	-1.90948
H	-0.25359	-2.19890	-1.11058
H	-0.77368	0.40361	2.16555
H	1.71674	-0.51880	2.33686
H	-4.80719	0.87172	1.15800
H	-4.33106	1.16072	-0.53502
H	-4.80399	-0.46296	-0.02253
H	-0.57712	1.32710	-1.47104
H	0.50258	-0.04880	-2.24081
H	3.70274	0.90609	0.35225
H	3.52798	-0.75349	-0.24163
H	3.80052	0.56092	-1.37104
H	1.16699	3.49617	0.87695
H	2.15178	2.20865	1.56655
H	2.72687	3.11047	0.17204

TS10-1

C	-1.19919	-2.42739	-0.49213
C	-1.64364	-1.30522	0.42957
C	-1.44353	-0.13421	-0.27720
C	-0.66441	-0.42490	-1.44889
C	-0.41834	-1.75432	-1.54198
C	-0.06574	-1.68277	1.66631
C	1.06539	-1.68644	0.87665
C	1.80443	-0.50421	0.52273

H	-0.31085	0.33505	-2.12610
O	-1.46903	-3.59478	-0.37235
H	1.44708	-2.63119	0.51541
H	-0.43898	-2.63250	2.01993
H	-0.28005	-0.83753	2.30328
C	-1.91157	1.17016	0.16517
H	-2.40964	-1.43739	1.17670
H	0.12605	-2.27264	-2.31164
O	-1.79498	2.10461	-0.78058
O	-2.35946	1.39807	1.26500
C	-2.24053	3.39935	-0.42050
H	-2.07450	4.02120	-1.29188
H	-3.29540	3.38193	-0.16197
H	-1.67754	3.77643	0.42877
C	2.97389	-0.61897	-0.24573
C	3.68594	0.49763	-0.62415
C	3.24356	1.76580	-0.25395
C	2.09332	1.89906	0.50422
C	1.37828	0.77706	0.89640
H	3.31039	-1.60180	-0.54434
H	4.58595	0.38960	-1.21099
H	3.80138	2.64113	-0.55171
H	1.75251	2.87936	0.80239
H	0.50432	0.90149	1.51645

TS10-2

C	-1.84905	-1.84002	0.61995
C	-0.77837	-1.70326	-0.46753
C	0.32033	-1.00694	0.21921
C	-0.14167	-0.57893	1.48272
C	-1.44794	-0.92841	1.68024
C	-1.54960	-0.86882	-1.58239
C	-2.04048	0.37495	-0.99516
C	-1.16297	1.38958	-0.65495
H	0.46938	-0.02166	2.17496
O	-2.83275	-2.53799	0.54221
H	-3.09207	0.48259	-0.76986
H	-2.36084	-1.50155	-1.92766
H	-0.84773	-0.70844	-2.39898
C	1.70069	-1.13364	-0.20098
H	-0.48246	-2.64058	-0.92925
H	-2.05628	-0.70265	2.53966
O	2.57310	-0.73504	0.73191
O	2.04657	-1.54035	-1.28919
C	3.93852	-0.83804	0.37418
H	4.49585	-0.48398	1.23329
H	4.19932	-1.86898	0.15246
H	4.15755	-0.22808	-0.49817
C	-1.58804	2.53061	0.08770
C	-0.68167	3.42372	0.56480
C	0.70049	3.23546	0.31927
C	1.14102	2.16931	-0.41563
C	0.22561	1.22317	-0.90875
H	-2.64292	2.65432	0.28653
H	-1.00893	4.28018	1.13479
H	1.40758	3.96064	0.69450
H	2.19134	2.05643	-0.63645
H	0.55364	0.53632	-1.67132

TS11-1

C	-2.22803	-1.64821	-0.57440
C	-2.13424	-0.46309	0.36094
C	-1.34721	0.46989	-0.26840
C	-0.77629	-0.12806	-1.46056
C	-1.21521	-1.39336	-1.61583
C	-0.93507	-1.61130	1.73098
C	0.12940	-2.03614	0.97964
C	1.24664	-1.22151	0.61068
C	1.31492	0.08474	0.96164
C	2.40364	1.00758	0.52845
C	3.25408	0.43474	-0.59352
C	3.57901	-1.02333	-0.32086
C	2.30446	-1.84789	-0.25942
H	-0.08942	0.39369	-2.10654
O	-3.00510	-2.56525	-0.48718
H	4.24220	-1.42192	-1.08757
H	2.71002	0.51048	-1.53717
H	4.16423	1.02200	-0.70850
H	3.02964	1.23314	1.39825
H	1.96588	1.96156	0.23078
H	1.89735	-1.98096	-1.26509
H	2.52041	-2.85029	0.11225
H	0.59410	0.48867	1.65792
H	4.11176	-1.10240	0.62933
H	0.10534	-3.04302	0.58290
H	-1.70594	-2.31926	1.99594
H	-0.85580	-0.74262	2.36668
C	-1.19565	1.84394	0.18632
H	-2.88116	-0.24241	1.10519
H	-0.98281	-2.08434	-2.40700
O	-0.57481	2.61632	-0.71197
O	-1.58729	2.26251	1.25012
C	-0.44459	3.98124	-0.35591
H	0.07582	4.45306	-1.18079
H	-1.42247	4.43328	-0.21704
H	0.12324	4.08733	0.56421

TS11-2

C	-2.01661	-1.86765	-0.53553
C	-1.93560	-0.74562	0.49899
C	-1.26595	0.33471	-0.24524
C	-0.70037	-0.19803	-1.39291
C	-0.91521	-1.56810	-1.44412
C	-0.98478	-1.49117	1.52503
C	0.20740	-1.97205	0.80382
C	1.30027	-1.13241	0.56300
C	1.22842	0.18568	0.93096
C	2.24941	1.20364	0.55974
C	3.22677	0.71748	-0.49858
C	3.65925	-0.70913	-0.20696
C	2.45826	-1.63883	-0.25524
H	-0.11405	0.37284	-2.09504
O	-2.76032	-2.81607	-0.50959
H	4.41117	-1.03819	-0.92288
H	2.74990	0.75312	-1.48012
H	4.08596	1.38519	-0.54378

H	2.78881	1.48688	1.47008
H	1.74062	2.11233	0.23281
H	2.12774	-1.75268	-1.29116
H	2.73002	-2.63721	0.08807
H	0.48401	0.50173	1.64515
H	4.12246	-0.75408	0.78119
H	0.29917	-3.02832	0.59300
H	-1.56025	-2.32034	1.92655
H	-0.74671	-0.80912	2.33683
C	-1.32488	1.72807	0.15424
H	-2.85965	-0.47286	0.99608
H	-0.58932	-2.23789	-2.22264
O	-0.80834	2.55976	-0.75961
O	-1.78379	2.11662	1.20435
C	-0.88072	3.93701	-0.43840
H	-0.42580	4.45848	-1.27221
H	-1.91485	4.24705	-0.31786
H	-0.34360	4.14894	0.48200

TS12-1

C	1.63511	-1.97673	-0.50086
C	0.45854	-1.83010	0.44312
C	-0.49355	-1.10519	-0.23998
C	0.09342	-0.59222	-1.45640
C	1.36853	-1.01887	-1.58851
C	1.57015	-0.56847	1.68908
C	2.01979	0.44951	0.88077
C	1.17596	1.52035	0.52217
C	-0.14305	1.78795	0.80539
C	-0.47684	2.95617	0.07689
C	0.64876	3.31184	-0.58962
O	1.64871	2.45933	-0.33411
H	-0.43359	0.05947	-2.13398
O	2.55645	-2.74277	-0.37510
H	0.87899	4.12619	-1.25028
H	-1.42076	3.46850	0.05383
H	-0.76709	1.24549	1.49183
H	3.01576	0.43356	0.46489
H	2.27282	-1.31752	2.02093
H	0.71195	-0.41097	2.32508
C	-1.85637	-0.90705	0.22717
H	0.24231	-2.54521	1.22000
H	2.05823	-0.80877	-2.38683
O	-2.65424	-0.40248	-0.71742
O	-2.24232	-1.16704	1.34370
C	-4.00139	-0.19521	-0.33451
H	-4.49871	0.20426	-1.21017
H	-4.46083	-1.13154	-0.03129
H	-4.06222	0.50841	0.49126

TS12-2

C	1.74525	-1.81868	-0.52133
C	0.64340	-1.62246	0.52348
C	-0.42120	-0.94900	-0.23190
C	0.09485	-0.53256	-1.46189
C	1.42159	-0.88017	-1.58439
C	1.40756	-0.69943	1.57025
C	1.98384	0.44795	0.86200



C	1.15351	1.49256	0.55548
C	-0.22048	1.61263	0.77326
C	-0.63093	2.76105	0.06096
C	0.49130	3.25600	-0.52235
O	1.56864	2.52222	-0.23841
H	-0.47479	0.02509	-2.18847
O	2.69787	-2.55366	-0.40622
H	0.66021	4.12134	-1.13661
H	-1.61806	3.17931	-0.00262
H	-0.79755	1.04528	1.47966
H	3.02925	0.48674	0.60031
H	2.17951	-1.32075	2.01315
H	0.69395	-0.41127	2.33806
C	-1.79411	-0.89157	0.21546
H	0.33193	-2.51941	1.04926
H	2.07120	-0.66792	-2.41662
O	-2.64285	-0.47373	-0.73247
O	-2.15793	-1.17650	1.33730
C	-4.00173	-0.40085	-0.34533
H	-4.54078	-0.06486	-1.22328
H	-4.36349	-1.37518	-0.02944
H	-4.13423	0.30215	0.47287

#### TS13-1

C	1.26048	1.12211	-1.11057
C	2.28144	0.58933	-0.12027
N	3.09219	-0.20314	-0.70002
C	2.25349	0.98058	1.32343
C	-0.10651	0.58838	-0.72543
C	-1.05860	1.40770	-0.14517
C	-2.31289	0.92426	0.19969
C	-2.62485	-0.40776	-0.03848
C	-1.66915	-1.24242	-0.62772
C	-0.43402	-0.74882	-0.96614
H	1.29755	2.20372	-1.04388
H	1.54309	0.83692	-2.11584
H	1.43111	1.65101	1.51377
H	3.18742	1.46987	1.57952
H	2.13394	0.09964	1.94379
H	-0.84397	2.44791	0.03070
H	-3.02795	1.59225	0.63709
H	0.27860	-1.40509	-1.43655
N	4.94133	-1.35696	0.80687
N	4.13155	-0.80607	0.36332
H	-1.93155	-2.26582	-0.81717
O	-3.79162	-0.98029	0.25090
C	-4.84306	-0.22523	0.80566
H	-5.66763	-0.90933	0.92327
H	-4.56632	0.17489	1.77400
H	-5.13470	0.58069	0.14290

#### TS13-2

C	-0.40888	-0.37260	1.68019
C	-2.54287	0.93215	-0.05190
N	-1.78114	0.44636	0.62890
C	-3.53403	1.56225	-0.93310
C	0.82724	-0.34487	0.97202
C	1.72462	0.71554	1.14931

C	2.94278	0.73470	0.51352
C	3.28790	-0.32627	-0.33313
C	2.39500	-1.39695	-0.52736
C	1.19157	-1.40220	0.11305
H	-0.55852	0.30331	2.49824
H	-0.95000	-1.29480	1.75257
H	-3.66505	2.59491	-0.63841
H	-4.47400	1.03438	-0.84538
H	-3.18096	1.51622	-1.95469
H	1.46435	1.53064	1.80134
H	3.61481	1.55295	0.67548
H	0.51684	-2.22681	-0.03465
N	-7.86381	-0.88970	-0.41718
N	-6.89309	-0.42429	-0.47528
H	2.69390	-2.19608	-1.17758
O	4.42455	-0.41268	-0.98861
C	5.42489	0.58253	-0.87356
H	6.23446	0.25303	-1.50283
H	5.05666	1.53800	-1.22398
H	5.76814	0.66351	0.14952

TS14-1

C	0.79495	1.08496	-1.10619
C	1.86835	0.57480	-0.16143
N	2.65796	-0.21483	-0.77263
C	1.91071	0.98730	1.27615
C	-0.55294	0.56327	-0.63876
C	-1.46491	1.40403	-0.01775
C	-2.69232	0.91763	0.40136
C	-3.03872	-0.41460	0.21195
C	-2.11597	-1.25071	-0.41312
C	-0.89088	-0.77165	-0.83498
H	0.83618	2.16785	-1.06624
H	1.02125	0.77598	-2.11852
H	1.08222	1.63833	1.50372
H	2.84370	1.50606	1.47066
H	1.85198	0.11344	1.91484
H	-1.23431	2.44571	0.12635
H	-3.38827	1.58725	0.87353
H	-0.20583	-1.43864	-1.33082
N	3.76387	-0.78573	0.24308
N	4.60536	-1.31704	0.64994
H	-2.36229	-2.28430	-0.57848
C	-4.38849	-0.93913	0.63874
H	-4.83005	-0.31442	1.40516
H	-5.07115	-0.96125	-0.20528
H	-4.31256	-1.94821	1.02655

TS14-2

C	0.11927	-0.90510	1.32159
C	-2.14693	0.79096	0.01257
N	-1.35024	0.15899	0.50985
C	-3.18259	1.60940	-0.63070
C	1.35182	-0.55106	0.70615
C	2.14536	0.47370	1.24497
C	3.36075	0.77600	0.68122
C	3.82134	0.06970	-0.43482
C	3.02838	-0.94762	-0.97593

C	1.81192	-1.25536	-0.41742
H	-0.11744	-0.52683	2.29554
H	-0.36702	-1.82064	1.05138
H	-3.24873	2.56245	-0.12306
H	-4.13235	1.09563	-0.56870
H	-2.91838	1.76699	-1.66787
H	1.80222	1.02073	2.10516
H	3.96573	1.55782	1.10142
H	1.21163	-2.04184	-0.83931
N	-6.61712	-0.30180	-0.33516
N	-7.60573	-0.73054	-0.30147
H	3.37728	-1.49383	-1.83251
C	5.17030	0.37964	-1.02767
H	5.43593	1.41883	-0.88112
H	5.93031	-0.22872	-0.54554
H	5.19467	0.16126	-2.08769

