

Supplementary Informations

A joint Experimental/Theoretical Investigation of the MMA Polymerization initiated by Yttrium phenoxyamine Complexes

Jian Fang,^{a,b} Mathieu J.-L. Tschan,^c E. Brulé,^{c,d} Carine Robert,^c Christophe M. Thomas^{c,*}
and Laurent Maron^{b,*}

Cartesian coordinates of all computed complexes:

YT1_NL.xyz	C	-2.757082	-4.271715	-1.105338
119	C	-8.738740	2.350412	-1.316601
scf done: -2165.526199	C	-7.372367	4.411380	-1.022908
C -3.917312 -5.585821 1.386234	C	-2.441539	2.597637	2.096806
C -4.616770 -4.586174 2.109086	C	-4.379628	4.053178	2.618823
C -5.899327 -4.896105 2.637783	C	-6.947821	-2.595505	2.893851
C -6.455819 -6.138289 2.305631	C	-7.950384	-4.510714	4.109660
C -5.817123 -7.105714 1.521085	C	-5.606042	-9.604367	1.720839
C -4.521359 -6.806542 1.093563	C	-7.880801	-8.592409	1.715817
O -4.040995 -3.402613 2.256369	H	0.089642	-4.641705	5.877284
Y -2.572598 -2.043453 1.483865	H	-1.068554	-4.654346	4.511399
O -1.379273 -2.361970 3.400013	H	0.784731	0.318792	1.778055
C -0.131361 -2.301291 3.652723	H	-1.246450	-3.451801	5.805354
O 0.391401 -3.158107 4.549118	H	-4.554283	-3.588896	-2.068332
C -0.522982 -4.024692 5.219123	H	-4.730572	-3.929398	-0.343079
C -6.625354 -3.930697 3.590660	H	-2.969131	-5.307132	-1.412678
C -5.725037 -3.662122 4.814654	H	-2.082803	-3.853919	-1.860146
C -6.458806 -8.451127 1.155746	H	-2.073021	-6.317760	0.626673
C -6.536292 -8.583859 -0.378166	H	-1.913213	-5.237372	2.016608
C -2.459387 -5.387581 1.075411	H	-5.925945	-1.744290	-1.190216
N -2.049712 -4.250862 0.193832	H	-5.539421	-2.056460	0.507509
C -0.601406 -4.390101 -0.028507	H	-5.746081	3.700397	0.694791
O -3.646490 -0.218473 1.588561	H	-6.713273	0.276387	-1.666436
C -4.511234 0.549936 0.927488	H	-7.443036	-6.363560	2.687869
C -4.704828 1.923324 1.239925	H	-3.949087	-7.543347	0.531517
C -5.607429 2.653664 0.457095	H	-4.000899	-1.383526	-2.762716
C -6.339683 2.116865 -0.606471	H	-3.212245	-0.272979	-1.620700
C -6.151441 0.758804 -0.868133	H	-2.355556	-1.723290	-2.175997
C -5.271313 -0.022969 -0.122916	H	-0.359886	-5.343774	-0.525253
C -3.951995 2.593412 2.400490	H	-0.234810	-3.567200	-0.642242
C -4.227053 1.836964 3.716247	H	-0.075208	-4.359194	0.929204
C -5.215699 -1.504504 -0.381745	H	-6.219767	-2.965251	5.502081
N -3.879827 -2.063353 -0.748161	H	-5.527911	-4.591783	5.360347
C -3.330447 -1.323382 -1.889895	H	-4.770867	-3.228302	4.509218
C -7.320547 2.938883 -1.453124	H	-7.507251	-1.941497	3.573477
C -6.892307 2.889984 -2.933206	H	-6.036321	-2.073514	2.600649
O -0.585614 -1.169720 0.662632	H	-7.567956	-2.758675	2.004763
C 0.151407 -0.445657 2.217572	H	-8.405054	-3.798056	4.806002
C 0.760397 -1.414271 3.028353	H	-8.672051	-4.684572	3.303560
C 2.251869 -1.578900 3.152558	H	-7.804924	-5.451621	4.651575
C 0.081825 -0.827934 -0.538812	H	-8.299390	-9.560420	1.420088
C 1.562706 -1.212051 -0.511115	H	-7.894758	-8.548259	2.809986
C -0.111570 0.644642 -0.903058	H	-8.548105	-7.812643	1.333498
C -4.062102 -3.488569 -1.085424	H	-6.986164	-9.543024	-0.661348