TS15-1

C	0.98783	-1.17748	1.17008
C	2.03109	-0.57645	0.24264
N	2.61490	0.39665	0.81561
C	2.26493	-1.11463	-1.13389
C	-0.39128	-0.97993	0.56205
C	-1.09528	-2.05466	0.03922
C	-2.35425	-1.85473	-0.50535
C	-2.91254	-0.58916	-0.53767
C	-2.20266	0.47843	-0.01237
C	-0.94900	0.29291	0.53931
Cl	-2.89085	2.06839	-0.03975
H	1.22955	-2.23021	1.26486
H	1.06382	-0.72520	2.15052
H	1.58431	-1.92486	-1.34051
H	3.28659	-1.47236	-1.20807
H	2.10972	-0.33250	-1.86825
H	-0.68076	-3.04668	0.07176
H	-2.90458	-2.68786	-0.90101
H	-3.88721	-0.43016	-0.95734
H	-0.42793	1.13410	0.95965
N	3.70044	1.05692	-0.18348
N	4.47009	1.69034	-0.58640

TS15-2

C	-0.00685	-0.98750	-1.47893
C	-2.44548	-0.77229	0.63088
N	-1.60232	-0.86000	-0.12085
C	-3.53979	-0.65897	1.60369
C	1.20769	-0.81728	-0.77007
C	1.89129	-1.93563	-0.26831
C	3.09971	-1.76567	0.36931
C	3.62714	-0.48858	0.51510
C	2.95158	0.62654	0.02470
C	1.74670	0.47175	-0.61574
Cl	3.63567	2.20152	0.22197
H	-0.34179	-1.96758	-1.75187
H	-0.43735	-0.17214	-2.02398
H	-3.78507	-1.64291	1.98060
H	-4.40549	-0.22803	1.11920
H	-3.22568	-0.02459	2.42179

H	1.47388	-2.91878	-0.38772
H	3.63921	-2.61056	0.75222
H	4.57028	-0.35207	1.00998
H	1.22510	1.32956	-0.99741
N	-6.71530	0.88101	-0.17579
N	-7.64114	1.28286	-0.55480

TS16-1

C	1.53733	1.13237	-1.08654
C	2.53625	0.53376	-0.10759
N	3.30609	-0.27184	-0.71697
C	2.54039	0.90369	1.34251
C	0.12966	0.70008	-0.70796
C	-0.75390	1.60688	-0.13887
C	-2.03775	1.21232	0.19954
C	-2.41083	-0.09497	-0.03816
C	-1.55324	-1.01581	-0.61068
C	-0.27531	-0.60895	-0.94577
N	-3.76279	-0.52095	0.32470
O	-4.04882	-1.65689	0.11169
O	-4.47747	0.29733	0.81102
H	1.65153	2.20861	-1.01977
H	1.78677	0.83060	-2.09568
H	3.47871	1.39466	1.57961
H	2.44277	0.01417	1.95407
H	1.72247	1.57058	1.56339
H	-0.45933	2.62760	0.02668
H	-2.73498	1.90032	0.63299
H	-1.88466	-2.01816	-0.79148
H	0.39417	-1.31270	-1.40814
N	5.16924	-1.50455	0.74183
N	4.36421	-0.92484	0.32727

TS16-2

C	-0.53452	-0.30517	1.78574
C	-3.02393	-0.73572	-0.60021
N	-2.19919	-0.59868	0.16655
C	-4.09304	-0.91392	-1.59147
C	0.70227	-0.15345	1.14709
C	1.16184	1.13387	0.80073
C	2.39391	1.29008	0.21039
C	3.14565	0.14915	-0.02845
C	2.73325	-1.13598	0.29120
C	1.50030	-1.28524	0.88156
N	4.46626	0.31275	-0.66312
O	5.08861	-0.67901	-0.86274
O	4.79879	1.42277	-0.92400
H	-1.11643	0.54435	2.08253
H	-0.86053	-1.26174	2.14162
H	-3.82322	-0.40269	-2.50592
H	-5.01530	-0.50212	-1.20460
H	-4.22357	-1.96878	-1.79307
H	0.54962	1.99381	1.00023
H	2.77468	2.25295	-0.06131
H	3.36567	-1.97326	0.07921
H	1.14548	-2.26509	1.14250
N	-8.45790	1.01936	0.09360
N	-7.49631	0.60524	-0.16371

## TS17-1

C	2.57310	0.74904	0.11301
C	1.52187	0.43066	1.15203
O	1.85322	0.20314	2.31425
H	2.28237	1.45640	-0.65808
H	3.51442	1.02456	0.58097
C	0.10739	0.25100	0.70639
C	-0.67594	-0.73766	1.31482
C	-2.00418	-0.94019	0.94741
C	-2.60613	-0.13978	-0.05047
C	-1.82037	0.88495	-0.62414
C	-0.48421	1.06562	-0.27069
H	-0.23298	-1.35328	2.09339
H	-2.56322	-1.72906	1.43877
H	-2.24793	1.56652	-1.35101
H	0.08226	1.91700	-0.65177
O	1.51602	3.18419	-0.08422
Br	2.97026	-1.04624	-0.81549
H	1.93182	3.95427	0.33667
N	-3.93372	-0.36694	-0.46364
C	-4.59158	0.66175	-1.25207
H	-4.04003	0.84865	-2.17889
H	-5.59111	0.31244	-1.52792
H	-4.69202	1.62307	-0.71586
C	-4.80188	-1.13752	0.41012
H	-4.40877	-2.14906	0.55731
H	-4.93560	-0.67582	1.40593
H	-5.78467	-1.23472	-0.06061

## TS17-2

C	-2.48508	0.70299	0.69571
C	-1.45657	1.17303	-0.27142
O	-1.79417	1.79601	-1.29133
H	-2.21648	0.33281	1.67037
H	-3.43805	1.20601	0.62730
C	-0.04566	0.64975	-0.14743
C	0.86403	0.95181	-1.16224
C	2.19520	0.52808	-1.10873
C	2.66357	-0.22363	-0.01827
C	1.74504	-0.53366	1.00412
C	0.42568	-0.09859	0.94191
H	0.50717	1.53643	-2.00511
H	2.86316	0.80113	-1.91986
H	2.06157	-1.14517	1.84543
H	-0.24436	-0.35823	1.75389
O	-1.48964	2.44541	1.39444
Br	-3.14926	-1.29459	-0.14996
H	-1.84231	3.16863	0.84776
N	4.00216	-0.71124	0.06532
C	4.73061	-0.37204	1.28400
H	4.11267	-0.54898	2.16532
H	5.62505	-1.00278	1.36161
H	5.05043	0.68852	1.29961
C	4.83225	-0.56262	-1.11563
H	4.31478	-0.96350	-1.99222
H	5.11521	0.48778	-1.32829
H	5.75609	-1.13546	-0.97138

TS18-1

C	1.43373	0.90363	0.21750
C	0.26886	0.52282	1.10164
O	0.41209	0.44321	2.31828
H	1.18992	1.54550	-0.62664
H	2.25211	1.30768	0.80796
C	-1.01835	0.09923	0.45254
C	-1.69171	-1.01407	0.97769
C	-2.89201	-1.44461	0.40946
C	-3.43640	-0.74923	-0.67680
C	-2.77676	0.37627	-1.18253
C	-1.56051	0.79913	-0.63710
H	-1.26484	-1.53298	1.83186
H	-3.40203	-2.31847	0.81128
H	-4.37662	-1.07750	-1.11770
H	-3.21316	0.93520	-2.00841
H	-1.07012	1.72501	-0.95336
O	0.13487	3.16233	-0.39055
Br	2.15122	-0.86922	-0.51883
H	0.25522	4.03493	0.01771

TS18-2

C	-1.28493	0.91034	0.67526
C	-0.15599	1.11802	-0.26913
O	-0.31907	1.78211	-1.30487
H	-1.13785	0.49469	1.65715
H	-2.10319	1.60658	0.56923
C	1.10580	0.29804	-0.09815
C	2.08355	0.39049	-1.09735
C	3.27792	-0.32670	-1.00477
C	3.51526	-1.15363	0.09804
C	2.54736	-1.24932	1.10344
C	1.35449	-0.53029	1.00490
H	1.87834	1.03646	-1.94572
H	4.02370	-0.24175	-1.79358
H	4.44418	-1.71613	0.17517
H	2.72073	-1.88754	1.96799
H	0.62033	-0.61396	1.79820
O	0.04884	2.38312	1.37804
Br	-2.36629	-0.91151	-0.18020
H	-0.12495	3.16078	0.81986

TS19-1

C	2.27059	0.74238	-0.03139
C	1.19782	0.71166	1.03160
O	1.49437	0.78798	2.21989
H	2.01497	1.29486	-0.93246
H	3.21977	1.06777	0.38673
C	-0.21741	0.41868	0.61724
C	-0.96294	-0.47938	1.39315
C	-2.28449	-0.78294	1.06105
C	-2.85185	-0.15617	-0.04839
C	-2.13691	0.75850	-0.82013
C	-0.80637	1.03920	-0.49506
H	-0.50170	-0.93947	2.26265
H	-2.86259	-1.48922	1.64938
H	-2.61310	1.25395	-1.66128

H	-0.23591	1.82470	-1.00849
O	1.21422	3.06391	-0.82586
Br	2.56517	-1.20981	-0.55517
H	1.38533	3.98542	-0.57327
Cl	-4.53572	-0.52832	-0.47604

TS19-2

C	-2.13628	0.72209	0.71898
C	-1.10557	1.18636	-0.24240
O	-1.42508	1.83174	-1.25200
H	-1.88162	0.31057	1.67996
H	-3.09205	1.21865	0.64703
C	0.30468	0.65004	-0.11843
C	1.22191	0.99440	-1.11829
C	2.54699	0.55780	-1.07482
C	2.95579	-0.23334	-0.00305
C	2.07108	-0.58771	1.01405
C	0.75002	-0.14127	0.94811
H	0.86912	1.61237	-1.93832
H	3.25029	0.82782	-1.85721
H	2.40753	-1.20229	1.84357
H	0.06951	-0.41742	1.74505
O	-1.13660	2.40752	1.45035
Br	-2.80380	-1.27954	-0.18903
H	-1.48928	3.15223	0.93298
Cl	4.63771	-0.79543	0.07244

TS20-1

C	2.24315	0.42930	0.43018
C	0.91696	0.41840	1.15226
O	0.85580	0.14570	2.34631
H	2.36912	1.24297	-0.28246
H	3.06578	0.38275	1.13966
C	-0.34314	0.58361	0.34402
C	-1.42544	-0.25454	0.65169
C	-2.61108	-0.11396	-0.06086
C	-2.75636	0.84843	-1.06000
C	-1.67488	1.69205	-1.33546
C	-0.46137	1.56076	-0.65513
H	-1.33151	-0.99062	1.44308
H	-3.69637	0.94324	-1.59611
H	-1.78534	2.46697	-2.09121
H	0.36208	2.27021	-0.78372
O	1.86730	3.05900	0.15911
Br	2.32637	-1.33467	-0.59323
H	2.21052	3.79172	0.69547
Cl	-3.98407	-1.17740	0.31734

TS20-2

C	-2.03314	0.91833	0.56718
C	-0.74180	1.11728	-0.13598
O	-0.68076	1.78851	-1.17586
H	-2.09184	0.48077	1.54841
H	-2.81552	1.61302	0.30209
C	0.45784	0.29455	0.29125
C	1.63806	0.46073	-0.44531
C	2.77642	-0.25355	-0.09190
C	2.78785	-1.14032	0.98389

C	1.60723	-1.30016	1.71582
C	0.45477	-0.59037	1.37687
H	1.63120	1.14819	-1.28405
H	3.68977	-1.68799	1.23984
H	1.59120	-1.98764	2.55882
H	-0.44637	-0.73268	1.96118
O	-0.87126	2.35260	1.53841
Br	-2.92699	-0.90258	-0.52015
H	-0.92975	3.14615	0.97826
Cl	4.26757	-0.03278	-1.03357

TS21-1

C	2.89123	0.67299	-0.07564
C	1.83881	0.77963	1.00130
O	2.15435	0.94205	2.17504
H	2.65936	1.22366	-0.98756
H	3.86978	0.93592	0.31933
C	0.40206	0.50974	0.63487
C	-0.35485	-0.30128	1.49235
C	-1.69199	-0.57401	1.21141
C	-2.28294	-0.01790	0.06918
C	-1.53573	0.81346	-0.77564
C	-0.18932	1.06748	-0.50847
H	0.11345	-0.71342	2.38147
H	-2.27038	-1.21642	1.86891
H	-2.00392	1.26387	-1.64637
H	0.39706	1.78425	-1.09494
O	1.89568	2.98461	-0.97449
Br	3.01362	-1.30773	-0.53175
H	2.15870	3.90851	-0.83519
C	-3.73653	-0.25528	-0.20685
F	-4.17928	-1.45331	0.27116
F	-4.54493	0.68982	0.36808
F	-4.03638	-0.23629	-1.53414

TS21-2

C	2.74050	0.68277	-0.73975
C	1.75158	1.19086	0.23955
O	2.11199	1.82553	1.24058
H	2.45378	0.26592	-1.68885
H	3.72340	1.12499	-0.68197
C	0.31283	0.72514	0.13371
C	-0.57036	1.11285	1.14845
C	-1.91358	0.74304	1.11811
C	-2.39724	-0.02302	0.05116
C	-1.52713	-0.40885	-0.97733
C	-0.18668	-0.03457	-0.93334
H	-0.17218	1.70453	1.96662
H	-2.58185	1.04619	1.91867
H	-1.89693	-1.00306	-1.80816
H	0.46968	-0.34119	-1.73876
O	1.81365	2.39130	-1.46810
Br	3.31399	-1.35502	0.18591
H	2.20602	3.12654	-0.96583
C	-3.84685	-0.38801	-0.02895
F	-4.46972	-0.36901	1.18154
F	-4.56432	0.46345	-0.82776
F	-4.05208	-1.63156	-0.54913



## TS22-1

C	2.57813	0.63905	0.00785
C	1.50649	0.70869	1.06831
O	1.79682	0.81534	2.25431
H	2.38886	1.29498	-0.84535
H	3.55656	0.81738	0.44876
C	0.07355	0.46522	0.66380
C	-0.69678	-0.38776	1.47131
C	-2.02565	-0.65148	1.15776
C	-2.57912	-0.03342	0.03121
C	-1.83642	0.84090	-0.76962
C	-0.49795	1.08066	-0.46208
H	-0.24241	-0.83942	2.34800
H	-2.63065	-1.31842	1.76029
H	-2.30751	1.32384	-1.61788
H	0.10001	1.82837	-0.99739
O	1.58482	3.01008	-0.75200
Br	2.61758	-1.28109	-0.63821
H	1.79819	3.94293	-0.58981
N	-3.97694	-0.30493	-0.30588
O	-4.45777	0.23988	-1.30671
O	-4.62053	-1.07132	0.42450

## TS22-2

C	-2.37820	0.65698	0.79204
C	-1.37327	1.19689	-0.14999
O	-1.70444	1.91784	-1.09982
H	-2.11351	0.14555	1.69999
H	-3.34962	1.12620	0.76137
C	0.05363	0.69198	-0.06606
C	0.96204	1.16320	-1.02600
C	2.29488	0.76832	-1.01521
C	2.72479	-0.11240	-0.01749
C	1.84482	-0.59558	0.95679
C	0.51628	-0.18671	0.92634
H	0.58830	1.84442	-1.78340
H	2.99909	1.12822	-1.75613
H	2.20668	-1.27576	1.71856
H	-0.16258	-0.55983	1.68311
O	-1.40412	2.25155	1.65770
Br	-3.00673	-1.29385	-0.30896
H	-1.76462	3.04274	1.22040
N	4.12229	-0.53492	0.00992
O	4.88791	-0.09203	-0.85661
O	4.48387	-1.31718	0.89847

## TS23-1

Rh	-0.48199	-0.19444	-0.03549
C	2.50960	0.44561	0.88775
C	2.48074	1.92117	0.58866
O	2.36635	2.21340	-0.72612
C	2.25293	3.61209	-1.03463
H	1.35246	4.02301	-0.57227
H	2.18352	3.66616	-2.12142
H	3.12668	4.16034	-0.67287
O	2.60539	2.76863	1.44839
C	1.86310	-0.56555	0.08244

C	2.19616	-0.69059	-1.30469
H	1.79040	-1.55814	-1.82412
H	2.16542	0.21123	-1.90640
H	1.72488	-1.50472	0.61409
O	-0.52730	-0.84537	1.93488
C	-1.65611	-0.96481	2.50265
O	-2.80272	-0.73460	2.02291
Rh	-2.92290	-0.06721	0.07104
O	-2.97476	-2.02564	-0.59274
C	-1.87782	-2.61444	-0.80808
O	-0.70003	-2.15804	-0.67811
H	-1.94833	-3.65585	-1.15273
O	-2.72714	1.87862	0.73460
C	-1.55938	2.34801	0.85423
O	-0.45333	1.77592	0.61065
H	-1.48884	3.38408	1.21375
O	-2.90326	0.59402	-1.88633
C	-1.78547	0.70556	-2.46627
O	-0.62887	0.46606	-2.00272
H	-1.81664	1.05536	-3.50806
H	-1.62924	-1.31384	3.54442
C	4.37472	0.02983	0.75233
C	4.51130	-1.29245	1.43027
C	4.45165	-2.43891	0.74358
C	4.24473	-2.48485	-0.74785
C	4.07311	-1.09637	-1.37359
C	4.56237	0.01348	-0.65868
H	4.76375	0.94354	-1.18234
H	4.22243	-1.07962	-2.45366
H	3.38442	-3.12366	-0.98921
H	5.11083	-2.97861	-1.21820
H	4.57334	-3.39128	1.25544
H	4.65796	-1.29362	2.50768
H	2.35877	0.32705	1.95999
H	4.80358	0.87210	1.29400

TS23-2

Rh	0.40059	0.11266	0.10019
C	-1.56065	0.76205	0.36722
C	-1.90070	2.02927	-0.35887
O	-1.53898	3.10423	0.37172
C	-1.57882	4.36255	-0.32458
H	-0.90533	4.33455	-1.18424
H	-1.24520	5.10364	0.40194
H	-2.59368	4.58413	-0.66507
O	-2.37154	2.10375	-1.47875
C	-2.20882	0.46177	1.63338
C	-3.22620	1.16755	2.17018
H	-3.64859	0.89638	3.13462
H	-3.62946	2.05631	1.69472
H	-1.83264	-0.41562	2.15475
O	0.05408	-0.93182	-1.66108
C	1.03862	-1.50662	-2.22868
O	2.23985	-1.55580	-1.85424
Rh	2.76898	-0.58573	-0.09922
O	2.25793	-2.27355	0.99721
C	1.06749	-2.40294	1.38701
O	0.07723	-1.62627	1.19081

H	0.84244	-3.30482	1.97495
O	3.10084	1.14974	-1.17757
C	2.12452	1.92118	-1.38211
O	0.91713	1.79280	-1.00453
H	2.33685	2.82921	-1.96470
O	3.14384	0.43393	1.66059
C	2.17542	1.01566	2.22160
O	0.96066	1.07269	1.85183
H	2.40201	1.54707	3.15704
H	0.79750	-2.02753	-3.16671
C	-3.08940	-0.82408	-1.14125
C	-2.92106	-2.22538	-0.70305
C	-3.85836	-2.86309	0.01645
C	-5.16616	-2.23302	0.39782
C	-5.34465	-0.84579	-0.14578
C	-4.40603	-0.21876	-0.87700
H	-4.58306	0.77292	-1.28117
H	-6.30435	-0.36437	0.03243
H	-5.27271	-2.22424	1.49589
H	-5.99954	-2.87093	0.05679
H	-3.69712	-3.89355	0.32661
H	-1.98848	-2.71604	-0.96287
H	-2.24349	-0.19110	-0.49089
H	-2.66510	-0.58736	-2.11977

#### TS24-1

C	-0.61461	1.64866	-0.14318
C	0.48763	0.94566	-0.65308
H	0.71579	0.95698	-1.71111
C	1.41105	0.27025	0.26981
O	1.10384	0.15207	1.45186
C	-2.15769	0.56469	-0.13681
C	-1.90990	-0.62090	0.58183
C	-0.95283	-1.51089	0.05185
O	-0.34442	-1.22918	-1.00876
C	2.69763	-0.28811	-0.29293
H	-2.89530	1.24987	0.27046
H	-0.66170	-2.39630	0.63398
H	-1.01367	2.43637	-0.77523
H	-2.26681	-0.75770	1.59602
H	-2.20092	0.45166	-1.21511
H	-0.55594	1.89304	0.91218
H	3.28877	-0.73227	0.50695
H	2.46925	-1.04416	-1.04890
H	3.27747	0.50325	-0.77898

#### TS24-2

C	0.75154	-1.67447	-0.21648
C	-0.49935	-1.13745	-0.67004
H	-0.81638	-1.23246	-1.70080
C	-1.26352	-0.37172	0.25503
O	-0.73108	-0.10459	1.35824
C	1.98341	-0.49711	-0.03131
C	1.54628	0.67015	0.67761
C	0.73343	1.60285	-0.02931
O	0.32749	1.32989	-1.17091
C	-2.61052	0.20418	-0.11013
H	2.78383	-1.04385	0.46320

H	0.39075	2.50906	0.49246
H	1.19270	-2.40302	-0.89426
H	1.77655	0.83237	1.72258
H	2.21868	-0.27014	-1.06994
H	0.67913	-2.05127	0.80275
H	-3.32758	-0.01851	0.68369
H	-2.53294	1.29104	-0.19514
H	-2.98364	-0.19420	-1.05538

TS25-1

C	-1.36302	-0.72499	-0.11123
C	-0.10499	-0.78132	-0.06198
C	1.04857	-1.64243	-0.10354
C	2.24603	-1.02559	0.03436
C	2.14163	0.40688	0.20274
C	0.90905	0.90646	0.00911
C	0.13642	1.97561	-0.29637
C	-1.22795	2.05519	0.19098
C	-2.70038	-1.30803	0.05925
H	2.96631	1.01205	0.56154
H	3.19269	-1.55003	0.05749
H	0.92090	-2.70747	-0.25181
H	0.41426	2.56750	-1.16766
H	-1.82848	2.85460	-0.24140
H	-1.33714	2.02563	1.27658
H	-1.64673	0.99993	-0.12288
H	-3.35954	-1.06522	-0.77999
H	-2.65941	-2.39924	0.16606
H	-3.17510	-0.90848	0.96209

TS25-2

C	1.47400	-0.33747	-0.28689
C	0.16379	-0.47321	0.05919
C	-0.60815	-1.67563	0.06482
C	-1.96825	-1.34135	0.00532
C	-2.11946	0.05001	0.00484
C	-0.83732	0.65023	0.02402
C	-0.45535	1.96459	-0.08764
C	0.93204	2.34408	0.12381
C	2.53112	-1.32735	0.01983
H	-3.05898	0.58390	0.05393
H	-2.78141	-2.05515	-0.01669
H	-0.20011	-2.67388	-0.00716
H	-1.16739	2.68950	-0.47597
H	1.25889	2.27058	1.16402
H	1.21118	3.31491	-0.28653
H	1.53071	1.42478	-0.34266
H	3.22247	-0.86584	0.73853
H	2.17252	-2.26479	0.47331
H	3.13761	-1.54733	-0.86459

TS26-1

C	2.39349	-0.35892	0.61524
C	2.68213	-0.23934	-0.73662
C	3.35930	-1.40990	-1.18961
C	3.56973	-2.22037	-0.12833
C	3.14505	-1.55069	1.12669
O	0.83176	-2.34765	0.09759

C	0.68786	-1.15718	0.12575
C	-0.27787	-0.20390	0.01972
H	2.13147	0.47934	1.23853
H	2.40714	0.60301	-1.34913
H	3.59593	-1.62904	-2.21706
H	4.00308	-3.20683	-0.16337
H	4.02536	-1.19229	1.67053
H	2.58081	-2.19664	1.79273
C	-1.68613	-0.63536	-0.00362
C	-2.06962	-1.98394	0.02552
C	-2.70780	0.32214	-0.06907
C	-3.40439	-2.34629	-0.01774
H	-1.31427	-2.75030	0.08233
C	-4.04113	-0.04824	-0.11129
H	-2.45606	1.37093	-0.09269
C	-4.40290	-1.38580	-0.08630
H	-3.66458	-3.39487	0.00511
H	-4.80072	0.71854	-0.16403
H	-5.44287	-1.67498	-0.11775
C	-0.00082	1.25500	0.02479
C	0.15691	1.95740	-1.16819
C	0.02965	1.97372	1.21953
C	0.37494	3.32770	-1.16864
H	0.09282	1.41792	-2.10289
C	0.25212	3.34240	1.22535
H	-0.13035	1.44677	2.14999
C	0.43005	4.02313	0.02973
H	0.49620	3.85213	-2.10536
H	0.27853	3.87844	2.16294
H	0.60005	5.08969	0.03186

TS26-2

C	-2.33885	-0.39799	-0.46142
C	-2.31071	-0.40498	0.99301
C	-2.76622	-1.64801	1.45548
C	-3.20142	-2.37380	0.38399
C	-3.27635	-1.52754	-0.83445
O	-0.84056	-2.24513	-0.68430
C	-0.86354	-1.02398	-0.49868
C	0.18165	-0.15591	-0.16032
H	-2.44250	0.55111	-0.96637
H	-1.95294	0.40997	1.59806
H	-2.68790	-2.00237	2.46936
H	-3.51768	-3.40442	0.41797
H	-4.29251	-1.13923	-0.94998
H	-2.99236	-2.05299	-1.73946
C	1.57223	-0.60788	-0.10196
C	1.92366	-1.96892	-0.13078
C	2.61649	0.32346	0.02014
C	3.24279	-2.36434	-0.00602
H	1.14567	-2.70118	-0.26309
C	3.93450	-0.08001	0.13485
H	2.39382	1.37870	0.02418
C	4.25847	-1.42820	0.12847
H	3.48024	-3.41824	-0.02600
H	4.71174	0.66494	0.22548
H	5.28760	-1.74443	0.21521
C	-0.05419	1.31077	-0.08833

C	0.06494	2.00120	1.11829
C	-0.34703	2.04538	-1.23650
C	-0.12999	3.37196	1.18105
H	0.32330	1.45087	2.01262
C	-0.54846	3.41661	-1.17723
H	-0.40581	1.53216	-2.18621
C	-0.44414	4.08482	0.03290
H	-0.03497	3.88380	2.12767
H	-0.77685	3.96371	-2.08035
H	-0.59740	5.15275	0.08024

TS27-1

C	-1.33552	0.76350	-0.68383
C	-1.48712	0.97853	0.66168
C	-2.54062	0.13951	1.16738
C	-3.06106	-0.56303	0.14337
C	-2.41722	-0.15942	-1.13475
O	-0.43451	-1.72942	0.00473
C	0.13881	-0.69753	-0.04549
C	1.31080	-0.05258	0.00806
Cl	1.58738	1.63811	-0.06907
Cl	2.72518	-1.03765	0.09421
H	-0.74119	1.36496	-1.35043
H	-0.90698	1.67045	1.25026
H	-2.81841	0.06054	2.20486
H	-3.83396	-1.31072	0.21381
H	-3.12076	0.39559	-1.76324
H	-2.06461	-1.00725	-1.71916

TS27-2

C	-1.12976	0.80746	-0.58452
C	-1.27138	0.95251	0.86385
C	-2.21961	0.04212	1.31922
C	-2.75728	-0.59445	0.22445
C	-2.41490	0.13351	-1.02271
O	-0.60954	-1.52493	-0.47219
C	-0.11391	-0.39333	-0.41057
C	1.16316	-0.05304	-0.01669
Cl	1.77904	1.55495	-0.09978
Cl	2.34133	-1.26844	0.20121
H	-0.75233	1.64627	-1.15381
H	-0.65426	1.59366	1.47138
H	-2.39274	-0.21949	2.34898
H	-3.42650	-1.43898	0.26303
H	-3.17680	0.89017	-1.22808
H	-2.30524	-0.51143	-1.88643

TS28-1

C	-1.73864	0.89812	0.18236
C	-1.02776	0.83992	-1.14122
C	-1.02236	1.04997	1.43180
C	0.08467	1.70102	-1.46960
C	0.25820	1.54422	1.66484
C	1.08000	2.16386	-0.64143
C	1.20881	2.01009	0.75781
O	-2.95033	0.64042	0.17701
H	0.18558	1.94292	-2.52678
H	1.88383	2.71796	-1.12506

H	2.13610	2.38160	1.18992
H	0.55944	1.57351	2.71143
C	-0.43864	-1.66221	0.99948
H	-1.65343	0.85252	2.29396
C	-0.52426	-0.99215	-1.23754
H	-1.78212	0.82065	-1.92644
C	0.41068	-1.20050	-0.07823
C	-1.72268	-1.70302	-0.88475
H	-0.15058	-1.03200	-2.25632
C	-1.67585	-2.03647	0.47211
H	-0.12379	-1.81480	2.02254
H	-2.57912	-1.83079	-1.53439
H	-2.49455	-2.46309	1.03916
C	1.75892	-1.02528	-0.06184
C	2.59837	-1.30166	1.15821
C	2.54844	-0.67948	-1.29643
H	1.93137	-0.27191	-2.09824
H	3.05749	-1.57735	-1.67774
H	3.32960	0.05394	-1.06618
H	2.00811	-1.49332	2.05577
H	3.25855	-0.45007	1.36180
H	3.24874	-2.17165	0.98701

TS28-2

C	1.67989	-0.95750	0.39317
C	1.06731	-0.87670	-1.01111
C	0.86099	-1.01269	1.59254
C	-0.01816	-1.83945	-1.33907
C	-0.49292	-1.25379	1.71135
C	-1.12681	-2.08054	-0.59963
C	-1.42718	-1.55675	0.70564
O	2.90483	-0.83321	0.47073
H	0.06058	-2.32698	-2.30908
H	-1.89831	-2.70864	-1.04446
H	-2.44973	-1.70935	1.04495
H	-0.90465	-1.14822	2.71468
C	0.44475	1.84903	0.75334
H	1.44156	-0.86239	2.49887
C	0.64463	0.69793	-1.26983
H	1.90655	-1.03961	-1.69135
C	-0.33029	1.15092	-0.18796
C	1.85994	1.51079	-1.00350
H	0.27230	0.74279	-2.29554
C	1.73871	2.11821	0.21497
H	0.08507	2.23007	1.70087
H	2.75079	1.47907	-1.61818
H	2.50724	2.69400	0.71775
C	-1.69039	0.87381	-0.10860
C	-2.49996	1.38461	1.06042
C	-2.49393	0.54402	-1.34089
H	-1.91285	0.01432	-2.09691
H	-2.85960	1.48022	-1.79095
H	-3.37348	-0.06067	-1.09683
H	-1.94945	1.33003	2.00259
H	-3.42265	0.80646	1.17345
H	-2.79161	2.43327	0.89925

TS29-1

C	-1.65638	0.46812	-0.58087
C	-0.61194	0.23593	-1.63814
C	-1.36242	1.05979	0.71991
C	0.40616	1.21005	-1.96214
C	-0.23859	1.82368	1.04977
C	1.07326	2.04705	-1.10312
C	0.84480	2.23875	0.27841
O	-2.77310	-0.02208	-0.80622
H	0.73555	1.21108	-3.00025
H	1.88820	2.63042	-1.53013
H	1.56816	2.87013	0.79118
H	-0.21246	2.16588	2.08427
C	-0.24391	-1.49776	1.17510
C	0.16186	-1.40619	-1.12263
H	-1.13051	-0.12130	-2.52668
C	0.78026	-1.13413	0.22197
C	-0.96514	-2.25871	-0.85139
H	0.79312	-1.60417	-1.98395
C	-1.22758	-2.24326	0.52095
H	-0.19503	-1.32975	2.24226
H	-1.59176	-2.71388	-1.60767
H	-2.09076	-2.69328	0.99704
C	2.03525	-0.67608	0.47784
C	2.55244	-0.47365	1.87839
C	3.06535	-0.47885	-0.60242
H	2.63181	-0.42342	-1.60175
H	3.78601	-1.31032	-0.58708
H	3.63822	0.43981	-0.43195
H	1.77348	-0.53869	2.63989
H	3.03100	0.50903	1.96612
H	3.32252	-1.22221	2.11518
C	-2.50284	0.98449	1.70908
H	-3.28664	1.70851	1.44917
H	-2.97538	-0.00012	1.68279
H	-2.16414	1.20348	2.72717

TS29-2

C	1.65643	-0.53076	-0.52106
C	0.66816	-0.07446	-1.59987
C	1.24835	-1.20300	0.71467
C	-0.32915	-1.06593	-2.07971
C	0.00681	-1.76363	0.96679
C	-1.14359	-1.81256	-1.29780
C	-1.11999	-1.88626	0.13649
O	2.82917	-0.17698	-0.67724
H	-0.46288	-1.12112	-3.15846
H	-1.92490	-2.39122	-1.78981
H	-1.97592	-2.38179	0.59021
H	-0.13603	-2.13363	1.98210
C	0.21347	1.56897	1.22012
C	-0.01013	1.34739	-1.09315
H	1.30203	0.22519	-2.43744
C	-0.69994	1.12666	0.24808
C	1.11717	2.25542	-0.76011
H	-0.65030	1.67906	-1.91317
C	1.26375	2.30870	0.59845
H	0.08759	1.46681	2.29073
H	1.79998	2.66209	-1.49550



H	2.06313	2.81011	1.13226
C	-1.93893	0.53843	0.47030
C	-2.45601	0.37234	1.88011
C	-2.99817	0.51279	-0.60191
H	-2.58153	0.45806	-1.60850
H	-3.59950	1.43304	-0.53535
H	-3.68451	-0.32983	-0.46783
H	-1.66618	0.09377	2.58188
H	-3.23120	-0.39978	1.91933
H	-2.91147	1.30795	2.23792
C	2.35284	-1.33543	1.73765
H	3.11621	-2.04507	1.39402
H	2.86955	-0.38200	1.88165
H	1.96610	-1.68779	2.69952

TS30-1

C	-1.41448	-1.48562	-0.14826
C	-1.00142	-1.00479	1.20899
C	-0.50694	-1.44413	-1.27556
C	0.30499	-1.26675	1.75982
C	0.88118	-1.35097	-1.31011
C	1.51553	-1.33030	1.11443
C	1.81379	-1.25959	-0.27199
O	-2.61025	-1.76889	-0.30749
H	0.34078	-1.34250	2.84589
H	2.38587	-1.43580	1.76310
H	1.30731	-1.34790	-2.31301
C	-1.18780	1.28592	-1.23056
H	-1.01739	-1.62617	-2.21739
C	-1.31479	0.89200	1.06798
H	-1.80460	-1.22179	1.91114
C	-0.38844	1.34567	-0.02557
C	-2.63259	0.97773	0.50838
H	-1.13626	1.18056	2.09911
C	-2.53079	1.14943	-0.87630
H	-0.82000	1.44914	-2.23409
H	-3.54975	0.79736	1.05431
H	-3.36139	1.12193	-1.57144
C	0.90533	1.74794	0.09817
C	1.72498	2.21208	-1.07674
C	1.59148	1.89781	1.42947
H	1.06381	1.39820	2.24269
H	1.68671	2.96388	1.68437
H	2.60993	1.49207	1.38926
H	1.24276	2.03229	-2.03888
H	2.69765	1.70428	-1.08530
H	1.93518	3.28847	-0.99721
C	3.28442	-1.17484	-0.62778
H	3.74707	-0.27417	-0.19967
H	3.84382	-2.03194	-0.22931
H	3.44390	-1.14637	-1.70981

TS30-2

C	-1.50859	-1.38530	-0.38079
C	-1.14328	-0.98000	1.05259
C	-0.54287	-1.32180	-1.46836
C	0.12276	-1.54615	1.59927
C	0.81886	-1.14546	-1.42283

C	1.33954	-1.51288	1.01496
C	1.68531	-1.02224	-0.30559
O	-2.69073	-1.65134	-0.60454
H	0.05778	-1.96314	2.60258
H	2.18262	-1.86800	1.60898
H	1.30631	-1.04834	-2.39321
C	-1.09162	1.66917	-0.95600
H	-1.00976	-1.45062	-2.44139
C	-1.21518	0.64791	1.13999
H	-1.98042	-1.32655	1.66363
C	-0.28022	1.26726	0.10516
C	-2.57071	1.05406	0.67091
H	-0.99828	0.90794	2.17923
C	-2.47234	1.59006	-0.57778
H	-0.73862	2.07768	-1.89496
H	-3.48504	0.80966	1.19704
H	-3.30013	1.89701	-1.20700
C	1.11771	1.35640	0.17769
C	1.86868	2.01150	-0.95838
C	1.80312	1.44587	1.51826
H	1.30696	0.85443	2.28879
H	1.80680	2.49615	1.84875
H	2.84988	1.12887	1.46062
H	1.50849	1.68086	-1.93618
H	2.93905	1.79366	-0.89726
H	1.75833	3.10504	-0.91063
C	3.17204	-0.96335	-0.59664
H	3.71461	-0.38880	0.16344
H	3.60835	-1.97281	-0.59928
H	3.37964	-0.51251	-1.57156

#### TS31-1

C	-0.47711	1.51482	-0.71907
C	-1.64348	1.41450	-0.00039
C	-2.35738	0.20802	0.17741
C	-1.89125	-1.02485	-0.29503
C	-0.20341	-1.39616	0.76879
C	0.86087	-0.70606	0.18511
O	1.38776	-1.17758	-0.97076
C	1.53011	0.46108	0.74164
O	2.56695	0.89578	0.22191
H	-1.97084	2.27906	0.57454
H	0.10216	2.43188	-0.71497
H	-3.17954	0.20843	0.88981
H	-2.49436	-1.90481	-0.08441
H	-1.36274	-1.07876	-1.24409
H	-0.49243	-1.08531	1.76647
H	-0.24525	-2.46603	0.58633
H	-0.18275	0.77265	-1.45085
H	1.11834	0.87312	1.67749
H	2.15961	-0.60394	-1.16032

#### TS31-2

C	-0.02907	1.34359	-0.55243
C	-1.39622	1.48515	-0.05534
C	-2.24982	0.44343	0.04979
C	-1.82488	-0.95723	-0.26101
C	-0.58017	-1.37947	0.61166

C	0.68231	-0.71962	0.20189
O	1.42272	-1.28428	-0.71128
C	1.28966	0.52638	0.64814
O	2.47262	0.71342	0.17719
H	-1.70707	2.46368	0.30630
H	0.56193	2.25602	-0.57355
H	-3.24047	0.59856	0.47002
H	-2.63339	-1.66472	-0.05871
H	-1.54232	-1.08118	-1.31421
H	-0.79490	-1.15072	1.65798
H	-0.42685	-2.45813	0.51162
H	0.08666	0.79415	-1.48761
H	0.95207	0.97245	1.59043
H	2.23089	-0.61661	-0.68581

TS32-1

C	0.56537	1.52475	0.76597
C	1.72930	1.37259	0.05470
C	2.37365	0.13198	-0.16382
C	1.82627	-1.08930	0.25172
C	0.14632	-1.35989	-0.82957
C	-0.91789	-0.69503	-0.19726
C	-1.49224	0.54519	-0.72527
O	-2.52136	1.04666	-0.26307
H	2.12493	2.23808	-0.47487
H	0.05254	2.48029	0.79384
H	3.20876	0.11167	-0.86060
H	2.39366	-1.99007	0.02737
H	1.28984	-1.13998	1.19881
H	0.43530	-0.98351	-1.80504
H	0.17779	-2.44474	-0.74970
H	0.19456	0.76656	1.44410
H	-0.99455	0.95193	-1.62319
H	-2.33936	-0.69460	1.23385
N	-1.47520	-1.15784	0.97244
H	-1.43092	-2.14584	1.17411

TS32-2

C	0.05188	-1.36361	-0.58986
C	1.43136	-1.47375	-0.11723
C	2.25781	-0.41455	0.02720
C	1.79595	0.98826	-0.21919
C	0.54929	1.35409	0.67510
C	-0.72580	0.73089	0.21600
C	-1.25407	-0.58778	0.61046
O	-2.43166	-0.89807	0.23248
H	1.78022	-2.45445	0.20343
H	-0.50008	-2.29960	-0.63094
H	3.25635	-0.55870	0.43237
H	2.59319	1.70253	0.00620
H	1.51057	1.14826	-1.26877
H	0.75822	1.04390	1.70108
H	0.42301	2.44298	0.67680
H	-0.08632	-0.80001	-1.51437
H	-0.83051	-0.96902	1.55704
H	-2.36225	0.84573	-0.87783
N	-1.49713	1.35251	-0.66240

H	-1.24767	2.21410	-1.12289
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TS33-1

C	-0.64980	1.58823	-0.70357
C	-1.80971	1.60114	0.02018
C	-2.65821	0.47418	0.18736
C	-2.36448	-0.79403	-0.31313
C	-0.73957	-1.43574	0.79739
C	0.41566	-0.93006	0.18906
O	0.79223	-1.49450	-0.97996
C	1.22256	0.11988	0.73343
H	-2.04300	2.48833	0.60589
H	0.03167	2.43112	-0.68338
H	-3.47336	0.56555	0.90218
H	-3.07778	-1.59154	-0.12271
H	-1.81339	-0.90587	-1.24356
H	-0.98012	-1.06823	1.78773
H	-0.97432	-2.47895	0.61050
H	-0.41119	0.80191	-1.40914
H	0.86070	0.56483	1.65938
H	1.65340	-1.07724	-1.22000
S	2.71193	0.53028	0.09302

TS33-2

C	-0.23755	1.28210	-0.61757
C	-1.55414	1.61364	-0.09349
C	-2.53476	0.69648	0.06798
C	-2.29628	-0.75931	-0.17370
C	-1.08126	-1.26774	0.69098
C	0.23773	-0.82097	0.16676
O	0.72971	-1.54377	-0.81327
C	1.03935	0.26151	0.65071
H	-1.71942	2.63545	0.24260
H	0.48964	2.08686	-0.63543
H	-3.48503	0.99854	0.50125
H	-3.17795	-1.34910	0.08961
H	-2.06339	-0.97470	-1.22448
H	-1.20922	-0.92799	1.72050
H	-1.07491	-2.36162	0.68025
H	-0.19685	0.68797	-1.52928
H	0.70564	0.73258	1.57347
H	1.66915	-1.17242	-0.94463
S	2.67414	0.37252	0.11765

TS34-1

C	-4.84684	-0.25581	-0.43144
C	-3.56774	-1.05525	-0.76578
C	-2.69615	-0.36127	-1.82483
C	-2.4194	1.08592	-1.50108
C	-3.59527	1.89738	-1.01379
C	-4.43336	1.15606	0.04047
H	-1.74882	-0.88331	-1.985
H	-2.96253	-1.19474	0.13682
H	-3.8145	-2.05251	-1.14101
H	-5.40903	-0.13264	-1.37285
H	-1.57254	0.98334	-0.52022
H	-3.26276	2.87114	-0.64268

H	-4.1983	2.09278	-1.9147
H	-3.84942	1.09513	0.96538
H	-5.31081	1.77073	0.25908
H	-3.21531	-0.33559	-2.79687
C	-5.82915	-0.9948	0.54494
C	-5.20154	-1.24317	1.93318
H	-4.92444	-0.30892	2.43204
H	-5.91817	-1.76065	2.58148
H	-4.30585	-1.8698	1.87122
C	-7.11452	-0.15495	0.72373
H	-7.56911	0.08865	-0.24459
H	-7.85493	-0.71586	1.3051
H	-6.92952	0.78256	1.25677
C	-6.24536	-2.35315	-0.06413
H	-5.41161	-3.05996	-0.11699
H	-7.025	-2.81953	0.54858
H	-6.6496	-2.2291	-1.0765
O	-1.63993	1.72816	-2.47601
C	-0.5151	2.24344	-1.84908
O	0.2578	2.98323	-2.38488
C	-0.46484	1.68292	-0.46049
C	-0.69628	2.60418	0.69208
O	-1.58554	2.44442	1.51137
O	0.20059	3.59487	0.71357
C	0.15133	4.46691	1.86124
H	-0.81361	4.97716	1.91167
H	0.3094	3.88993	2.77492
H	0.95866	5.182	1.708
Rh	0.97958	0.15824	-0.08045
Rh	2.72206	-1.50558	0.33417
O	2.9416	-0.69748	2.22123
C	2.2187	0.28797	2.5629
C	2.43539	0.86675	3.94342
O	1.33045	0.85572	1.84031
H	3.05787	1.76435	3.85704
H	1.47984	1.1596	4.38447
H	2.94871	0.14501	4.58028
O	1.24555	-2.75343	1.06491
C	0.04298	-2.35612	1.08941
O	-0.38189	-1.22195	0.6739
C	-0.99526	-3.30158	1.65244
H	-1.56901	-2.79672	2.43489
H	-1.69452	-3.59023	0.86115
H	-0.51497	-4.19353	2.0557
O	4.10845	-0.17693	-0.40607
C	3.70072	0.95885	-0.80554
C	4.73596	1.93432	-1.31672
O	2.49213	1.36704	-0.79691
H	5.59404	1.39542	-1.72239
H	4.29613	2.59355	-2.06721
H	5.08038	2.55126	-0.47906
O	0.75054	-0.67661	-1.96591
C	1.51603	-1.64191	-2.31575
O	2.39205	-2.19821	-1.58793
C	1.36943	-2.13837	-3.73637
H	1.95646	-1.48842	-4.39488
H	1.74936	-3.15744	-3.82299
H	0.32697	-2.0838	-4.05721

## TS34-2

C	-5.15456	-0.65453	-0.44302
C	-3.84088	-1.46318	-0.3643
C	-2.9238	-1.2274	-1.58192
C	-2.72059	0.21899	-1.88756
C	-3.92193	1.11341	-1.82315
C	-4.80775	0.84374	-0.59311
H	-1.94975	-1.71401	-1.47582
H	-3.28923	-1.18802	0.54197
H	-4.04164	-2.53585	-0.30087
H	-5.67072	-0.96127	-1.36884
H	-1.27772	0.21207	-0.23099
H	-3.63782	2.16519	-1.91005
H	-4.49073	0.86881	-2.73959
H	-4.28197	1.19858	0.30028
H	-5.71393	1.4462	-0.69605
H	-3.39284	-1.65166	-2.48774
C	-6.16408	-0.9646	0.71914
C	-5.58586	-0.61968	2.10824
H	-5.31739	0.4379	2.19375
H	-6.3294	-0.83323	2.88484
H	-4.6932	-1.20883	2.34113
C	-7.46537	-0.15785	0.50642
H	-7.87926	-0.32285	-0.49632
H	-8.22446	-0.46907	1.23265
H	-7.3156	0.91791	0.63937
C	-6.53944	-2.46392	0.69254
H	-5.69287	-3.11074	0.94246
H	-7.32783	-2.66864	1.42539
H	-6.91752	-2.7637	-0.2929
O	-1.65947	0.5459	-2.61327
C	-1.08266	1.69797	-1.82444
O	-0.72294	2.68283	-2.391
C	-1.2587	1.27332	-0.45918
C	-1.41418	2.17124	0.69146
O	-1.83763	1.79475	1.77594
O	-1.11721	3.45809	0.4156
C	-1.26127	4.37898	1.5084
H	-2.29754	4.40816	1.85651
H	-0.61342	4.08735	2.33885
H	-0.96314	5.34822	1.10846
Rh	1.11595	0.07124	-0.05583
Rh	3.26033	-0.94095	0.35943
O	3.78624	0.73878	1.42333
C	2.93865	1.68267	1.53671
C	3.34475	2.88654	2.35438
O	1.76701	1.69522	1.03507
H	2.98967	3.80146	1.87457
H	2.87305	2.81873	3.34088
H	4.4278	2.91306	2.4813
O	2.46341	-1.76945	2.07282
C	1.24126	-1.54852	2.35614
O	0.43516	-0.83745	1.6714
C	0.69044	-2.2072	3.59988
H	1.47635	-2.31216	4.35029
H	-0.14895	-1.63122	3.99305
H	0.33332	-3.21009	3.33943

O	3.94919	-0.05624	-1.36765
C	3.14787	0.66443	-2.04891
C	3.70026	1.33046	-3.28685
O	1.92657	0.88819	-1.76469
H	4.41282	0.66858	-3.78387
H	2.89021	1.61062	-3.96153
H	4.2354	2.23828	-2.98685
O	0.59583	-1.63843	-1.11512
C	1.45574	-2.57642	-1.22764
O	2.62692	-2.5726	-0.73501
C	1.03079	-3.80305	-2.00304
H	0.30084	-4.36639	-1.41156
H	0.54646	-3.50456	-2.93644
H	1.8913	-4.44065	-2.20839

TS35-1

C	-0.78947	-0.27118	0.85070
C	-0.35433	-2.13994	-1.35112
C	-0.85396	-1.14089	-2.14306
C	-2.10497	-0.51925	-1.93929
C	-2.93500	-0.75224	-0.82987
C	-2.10098	0.24560	0.62694
C	-4.38054	-0.26581	-0.84256
C	-4.52560	1.25438	-0.98524
C	-2.37564	1.72690	0.35511
C	-3.88127	1.99960	0.18732
C	-1.82018	2.56599	1.52120
C	-0.71494	-1.47992	1.66311
C	0.40986	0.35040	0.28290
C	1.72231	-1.23928	1.59665
O	-1.67999	-2.16454	2.02242
O	0.33200	1.28649	-0.53191
N	0.57709	-1.86113	2.03347
C	1.71630	-0.19447	0.72564
C	2.98831	0.35683	0.20710
C	3.16576	1.73890	0.01522
C	4.06234	-0.49783	-0.09919
C	4.38217	2.24173	-0.44226
C	5.28123	0.00741	-0.55078
C	5.44714	1.38220	-0.72324
C	1.00950	-2.72703	-1.50989
H	-2.80815	-1.70890	-0.32450
H	-2.80182	-0.17841	1.35053
H	-4.85919	-0.58159	0.09316
H	-4.91798	-0.77833	-1.65178
H	-4.07309	1.59165	-1.92808
H	-5.59086	1.50896	-1.04956
H	-1.84676	2.02232	-0.55261
H	-4.02706	3.07978	0.05805
H	-4.40250	1.72659	1.11837
H	-0.73430	2.46961	1.58743
H	-2.25821	2.25384	2.47781
H	-0.21369	-0.73291	-2.92239
H	-2.37398	0.28001	-2.62613
H	2.64624	-1.65108	1.98975
H	2.34092	2.41019	0.21848
H	3.93193	-1.57314	-0.00440
H	4.49924	3.31378	-0.57920

H	6.09517	-0.67534	-0.78158
H	6.39290	1.77948	-1.08236
H	0.62829	-2.66608	2.64397
H	1.65145	-2.11294	-2.14843
H	1.49740	-2.83636	-0.53464
H	0.94319	-3.73630	-1.94298
H	-1.00275	-2.63064	-0.63103
H	-2.06045	3.62547	1.37138

TS35-2

C	-0.85405	0.83186	-0.36346
C	-0.46111	1.17726	2.25561
C	-0.56285	-0.19067	2.46733
C	-1.55558	-0.94553	1.85720
C	-2.65805	-0.30369	1.11404
C	-2.21699	0.22378	-0.35793
C	-3.95445	-1.13766	1.06251
C	-3.94194	-2.22462	-0.01234
C	-2.38071	-0.85982	-1.46934
C	-3.73103	-1.58401	-1.38509
C	-2.19797	-0.21650	-2.85131
C	-0.73002	2.25535	-0.60920
C	0.28878	-0.03682	-0.27185
C	1.69965	1.88426	-0.72272
O	-1.65327	3.07458	-0.64308
O	0.11455	-1.24947	0.03063
N	0.59084	2.69001	-0.79655
C	1.62899	0.55194	-0.44760
C	2.86160	-0.26281	-0.35370
C	2.99628	-1.27135	0.61773
C	3.94798	-0.02285	-1.21350
C	4.18391	-1.99117	0.73598
C	5.13757	-0.73941	-1.08963
C	5.26250	-1.72683	-0.11103
C	0.74453	1.97632	2.62404
H	-2.89896	0.62983	1.63346
H	-2.93321	1.02635	-0.56746
H	-4.78647	-0.45205	0.85194
H	-4.14926	-1.56310	2.05509
H	-3.13552	-2.94578	0.18506
H	-4.88384	-2.78639	0.01776
H	-1.59821	-1.60830	-1.32581
H	-3.77440	-2.34497	-2.17527
H	-4.55045	-0.87609	-1.58701
H	-1.19727	0.21294	-2.96460
H	-2.92729	0.58813	-3.01259
H	0.27633	-0.70903	2.92549
H	-1.54009	-2.02624	1.95817
H	2.64831	2.39211	-0.86124
H	2.15680	-1.49443	1.26395
H	3.84930	0.71705	-2.00388
H	4.26694	-2.76443	1.49572
H	5.96137	-0.53587	-1.76910
H	6.18591	-2.29215	-0.01712
H	0.68831	3.68018	-0.98175
H	1.62555	1.34784	2.78172
H	0.97171	2.70834	1.84130
H	0.55056	2.55073	3.54247



H	-1.33710	1.75367	1.97863
H	-2.33739	-0.96134	-3.64401

TS36-1

C	1.07531	0.76666	0.07601
C	0.33860	0.46898	1.31303
C	0.42584	1.19948	-1.11132
C	-0.72252	1.30195	1.80117
C	-0.80596	1.84002	-1.25938
C	-1.64122	2.03371	1.09518
C	-1.73083	2.20939	-0.29958
H	-0.84957	1.28172	2.88152
H	-2.40909	2.53111	1.68426
H	-2.59672	2.76233	-0.65616
H	-1.05337	2.11209	-2.28322
C	-0.45020	-1.41921	-1.34893
H	1.03732	1.15987	-2.00851
C	-0.38373	-1.35310	0.97716
H	1.00071	0.15900	2.11719
C	-1.28436	-1.15194	-0.19478
C	0.74277	-2.05556	0.47651
H	-0.76715	-1.54801	1.97261
C	0.71513	-2.03863	-0.92441
H	-0.73886	-1.27832	-2.38160
H	1.54473	-2.45329	1.08618
H	1.50681	-2.39864	-1.56975
C	-2.60211	-0.84231	-0.18069
C	-3.41702	-0.71383	-1.43670
C	-3.39311	-0.72314	1.09076
H	-2.76638	-0.63432	1.97890
H	-4.03305	-1.60778	1.20997
H	-4.05609	0.14773	1.05233
H	-2.81402	-0.72242	-2.34536
H	-3.99128	0.21901	-1.41660
H	-4.14371	-1.53398	-1.50122
C	2.42053	0.39269	0.03097
C	3.10919	-0.09721	1.17704
N	3.64701	-0.50387	2.12489
C	3.16889	0.46754	-1.17897
N	3.74423	0.51686	-2.18761

TS36-2

C	1.07547	0.45782	0.49130
C	0.34199	-0.72349	1.08275
C	0.39987	1.61097	-0.00203
C	-0.57988	-0.38860	2.20802
C	-0.87726	2.06485	0.30693
C	-1.54538	0.54909	2.20358
C	-1.81350	1.51498	1.16996
H	-0.49211	-1.02657	3.08413
H	-2.21325	0.58076	3.06265
H	-2.74888	2.06114	1.27013
H	-1.19342	2.95405	-0.23481
C	-0.56881	-0.21335	-1.99132
H	1.00253	2.27337	-0.61729
C	-0.37945	-1.56926	-0.11238
H	1.08401	-1.42143	1.47445
C	-1.31044	-0.65667	-0.88713

C	0.68764	-1.88107	-1.09868
H	-0.83783	-2.43921	0.36150
C	0.58991	-1.03060	-2.15537
H	-0.88868	0.53706	-2.70332
H	1.49089	-2.58335	-0.91077
H	1.28977	-0.95195	-2.97808
C	-2.59199	-0.26895	-0.54460
C	-3.37559	0.65721	-1.43820
C	-3.42196	-1.07057	0.41952
H	-2.82152	-1.59524	1.16315
H	-3.99220	-1.81946	-0.14850
H	-4.14764	-0.44008	0.94173
H	-2.74928	1.41867	-1.90712
H	-4.16066	1.16517	-0.87085
H	-3.86856	0.08379	-2.23483
C	2.43746	0.30785	0.26579
C	3.15742	-0.86211	0.65201
N	3.73030	-1.82354	0.96679
C	3.20047	1.32112	-0.39016
N	3.79698	2.15038	-0.94280

TS36-3

C	-1.01076	0.66250	0.57296
C	-0.24278	1.21400	-0.59603
C	-0.43604	0.18557	1.73173
C	0.83723	2.20045	-0.30941
C	0.87597	0.42025	2.24926
C	1.73044	2.19920	0.69828
C	1.82957	1.27906	1.80326
H	0.92233	3.00199	-1.04055
H	2.47832	2.99030	0.68605
H	2.74160	1.34745	2.39211
H	1.11115	-0.14081	3.15103
C	0.43126	-2.01626	-0.08159
H	-1.09365	-0.37340	2.39336
C	0.18297	-0.11053	-1.44409
H	-0.95066	1.71083	-1.26472
C	1.19470	-0.94325	-0.67467
C	-1.01166	-1.00668	-1.50421
H	0.51022	0.22776	-2.43006
C	-0.80461	-2.12176	-0.69290
H	0.81507	-2.72651	0.64017
H	-1.82848	-0.87048	-2.20153
H	-1.53705	-2.89575	-0.50088
C	2.53197	-0.76607	-0.60573
C	3.42938	-1.64365	0.22330
C	3.26526	0.25410	-1.43011
H	2.60307	0.90611	-2.00039
H	3.93546	-0.25843	-2.13334
H	3.89361	0.88749	-0.79409
H	2.88741	-2.31155	0.89419
H	4.09243	-1.02115	0.83496
H	4.07302	-2.25489	-0.42232
C	-2.32747	0.25968	0.20080
C	-3.07806	0.94071	-0.80212
N	-3.66911	1.47730	-1.64796
C	-3.04908	-0.68236	0.99108
N	-3.57999	-1.50140	1.62184

## TS37-1

C	-2.46391	4.15163	0.09939
C	-2.61877	2.77026	0.03591
C	-1.49245	1.95196	0.01315
C	-0.20457	2.53220	0.05418
C	-0.05476	3.91844	0.11609
C	-1.19027	4.72135	0.13889
C	-1.46760	0.50287	-0.04926
Au	-3.20158	-0.67983	-0.07008
P	-5.21458	-1.92856	-0.08147
C	0.85828	1.59215	0.02297
C	1.87883	0.89093	-0.00515
Au	3.61458	-0.13116	-0.05991
P	5.69737	-1.24892	-0.12894
C	-0.36319	-0.18647	-0.07165
C	0.24611	-1.52419	-0.05160
C	0.67836	-1.99209	1.33435
H	6.05141	-1.88347	-1.33218
H	5.90822	-2.29086	0.79063
H	6.83833	-0.46075	0.09968
H	-0.53671	-2.19159	-0.44472
H	1.06869	-1.58060	-0.77422
H	-6.40692	-1.20028	-0.23713
H	-5.51721	-2.68298	1.06569
H	-5.37082	-2.90187	-1.08405
H	1.08469	-3.00767	1.28632
H	1.44597	-1.33065	1.75212
H	-0.17251	-1.99239	2.02494
H	0.93863	4.35762	0.14621
H	-1.08271	5.80166	0.18755
H	-3.61257	2.32756	0.00313
H	-3.34180	4.79211	0.11767

## TS37-2

C	-2.60690	4.13470	0.04988
C	-2.69624	2.74920	-0.00690
C	-1.52601	1.98931	0.00824
C	-0.28687	2.65764	0.08478
C	-0.18675	4.04954	0.13647
C	-1.36553	4.78113	0.12024
C	-1.36615	0.54833	-0.04168
Au	-3.00713	-0.72590	-0.07438
P	-4.93123	-2.13129	-0.11082
C	0.74264	1.69543	0.07089
C	1.66629	0.85991	0.01474
Au	3.43650	-0.14183	-0.06777
P	5.55436	-1.17299	-0.16854
C	-0.10208	0.07221	-0.02612
C	0.31890	-1.36985	0.05145
C	0.67659	-1.83482	1.45862
H	6.12225	-1.33499	-1.44314
H	5.65982	-2.47608	0.34573
H	6.59620	-0.52455	0.51501
H	-0.55763	-1.93165	-0.30129
H	1.12407	-1.59556	-0.65942
H	-6.05783	-1.70898	0.61837
H	-4.79785	-3.44311	0.38038

H	-5.52776	-2.39455	-1.35766
H	0.91504	-2.90387	1.46279
H	1.54062	-1.29314	1.86454
H	-0.16521	-1.66762	2.14074
H	0.78054	4.54080	0.19093
H	-1.32569	5.86601	0.16357
H	-3.66471	2.25536	-0.06313
H	-3.51582	4.73100	0.03925

TS38-1

C	1.46587	0.93088	-0.63365
C	1.35974	-0.38745	0.13615
C	0.26872	-0.39754	1.29928
C	-1.02987	0.35375	1.01428
C	-0.75206	1.73113	0.37191
C	0.15528	1.69291	-0.87061
H	2.14708	1.54258	-0.02321
H	1.99330	0.73111	-1.57079
H	-1.52385	0.54139	1.98082
H	-1.70309	2.22043	0.12522
H	-0.27321	2.36033	1.13501
H	-0.37869	1.26046	-1.72077
H	0.39178	2.72233	-1.16677
H	0.85039	0.10540	2.08592
O	2.34206	-1.09572	0.30498
C	-1.98752	-0.55505	0.25121
H	-2.25324	-1.41661	0.86834
H	-2.90431	-0.04512	-0.06162
C	-1.34603	-1.14345	-1.10686
N	-0.07964	-1.55235	-0.75373
H	-2.01196	-1.98411	-1.37682
H	-1.41988	-0.33700	-1.85926
H	0.10195	-1.42007	1.64985

TS38-2

C	0.84495	1.30626	-0.66115
C	1.27799	-0.15558	0.06978
C	0.27364	-0.13584	1.39928
C	-1.18368	-0.09107	0.97056
C	-1.51798	1.26399	0.31719
C	-0.62967	1.57158	-0.90212
H	1.27840	1.99702	0.06233
H	1.44066	1.32627	-1.57410
H	-1.77798	-0.16596	1.89503
H	-2.57439	1.29436	0.02650
H	-1.37650	2.04831	1.07241
H	-0.99077	1.04645	-1.79075
H	-0.71665	2.63966	-1.14846
H	0.59966	0.73824	1.96251
O	2.48057	-0.02961	0.49983
C	-1.49236	-1.31756	0.10923
H	-1.44989	-2.21457	0.73832
H	-2.50409	-1.26896	-0.30950
C	-0.46575	-1.49195	-1.04729
N	0.90373	-1.21359	-0.72679
H	-0.51282	-2.51678	-1.43405
H	-0.76992	-0.85203	-1.89279
H	0.54075	-1.03906	1.94864

TS39-1

C	-0.80951	1.76649	0.25160
C	-1.28890	0.30050	0.21171
C	-0.53839	-0.49993	-0.96472
C	0.97409	-0.35367	-0.97093
C	1.34724	1.14795	-1.00586
C	0.69716	2.00979	0.09441
H	-1.35721	2.24926	-0.57085
H	-1.19508	2.20998	1.17380
H	1.33343	-0.80425	-1.90957
H	2.43868	1.25186	-0.97174
H	1.03603	1.53676	-1.98459
H	1.20153	1.85519	1.05137
H	0.86233	3.06608	-0.15095
H	-0.97819	-0.02520	-1.85398
O	-2.46921	0.03507	0.40161
C	1.60116	-1.19101	0.13146
H	1.32756	-2.23984	0.02046
H	2.69081	-1.09525	0.16201
C	1.14957	-0.74054	1.63914
N	-0.20515	-0.72441	1.50023
H	1.54009	-1.53534	2.29940
H	1.67169	0.21602	1.81685
F	-0.90848	-1.83694	-1.01305

TS39-2

C	0.13409	1.83361	0.04740
C	-1.03812	0.65350	0.26161
C	-0.56691	-0.39764	-0.99245
C	0.84200	-0.90458	-0.75850
C	1.85388	0.24157	-0.94479
C	1.59521	1.42383	0.00480
H	-0.19809	2.26459	-0.89837
H	-0.08941	2.54084	0.84695
H	1.01472	-1.63887	-1.55981
H	2.87073	-0.14225	-0.80857
H	1.78884	0.59252	-1.98318
H	1.98660	1.21763	1.00443
H	2.15899	2.29862	-0.34839
H	-0.70814	0.21781	-1.88214
O	-2.16255	1.16075	-0.08039
C	0.90891	-1.63476	0.58412
H	0.32734	-2.55940	0.51819
H	1.94043	-1.91469	0.82382
C	0.32079	-0.77548	1.74315
N	-0.87695	-0.05561	1.43053
H	0.10569	-1.42080	2.60192
H	1.09553	-0.07051	2.08763
F	-1.46147	-1.43584	-1.04945

TS40-1

C	-1.07065	0.20749	1.45758
C	-1.06284	-0.72672	0.23716
C	-0.51149	-0.02389	-1.09341
C	0.75117	0.80291	-0.88903
C	0.58039	1.79497	0.28406
C	0.12937	1.15436	1.61001

H	-1.99337	0.78888	1.33306
H	-1.21189	-0.40983	2.34915
H	0.89816	1.39109	-1.80663
H	1.51806	2.34525	0.43228
H	-0.16740	2.53366	-0.02508
H	0.96262	0.63072	2.08637
H	-0.14344	1.95527	2.30787
O	-1.97275	-1.53077	0.06910
C	1.95221	-0.12829	-0.81123
H	2.07722	-0.68987	-1.73810
H	2.87489	0.41554	-0.58748
C	1.90790	-1.23011	0.40481
N	0.65696	-1.71987	0.18466
H	2.73402	-1.92632	0.17759
H	2.10419	-0.66712	1.33248
H	-0.43254	-0.76165	-1.89371
F	-1.56595	0.84169	-1.44587

TS40-2

C	0.82210	-0.31093	1.44792
C	1.02767	0.73325	0.12333
C	0.46080	-0.27488	-1.11290
C	-0.98668	-0.65904	-0.86919
C	-1.11807	-1.57761	0.36350
C	-0.53799	-0.95032	1.64410
H	1.59669	-1.03786	1.20844
H	1.13923	0.30466	2.28914
H	-1.29043	-1.24289	-1.75104
H	-2.17247	-1.83404	0.51353
H	-0.59077	-2.51262	0.14864
H	-1.24694	-0.25730	2.10408
H	-0.39096	-1.74526	2.38982
O	2.28538	0.87914	-0.03241
C	-1.82532	0.61951	-0.82523
H	-1.82730	1.08497	-1.81779
H	-2.86847	0.39124	-0.57928
C	-1.26210	1.65060	0.19244
N	0.16363	1.79896	0.17410
H	-1.70054	2.63586	-0.00298
H	-1.59848	1.37768	1.20545
H	0.64307	0.30676	-2.01593
F	1.26626	-1.38672	-1.15948

TS41-1

C	1.41966	0.18292	-0.69817
C	0.81220	-0.97656	0.11533
C	-0.11730	-0.50814	1.31319
C	-1.03015	0.68193	1.02567
C	-0.26787	1.81913	0.30813
C	0.52031	1.38363	-0.94169
H	1.84954	-0.21722	-1.61973
H	-1.36884	1.08091	1.99497
H	-0.96682	2.62121	0.04032
H	0.43872	2.25197	1.02574
H	-0.14690	1.15769	-1.77788
H	1.15596	2.21062	-1.27850
H	0.65670	-0.24472	2.04797
O	1.43088	-2.01901	0.25380

C	-2.29783	0.20058	0.33408
H	-2.83162	-0.50993	0.96896
H	-2.97431	1.01533	0.05756
C	-1.99470	-0.56545	-1.06329
N	-0.97034	-1.42279	-0.75656
H	-2.94305	-1.07919	-1.30302
H	-1.78656	0.23298	-1.80001
H	-0.65402	-1.37054	1.71727
F	2.51674	0.62826	0.09248

TS41-2

C	1.26610	0.30909	-0.73106
C	0.58931	-1.05899	0.03864
C	-0.05668	-0.32190	1.38919
C	-1.12107	0.68218	0.98062
C	-0.49563	1.88182	0.24322
C	0.32925	1.46439	-0.99050
H	1.72848	-0.12025	-1.61913
H	-1.54748	1.06440	1.92188
H	-1.27544	2.58815	-0.06222
H	0.15825	2.41482	0.94270
H	-0.31336	1.22559	-1.84054
H	0.95619	2.30414	-1.31575
H	0.80855	0.11119	1.88808
O	1.55658	-1.78900	0.44300
C	-2.23047	-0.04169	0.21567
H	-2.74875	-0.72252	0.90130
H	-2.98082	0.66172	-0.16263
C	-1.66780	-0.88063	-0.96586
N	-0.42654	-1.56346	-0.73510
H	-2.40336	-1.63404	-1.27287
H	-1.55624	-0.22648	-1.84741
H	-0.44372	-1.15618	1.97396
F	2.27475	0.72666	0.11275

TS42-1

C	0.85521	-0.26026	-0.57871
C	0.35932	0.88800	0.03488
C	0.16927	0.84779	1.54477
C	-0.61766	-0.43566	1.95541
C	-0.80633	-1.25079	0.67214
C	0.59796	-1.58289	0.10663
H	1.16856	0.85302	1.99613
H	1.17762	-0.21370	-1.61242
H	-0.07475	-1.02011	2.70239
H	-1.58098	-0.17258	2.39974
H	1.33305	-1.81403	0.88224
H	0.60107	-2.40645	-0.60946
H	-0.32559	1.75972	1.88825
C	0.43383	2.22501	-0.64600
H	1.30483	2.77359	-0.26641
H	0.53787	2.13739	-1.73073
H	-0.44409	2.83763	-0.41980
H	-1.46581	-2.11340	0.81421
C	-1.29912	-0.28254	-0.42595
C	-2.39050	0.72038	-0.11119
H	-3.31833	0.14019	0.00093
H	-2.25108	1.28617	0.80835

H	-2.54761	1.41623	-0.93912
C	-1.49917	-0.84337	-1.82754
H	-2.51696	-1.25205	-1.87248
H	-1.44408	-0.05502	-2.58395
H	-0.81326	-1.64481	-2.10139
N	3.46868	-0.26456	-0.37344
H	3.82933	-0.20583	0.57708
H	3.85090	-1.11839	-0.77678
H	3.88166	0.51035	-0.88937

TS42-2

C	-0.88361	0.28364	0.89727
C	0.02994	0.79879	-0.09232
C	-0.54711	0.02830	-1.41498
C	-0.16839	-1.45604	-1.22394
C	0.52334	-1.45284	0.16174
C	-0.59190	-1.13508	1.17975
H	-1.61172	0.21359	-1.54331
H	-1.61537	0.86942	1.44092
H	-1.04148	-2.11374	-1.23663
H	0.50620	-1.80278	-2.00930
H	-1.48407	-1.77073	1.16036
H	-0.23196	-1.17951	2.22146
H	-0.01363	0.51414	-2.23608
C	0.16323	2.30351	-0.25668
H	-0.80357	2.76424	-0.48288
H	0.55474	2.76964	0.65228
H	0.84348	2.54352	-1.07782
H	1.09318	-2.35369	0.39531
C	1.33599	-0.12046	0.16400
C	2.38614	-0.00001	-0.95015
H	3.18396	-0.72644	-0.76154
H	2.00954	-0.18651	-1.95619
H	2.84752	0.99178	-0.94180
C	2.04160	0.21088	1.49396
H	2.83633	-0.51775	1.68192
H	2.51462	1.19582	1.43963
H	1.38717	0.21639	2.36975
N	-3.55597	0.18315	0.13244
H	-3.83066	-0.57851	-0.48620
H	-4.09412	0.06242	0.98990
H	-3.89376	1.04253	-0.29881

TS43-1

C	1.10519	-2.30821	-0.38521
C	2.03584	-1.68419	0.50836
C	3.38767	-2.12429	0.54088
C	3.76105	-3.14895	-0.30119
C	2.81583	-3.74439	-1.17450
C	1.47901	-3.34206	-1.23117
C	-0.02201	-0.71465	0.70941
C	1.36256	-0.67585	1.20362
H	4.10425	-1.65586	1.20752
H	4.78457	-3.50730	-0.30675
H	3.14406	-4.54818	-1.82706
H	0.77806	-3.81700	-1.90917
H	-0.96008	-1.88207	-0.76338
N	-0.13196	-1.71439	-0.20573



S	-1.23859	0.27504	1.31220
O	-0.76291	2.10701	-0.31130
C	-2.71477	-0.22542	0.43773
C	-2.82312	-0.07132	-0.95264
C	-3.77856	-0.69978	1.21745
C	-4.01740	-0.44408	-1.56821
H	-2.01320	0.37929	-1.51508
C	-4.96413	-1.06227	0.57951
H	-3.68393	-0.78919	2.29538
C	-5.08120	-0.93957	-0.80742
H	-4.12397	-0.32375	-2.64190
H	-5.79586	-1.43559	1.16849
H	-6.01038	-1.21625	-1.29609
C	1.88832	0.23999	2.24704
H	2.79832	-0.16173	2.69851
H	2.13182	1.21303	1.80150
H	1.15488	0.42035	3.04033
C	0.45688	1.94635	-0.59657
O	1.00950	0.84635	-0.86040
C	1.37176	3.19223	-0.49590
F	2.38971	3.11494	-1.35940
F	0.70144	4.32524	-0.70630
F	1.89577	3.24163	0.76336

TS43-2

C	-0.55512	2.31562	-0.47714
C	-1.60370	1.92468	0.41173
C	-2.81188	2.66145	0.45744
C	-2.93521	3.76482	-0.36514
C	-1.88088	4.12922	-1.23372
C	-0.67848	3.41773	-1.30881
C	0.18891	0.46500	0.57537
C	-1.18554	0.77004	1.09438
H	-3.61764	2.36210	1.12000
H	-3.84483	4.35505	-0.35661
H	-2.00940	4.99746	-1.87364
H	0.11072	3.72025	-1.98861
H	1.39125	1.46607	-0.81746
N	0.51575	1.44691	-0.30916
S	1.34383	-0.43262	1.49323
O	0.14555	-2.55500	-0.43595
C	2.84468	-0.24101	0.51318
C	3.06329	-1.08511	-0.58356
C	3.80620	0.68832	0.93242
C	4.26696	-0.97173	-1.28154
H	2.31051	-1.81243	-0.86896
C	5.00511	0.78041	0.22472
H	3.62654	1.31681	1.79935
C	5.23280	-0.04574	-0.87913
H	4.45243	-1.61899	-2.13329
H	5.76140	1.49223	0.54103
H	6.17029	0.02707	-1.42222
C	-1.85816	0.06817	2.21163
H	-1.80757	0.70093	3.10910
H	-2.91446	-0.09592	1.98023
H	-1.39931	-0.89424	2.44144
C	-0.90029	-1.94210	-0.46076
O	-1.05712	-0.62878	-0.48313

C	-2.26700	-2.67925	-0.46933
F	-3.06775	-2.20023	-1.43050
F	-2.10844	-3.98674	-0.63803
F	-2.87258	-2.46587	0.72679

TS44-1

C	1.17814	-2.30267	-0.39354
C	2.09599	-1.65351	0.49783
C	3.45820	-2.06529	0.53421
C	3.85141	-3.08795	-0.29920
C	2.91737	-3.71039	-1.16692
C	1.57223	-3.33688	-1.22862
C	0.01301	-0.74272	0.70561
C	1.40150	-0.66480	1.19396
H	4.16193	-1.57657	1.19873
H	4.88125	-3.42688	-0.30181
H	3.26187	-4.51428	-1.81028
H	0.88097	-3.83526	-1.89870
H	-0.90113	-1.94441	-0.75796
N	-0.06938	-1.73159	-0.22077
S	-1.22658	0.19867	1.33036
O	-0.84102	2.12614	-0.22635
C	-2.68709	-0.32029	0.44560
C	-2.77736	-0.19213	-0.94873
C	-3.76037	-0.78267	1.21937
C	-3.96197	-0.57727	-1.57381
H	-1.95890	0.24123	-1.51177
C	-4.93617	-1.15916	0.57186
H	-3.67885	-0.85388	2.29914
C	-5.03487	-1.06136	-0.81837
H	-4.05284	-0.47862	-2.65089
H	-5.77426	-1.52552	1.15575
H	-5.95625	-1.35000	-1.31451
C	1.90864	0.27592	2.22295
H	2.82823	-0.09762	2.67853
H	2.13165	1.24530	1.75938
H	1.17003	0.45584	3.01056
C	0.36562	1.99784	-0.57692
O	0.94056	0.93023	-0.89979
C	1.24414	3.27327	-0.49316
F	2.22834	3.25094	-1.40318
F	0.52942	4.39215	-0.66225
F	1.82340	3.33608	0.73875

TS44-2

C	-0.55571	2.31277	-0.51075
C	-1.57906	1.96256	0.42619
C	-2.78102	2.71359	0.48827
C	-2.92001	3.78756	-0.36670
C	-1.88985	4.11075	-1.28238
C	-0.69662	3.38592	-1.37468
C	0.20824	0.50383	0.58611
C	-1.15226	0.83383	1.13098
H	-3.56241	2.44432	1.19144
H	-3.82091	4.39025	-0.34898
H	-2.03186	4.95840	-1.94620
H	0.07167	3.65341	-2.09087
H	1.37278	1.44895	-0.88351

N	0.51088	1.43921	-0.35105
S	1.36595	-0.36580	1.51621
O	0.12100	-2.59621	-0.29802
C	2.85515	-0.22632	0.51454
C	3.01798	-1.06149	-0.59785
C	3.86111	0.65560	0.92899
C	4.21077	-0.98556	-1.31898
H	2.23209	-1.75601	-0.87617
C	5.04915	0.70953	0.19945
H	3.72190	1.28018	1.80560
C	5.22133	-0.10617	-0.92204
H	4.35231	-1.62532	-2.18463
H	5.83863	1.38681	0.51016
H	6.14944	-0.06112	-1.48392
C	-1.82571	0.13726	2.24912
H	-1.94013	0.82984	3.09317
H	-2.82975	-0.17168	1.94049
H	-1.28066	-0.74424	2.58878
C	-0.91459	-1.96354	-0.39897
O	-1.07095	-0.66631	-0.46065
C	-2.28274	-2.69956	-0.46815
F	-3.01504	-2.26717	-1.50766
F	-2.12270	-4.01903	-0.57445
F	-2.98023	-2.44476	0.66578

TS45-1

C	1.33663	-2.26497	-0.39442
C	2.20887	-1.55476	0.49901
C	3.60018	-1.86470	0.52792
C	4.06248	-2.85071	-0.31263
C	3.17128	-3.53562	-1.18036
C	1.80171	-3.26182	-1.23665
C	0.06243	-0.81160	0.72421
C	1.44572	-0.63451	1.21001
H	4.26844	-1.33098	1.19454
H	5.11377	-3.11463	-0.32180
H	3.57054	-4.30793	-1.83045
H	1.14528	-3.80254	-1.90824
H	-0.77038	-2.10768	-0.71445
N	0.05251	-1.78412	-0.21975
S	-1.21788	0.07010	1.34239
O	-0.97534	2.10459	-0.11298
C	-2.65066	-0.48637	0.44341
C	-2.71350	-0.39829	-0.95556
C	-3.73478	-0.93701	1.20910
C	-3.88034	-0.81349	-1.59308
H	-1.88357	0.01344	-1.51834
C	-4.89265	-1.34516	0.54880
H	-3.67304	-0.97849	2.29152
C	-4.96368	-1.28755	-0.84537
H	-3.94787	-0.75172	-2.67440
H	-5.73772	-1.70557	1.12617
H	-5.87057	-1.60243	-1.35201
C	1.88215	0.33082	2.24736
H	2.84749	0.04111	2.66664
H	1.99077	1.32967	1.80591
H	1.15221	0.41110	3.05936
C	0.20681	2.04154	-0.55850

O	0.81657	1.03024	-0.96455
C	1.01289	3.36810	-0.49247
F	1.95424	3.42631	-1.44945
F	0.22695	4.45131	-0.61330
F	1.64659	3.45923	0.70842

TS45-2

C	-0.49842	2.32845	-0.56142
C	-1.50544	2.09573	0.43628
C	-2.65265	2.93806	0.50150
C	-2.75337	3.96642	-0.40844
C	-1.74038	4.16650	-1.38053
C	-0.60089	3.35893	-1.47795
C	0.18750	0.53788	0.60155
C	-1.12823	0.98942	1.18469
H	-3.41972	2.76667	1.24850
H	-3.60887	4.63156	-0.39229
H	-1.85251	4.98546	-2.08436
H	0.15563	3.53675	-2.23306
H	1.36090	1.33977	-0.94176
N	0.51006	1.39467	-0.39438
S	1.30354	-0.39584	1.50306
O	0.08719	-2.55438	-0.44293
C	2.80794	-0.28644	0.51896
C	2.94629	-1.06104	-0.63950
C	3.84709	0.52178	0.99617
C	4.15093	-0.99801	-1.34232
H	2.12955	-1.69541	-0.96741
C	5.04573	0.56288	0.28357
H	3.72199	1.10582	1.90200
C	5.19556	-0.19199	-0.88283
H	4.27294	-1.58807	-2.24546
H	5.85933	1.18649	0.64068
H	6.13103	-0.15454	-1.43289
C	-1.80912	0.36106	2.33486
H	-2.59835	1.00447	2.72615
H	-2.25975	-0.58588	2.01224
H	-1.10234	0.12724	3.13868
C	-0.98186	-1.95312	-0.45303
O	-1.21039	-0.68554	-0.44881
C	-2.30492	-2.77418	-0.43728
F	-3.17573	-2.33345	-1.36358
F	-2.08728	-4.07788	-0.65375
F	-2.89987	-2.64913	0.77611

TS46-1

C	1.36279	-2.25732	-0.39413
C	2.22875	-1.53563	0.49672
C	3.62388	-1.82931	0.52320
C	4.09544	-2.81149	-0.31644
C	3.21005	-3.50864	-1.18071
C	1.83725	-3.25085	-1.23499
C	0.07386	-0.81950	0.72711
C	1.45626	-0.62545	1.20977
H	4.28702	-1.28692	1.18795
H	5.14956	-3.06372	-0.32735
H	3.61685	-4.27787	-1.82976
H	1.18558	-3.80072	-1.90374

H	-0.74705	-2.13119	-0.70457
N	0.07395	-1.79021	-0.21848
S	-1.21417	0.04818	1.34770
O	-1.00075	2.10293	-0.08656
C	-2.64081	-0.51635	0.44484
C	-2.69866	-0.43113	-0.95461
C	-3.72566	-0.97072	1.20730
C	-3.86102	-0.85293	-1.59576
H	-1.86758	-0.01888	-1.51548
C	-4.87904	-1.38555	0.54331
H	-3.66741	-1.01070	2.28994
C	-4.94500	-1.33075	-0.85122
H	-3.92434	-0.79438	-2.67751
H	-5.72437	-1.74943	1.11812
H	-5.84823	-1.65136	-1.36081
C	1.88286	0.34573	2.24553
H	2.85637	0.07251	2.65678
H	1.96999	1.34739	1.80564
H	1.15761	0.41051	3.06316
C	0.17403	2.05094	-0.55275
O	0.78592	1.04867	-0.97584
C	0.96930	3.38482	-0.49310
F	1.89113	3.45901	-1.46833
F	0.17153	4.46232	-0.59146
F	1.62599	3.47503	0.69520

TS46-2

C	-0.49324	2.32959	-0.56618
C	-1.50050	2.10459	0.43419
C	-2.64141	2.95631	0.50197
C	-2.73584	3.98509	-0.40737
C	-1.72248	4.17777	-1.38138
C	-0.58964	3.36182	-1.48173
C	0.18028	0.53285	0.59445
C	-1.13001	0.99738	1.18249
H	-3.40798	2.79060	1.25066
H	-3.58595	4.65702	-0.38962
H	-1.82966	4.99798	-2.08447
H	0.16696	3.53466	-2.23780
H	1.35806	1.32958	-0.94960
N	0.50715	1.38785	-0.40262
S	1.29618	-0.39708	1.50192
O	0.08493	-2.56789	-0.43853
C	2.80269	-0.29098	0.52072
C	2.94617	-1.07230	-0.63262
C	3.83863	0.52300	0.99517
C	4.15238	-1.01069	-1.33286
H	2.13146	-1.70974	-0.95947
C	5.03902	0.56266	0.28539
H	3.70921	1.11329	1.89631
C	5.19382	-0.19918	-0.87581
H	4.27792	-1.60548	-2.23243
H	5.84982	1.19115	0.64030
H	6.13041	-0.16240	-1.42405
C	-1.81379	0.37230	2.33244
H	-2.60416	1.01643	2.72006
H	-2.26222	-0.57630	2.01158
H	-1.10848	0.14170	3.13858

C	-0.98091	-1.96079	-0.45125
O	-1.20436	-0.69275	-0.44940
C	-2.30782	-2.77582	-0.43657
F	-3.17510	-2.33323	-1.36558
F	-2.09559	-4.08130	-0.65109
F	-2.90521	-2.64732	0.77496

TS47-1

C	1.37610	-2.25308	-0.39421
C	2.23875	-1.52589	0.49565
C	3.63572	-1.81143	0.52104
C	4.11207	-2.79138	-0.31837
C	3.22979	-3.49429	-1.18134
C	1.85544	-3.24452	-1.23471
C	0.07973	-0.82331	0.72846
C	1.46159	-0.62081	1.20969
H	4.29612	-1.26497	1.18517
H	5.16755	-3.03776	-0.33002
H	3.64047	-4.26169	-1.83009
H	1.20638	-3.79869	-1.90241
H	-0.73498	-2.14234	-0.70012
N	0.08489	-1.79300	-0.21802
S	-1.21222	0.03704	1.35044
O	-1.01356	2.10211	-0.07327
C	-2.63577	-0.53160	0.44563
C	-2.69152	-0.44670	-0.95397
C	-3.72056	-0.98896	1.20638
C	-3.85160	-0.87178	-1.59697
H	-1.86020	-0.03323	-1.51370
C	-4.87166	-1.40708	0.54051
H	-3.66375	-1.02907	2.28909
C	-4.93548	-1.35257	-0.85414
H	-3.91312	-0.81396	-2.67887
H	-5.71680	-1.77354	1.11395
H	-5.83686	-1.67601	-1.36521
C	1.88314	0.35340	2.24458
H	2.86122	0.08941	2.65093
H	1.95808	1.35652	1.80574
H	1.16100	0.40956	3.06563
C	0.15724	2.05551	-0.55002
O	0.76972	1.05771	-0.98188
C	0.94728	3.39287	-0.49328
F	1.86071	3.47413	-1.47606
F	0.14412	4.46751	-0.58233
F	1.61353	3.48339	0.68957

TS47-2

C	-0.48946	2.33023	-0.56842
C	-1.49723	2.10933	0.43290
C	-2.63446	2.96634	0.50192
C	-2.72491	3.99568	-0.40679
C	-1.71099	4.18445	-1.38139
C	-0.58194	3.36371	-1.48314
C	0.17669	0.52987	0.59086
C	-1.13081	1.00132	1.18104
H	-3.40107	2.80370	1.25119
H	-3.57191	4.67148	-0.38823
H	-1.81498	5.00561	-2.08383

H	0.17506	3.53396	-2.23936
H	1.35739	1.32366	-0.95314
N	0.50632	1.38395	-0.40659
S	1.29211	-0.39859	1.50145
O	0.08276	-2.57456	-0.43666
C	2.79977	-0.29442	0.52181
C	2.94570	-1.07916	-0.62892
C	3.83420	0.52238	0.99473
C	4.15266	-1.01843	-1.32792
H	2.13191	-1.71804	-0.95519
C	5.03543	0.56117	0.28631
H	3.70273	1.11585	1.89348
C	5.19261	-0.20425	-0.87221
H	4.27987	-1.61565	-2.22565
H	5.84491	1.19205	0.64002
H	6.12973	-0.16792	-1.41958
C	-1.81640	0.37827	2.33089
H	-2.60838	1.02226	2.71535
H	-2.26233	-0.57205	2.01168
H	-1.11221	0.15113	3.13906
C	-0.98125	-1.96422	-0.45054
O	-1.20169	-0.69581	-0.44971
C	-2.31038	-2.77571	-0.43636
F	-3.17589	-2.33161	-1.36642
F	-2.10136	-4.08206	-0.65028
F	-2.90862	-2.64552	0.77441

#### TS48-1

C	1.17268	0.81063	-0.36918
C	1.17268	-0.81063	-0.36918
C	0.00000	-1.37863	0.28448
C	-1.17268	-0.81063	-0.36918
C	-1.17268	0.81063	-0.36918
C	0.00000	1.37863	0.28448
H	0.00000	-2.38911	0.66703
H	-2.15347	-1.26447	-0.27872
H	2.15347	-1.26447	-0.27872
H	2.15347	1.26447	-0.27872
C	0.76097	-0.00000	-1.57902
H	1.34013	-0.00000	-2.49651
C	-0.76097	0.00000	-1.57902
H	-1.34013	0.00000	-2.49651
H	0.00000	2.38911	0.66703
N	0.00000	-0.57932	2.08347
N	0.00000	0.57932	2.08347
H	-2.15347	1.26447	-0.27872

#### TS48-2

C	0.38862	1.14571	-0.70511
C	1.93310	1.14265	0.72259
C	1.94222	-0.00310	1.51063
C	1.93152	-1.14614	0.71874
C	0.38697	-1.14218	-0.70908
C	-0.40130	0.00223	-0.65431
H	1.88743	-0.00489	2.59498
H	1.96589	-2.16969	1.07198
H	1.96897	2.16496	1.07928
H	0.03294	2.16902	-0.71054

C	1.84545	0.78499	-0.73260
H	2.50372	1.29225	-1.44337
C	1.84433	-0.78347	-0.73524
H	2.50189	-1.28926	-1.44771
H	-1.47797	0.00276	-0.51550
N	-4.38131	0.00064	0.07359
N	-5.42414	-0.00127	0.43999
H	0.02982	-2.16497	-0.71795

TS49-1

C	-1.51279	0.31952	-1.08005
C	-1.10075	-0.99286	-0.75672
C	-1.98993	-1.75993	0.03583
C	-3.22035	-1.25517	0.44882
C	-3.62910	0.04821	0.11108
C	-2.74873	0.82039	-0.65618
S	0.45023	-1.61767	-1.28086
C	1.88708	-0.24972	0.38815
Cl	2.03571	-1.52835	1.63657
C	1.18183	0.87530	0.77096
C	1.15568	2.17529	0.13820
O	1.78808	2.51418	-0.87267
C	0.28688	3.23088	0.83613
Cl	3.32424	-0.15352	-0.61988
H	0.94322	3.94828	1.34483
H	-0.27722	3.78289	0.07815
H	-0.40644	2.80780	1.56899
H	0.50163	0.72585	1.60146
H	-1.69233	-2.76653	0.31560
H	-3.87820	-1.88226	1.05062
C	-4.96849	0.58627	0.56371
H	-3.03227	1.83502	-0.93351
H	-0.85665	0.93332	-1.68898
H	-5.11636	1.61651	0.22230
H	-5.05888	0.58491	1.65838
H	-5.80199	-0.01380	0.17396

TS49-2

C	-1.62273	0.68323	-1.01562
C	-1.22418	-0.62748	-0.71173
C	-2.11076	-1.45462	-0.00571
C	-3.37217	-0.98703	0.36794
C	-3.78153	0.31922	0.05888
C	-2.88465	1.14544	-0.63232
S	0.36372	-1.24049	-1.24201
C	1.53962	-0.50182	0.09479
Cl	1.31953	-1.78294	1.63377
C	1.31743	0.81746	0.58661
C	1.96936	2.02694	0.22577
O	2.88597	2.20306	-0.60896
C	1.46332	3.28161	0.96636
Cl	3.16541	-0.85176	-0.60856
H	2.30219	3.72377	1.51738
H	1.13517	4.02366	0.22843
H	0.64390	3.08276	1.66591
H	0.49734	0.88954	1.29122
H	-1.79555	-2.45873	0.25890
H	-4.04408	-1.64350	0.91793



C	-5.16060	0.81057	0.43912
H	-3.17355	2.16687	-0.87245
H	-0.93551	1.33312	-1.54644
H	-5.18861	1.90274	0.51317
H	-5.48043	0.39854	1.40271
H	-5.91079	0.51345	-0.30626

TS50-1

C	-1.04891	0.23419	-0.62373
C	-0.07348	1.34339	-0.69345
C	-0.01525	2.08623	0.50835
C	1.13030	0.95485	-1.28692
C	1.83090	-0.31861	0.00806
C	3.00238	-0.78251	-0.35537
C	0.85303	-0.35200	0.99282
C	0.65914	0.83562	1.74559
C	-0.43545	-0.88163	0.47599
F	-0.32682	-2.05145	-0.17123
F	-1.22501	-0.41813	-1.78540
H	1.94601	1.66793	-1.27193
F	-1.36894	-1.02855	1.43445
F	-2.26325	0.59937	-0.17391
H	3.48388	-0.46695	-1.27099
H	3.51496	-1.50870	0.26159
H	1.09288	0.31167	-2.15731
H	1.56051	1.32790	2.08905
H	-0.13793	0.80746	2.47823
H	0.73705	2.86524	0.54564
H	-0.95714	2.36712	0.96246

TS50-2

C	-1.11688	0.47143	-0.63017
C	-0.10420	1.43156	-0.47849
C	0.00265	2.00201	0.79892
C	1.17410	1.01563	-1.09939
C	1.78043	-0.16925	-0.21800
C	2.96525	-0.68414	-0.49605
C	0.87472	-0.50573	0.88685
C	0.74173	0.51096	1.84970
C	-0.33705	-1.06233	0.43915
F	-0.33410	-2.03098	-0.46880
F	-1.31790	-0.11087	-1.80861
H	1.89831	1.82830	-1.09303
F	-1.31397	-1.28932	1.31327
F	-2.29045	0.64849	-0.02993
H	3.55094	-0.31559	-1.32917
H	3.38124	-1.48798	0.09398
H	1.05206	0.64673	-2.11580
H	1.65836	0.98089	2.17918
H	-0.01204	0.38516	2.61730
H	0.80221	2.71738	0.93985
H	-0.90775	2.22837	1.33923

TS51-1

C	1.16194	-2.07482	0.31200
C	0.00181	-1.52354	0.78757
C	0.06779	-0.93407	2.15743
C	1.05794	0.32312	2.09862

C	1.33192	0.65681	0.66495
C	2.28464	-0.09654	0.06487
C	3.44396	-0.36483	-0.46744
C	0.21899	1.08873	-0.10255
H	1.99188	0.06224	2.58936
H	0.47271	-1.65318	2.86537
C	-0.89575	-0.89396	-0.11062
H	1.25514	-2.40965	-0.71026
H	0.60366	1.15804	2.62410
H	-0.90538	-0.60850	2.51115
H	3.69563	-1.34860	-0.83949
H	4.19160	0.41498	-0.55841
H	1.89133	-2.44153	1.02189
Cl	0.45999	1.46123	-1.77352
Cl	-0.90017	2.17979	0.65317
Cl	-0.89860	-1.39463	-1.76943
Cl	-2.49864	-0.49694	0.42314

TS51-2

C	-1.25269	-1.66193	0.70014
C	0.01029	-1.70629	-0.11208
C	-0.11887	-2.08547	-1.42200
C	-1.26300	-0.08774	-2.08172
C	-1.35777	0.35130	-0.78759
C	-2.13507	-0.52175	0.12481
C	-3.43231	-0.42617	0.36253
C	-0.32533	1.09659	-0.18483
H	-2.05465	-0.70110	-2.48485
H	-0.96579	-2.69636	-1.70242
C	1.02463	-0.81088	0.27880
H	-1.05444	-1.46837	1.75247
H	-0.57358	0.36883	-2.77859
H	0.70751	-2.03814	-2.11456
H	-3.94004	-1.15156	0.98606
H	-4.02018	0.38385	-0.04623
H	-1.80216	-2.59866	0.61934
Cl	-0.59456	1.76153	1.38688
Cl	0.70495	2.08158	-1.15676
Cl	1.41524	-0.59933	1.94804
Cl	2.40402	-0.59580	-0.73696

I-28

C	-2.10085	0.95862	0.19252
C	-1.37994	0.81313	-1.14152
C	-1.37124	1.04762	1.44255
C	-0.2925	1.7602	-1.46881
C	-0.07991	1.54891	1.67124
C	0.68089	2.23536	-0.64586
C	0.84565	2.02554	0.76085
O	-3.32444	0.78312	0.18492
H	-0.23944	2.05609	-2.51543
H	1.44792	2.85362	-1.11162
H	1.78466	2.38521	1.17768
H	0.23969	1.5462	2.71274
C	-0.80829	-1.48698	1.02223
H	-2.00889	0.88137	2.30643
C	-0.89992	-0.80684	-1.21189
H	-2.15855	0.87096	-1.90534

C	0.04915	-1.0603	-0.05313
C	-2.09287	-1.60509	-0.85728
H	-0.50382	-0.95253	-2.21723
C	-2.03845	-1.93296	0.47711
H	-0.49004	-1.66069	2.04114
H	-2.94347	-1.74855	-1.51195
H	-2.83572	-2.39616	1.04643
C	1.40012	-0.9058	-0.03392
C	2.23259	-1.2115	1.18536
C	2.19898	-0.58727	-1.27041
H	1.59143	-0.17602	-2.0774
H	2.69391	-1.49737	-1.64138
H	2.99212	0.13514	-1.04621
H	1.63909	-1.3486	2.09153
H	2.94659	-0.39964	1.36955
H	2.82556	-2.12482	1.02707

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C	-1.90949	0.44931	-0.71773
C	-0.86505	0.21712	-1.775
C	-1.61554	1.04098	0.58305
C	0.15305	1.19124	-2.099
C	-0.4917	1.80487	0.91292
C	0.82015	2.02824	-1.23998
C	0.59169	2.21994	0.14155
O	-3.02621	-0.04089	-0.94308
H	0.48244	1.19227	-3.13711
H	1.63508	2.61161	-1.66699
H	1.31505	2.85132	0.65432
H	-0.46557	2.14707	1.94741
C	-0.49703	-1.51657	1.03824
C	-0.09125	-1.425	-1.25949
H	-1.38362	-0.14011	-2.66354
C	0.52715	-1.15294	0.08511
C	-1.21825	-2.27752	-0.98825
H	0.54001	-1.62298	-2.12081
C	-1.48069	-2.26207	0.38409
H	-0.44814	-1.34856	2.1054
H	-1.84487	-2.73269	-1.74453
H	-2.34387	-2.71209	0.86018
C	1.78214	-0.69489	0.34098
C	2.29932	-0.49246	1.74153
C	2.81224	-0.49766	-0.73928
H	2.3787	-0.44223	-1.73861
H	3.5329	-1.32913	-0.72394
H	3.38511	0.421	-0.56881
H	1.52037	-0.5575	2.50303
H	2.77789	0.49022	1.82926
H	3.06941	-1.24102	1.97832
C	-2.75595	0.96568	1.57222
H	-3.53975	1.6897	1.31231
H	-3.22849	-0.01893	1.54593
H	-2.41725	1.18467	2.59031

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C	-1.79452	-1.65203	-0.14835
C	-1.40795	-1.06569	1.20165
C	-0.90664	-1.55477	-1.28986

C	-0.08673	-1.42971	1.76109
C	0.4946	-1.46782	-1.32311
C	1.10375	-1.52965	1.11731
C	1.40995	-1.39703	-0.28489
O	-2.96593	-2.02256	-0.28322
H	-0.07047	-1.58069	2.83962
H	1.97041	-1.72605	1.74996
H	0.92041	-1.43171	-2.32553
C	-1.52188	0.99968	-1.23835
H	-1.41338	-1.7767	-2.22509
C	-1.64158	0.59239	1.05877
H	-2.19445	-1.3721	1.89505
C	-0.72593	1.09892	-0.04447
C	-2.99643	0.76887	0.48591
H	-1.48504	1.00443	2.05629
C	-2.89236	0.94018	-0.87264
H	-1.16391	1.1829	-2.24237
H	-3.91386	0.60812	1.03834
H	-3.71982	0.95895	-1.57227
C	0.56173	1.52406	0.06928
C	1.35955	2.01574	-1.11065
C	1.25142	1.69991	1.39585
H	0.73073	1.21019	2.21931
H	1.34393	2.77041	1.63289
H	2.27191	1.29788	1.35907
H	0.88296	1.8132	-2.07133
H	2.35146	1.54688	-1.12132
H	1.52707	3.10023	-1.03709
C	2.88378	-1.30133	-0.61488
H	3.34007	-0.41548	-0.14946
H	3.43664	-2.17067	-0.2326
H	3.06051	-1.23895	-1.6929