H	-7.146320	-7.782255	-0.808167	C	-6.243286	-8.917867	-0.121213
H	-5.544948	-8.533155	-0.840055	C	-2.485138	-5.301873	1.176271
H	-6.050452	-10.574062	1.466472	N	-2.196723	-4.183030	0.222158
H	-4.587803	-9.591267	1.319107	C	-0.756957	-4.238977	-0.083820
H	-5.534272	-9.537985	2.811443	O	-3.779842	-0.195586	1.681665
H	-1.880749	3.013069	2.943296	C	-4.540716	0.630371	0.966216
H	-2.082786	1.586285	1.902463	C	-4.669549	2.011439	1.278654
H	-2.227428	3.212406	1.215168	C	-5.441446	2.806558	0.422458
H	-3.821542	4.467210	3.465689	C	-6.114278	2.325335	-0.705796
H	-4.166725	4.683954	1.748717	C	-6.015525	0.954720	-0.952208
H	-5.446081	4.138707	2.854155	C	-5.260973	0.111231	-0.139587
H	-3.675722	2.302997	4.542153	C	-4.009066	2.613346	2.530186
H	-5.294224	1.872928	3.961773	C	-4.497716	1.863382	3.786468
H	-3.928608	0.790580	3.642826	C	-5.304966	-1.374123	-0.375930
H	-8.076437	4.957896	-1.659741	N	-4.008555	-2.022891	-0.738218
H	-7.711087	4.522037	0.012620	C	-3.464196	-1.379103	-1.938388
H	-6.395534	4.897985	-1.116936	C	-6.947877	3.219624	-1.633353
H	-7.588342	3.464354	-3.556280	C	-6.392586	3.133037	-3.068784
H	-5.890318	3.312517	-3.064047	O	-0.620025	-1.044562	0.758269
H	-6.873812	1.864440	-3.315479	C	0.159923	-0.603648	1.956440
H	-9.454511	2.921631	-1.919902	C	0.774463	-1.723802	2.703491
H	-8.778818	1.308859	-1.650620	C	2.265836	-1.888384	2.770671
H	-9.072896	2.377646	-0.274225	C	-0.179770	-0.532663	-0.515775
H	-0.816768	-0.057456	2.522407	C	1.266482	-0.910892	-0.822816
H	2.771750	-0.695861	2.768403	C	-0.442224	0.963209	-0.649631
H	2.637064	-2.451572	2.606972	C	-4.263513	-3.456383	-0.987745
H	2.549611	-1.703294	4.198465	C	-2.990083	-4.291424	-1.023500
H	-0.388320	-1.425554	-1.338745	C	-8.414755	2.745524	-1.628680
H	2.011750	-1.072247	-1.500510	C	-6.922420	4.692616	-1.202715
H	1.691529	-2.257265	-0.216895	C	-2.476432	2.508684	2.422346
H	2.125021	-0.596115	0.197000	C	-4.353857	4.098700	2.722069
H	0.303497	0.855816	-1.894890	C	-7.208772	-2.820521	2.798544
H	0.392716	1.302084	-0.187173	C	-8.105682	-4.745276	4.079683
H	-1.172252	0.908242	-0.905941	C	-5.249470	-9.739138	2.035222
YT1_NLb.xyz				C	-7.605595	-8.937189	1.961553
119				H	-0.004242	-4.994346	5.472301
scf done: -2165.534054				H	-1.459111	-4.524317	4.543550
C	-3.920584	-5.608489	1.506815	H	0.912598	0.112826	1.621605
C	-4.713201	-4.644429	2.179889	H	-0.809585	-3.431504	5.784642
C	-5.975790	-5.036797	2.700196	H	-4.806071	-3.590202	-1.939729
C	-6.415251	-6.338486	2.427101	H	-4.912618	-3.826202	-0.191067
C	-5.681101	-7.283763	1.702177	H	-3.262249	-5.338292	-1.217905
C	-4.413230	-6.890141	1.268853	H	-2.356968	-3.973084	-1.858148
O	-4.245432	-3.406641	2.286538	H	-2.023679	-6.216920	0.771212
Y	-2.763295	-2.058429	1.565667	H	-1.941551	-5.050240	2.096307
O	-1.409188	-2.426445	3.233611	H	-6.034164	-1.582942	-1.176400
C	-0.112209	-2.552084	3.329221	H	-5.659197	-1.887307	0.525314
O	0.358768	-3.601469	4.065150	H	-5.526312	3.860180	0.655283
C	-0.540317	-4.161877	5.012623	H	-6.551200	0.513094	-1.791166
C	-6.810131	-4.088173	3.578016	H	-7.385188	-6.629997	2.807846
C	-5.981830	-3.685801	4.815884	H	-3.772672	-7.598708	0.745786
C	-6.195747	-8.698643	1.403858	H	-4.171547	-1.449051	-2.781070
				H	-3.278142	-0.322651	-1.737774
				H	-2.528551	-1.854493	-2.241360

H	-0.482449	-5.199474	-0.548172
H	-0.488882	-3.431119	-0.767119
H	-0.173934	-4.114098	0.832456
H	-6.556417	-2.998028	5.447920
H	-5.731190	-4.567197	5.416590
H	-5.053897	-3.191383	4.522301
H	-7.847232	-2.181041	3.419749
H	-6.327484	-2.243713	2.516217
H	-7.772279	-3.077381	1.893973
H	-8.642760	-4.035903	4.718206
H	-8.777319	-5.018842	3.258102
H	-7.910616	-5.641613	4.678493
H	-7.934376	-9.952265	1.713625
H	-7.635030	-8.838990	3.051883
H	-8.335215	-8.240270	1.535494
H	-6.599600	-9.928207	-0.355091
H	-6.919752	-8.200325	-0.597818
H	-5.255385	-8.800081	-0.578188
H	-5.602803	-10.756708	1.829914
H	-4.231989	-9.655872	1.640107
H	-5.196116	-9.609417	3.121133
H	-2.002266	2.903133	3.329397
H	-2.166798	1.470848	2.294081
H	-2.108572	3.090285	1.569356
H	-3.873125	4.462608	3.636588
H	-3.993230	4.720485	1.895050
H	-5.431678	4.260902	2.831229
H	-4.021653	2.278742	4.683014
H	-5.582106	1.970704	3.900161
H	-4.261770	0.799879	3.728610
H	-7.520675	5.291621	-1.897803
H	-7.343801	4.831757	-0.201560
H	-5.905575	5.099862	-1.205334
H	-6.980659	3.760169	-3.749476
H	-5.352255	3.473660	-3.105759
H	-6.421838	2.108485	-3.453228
H	-9.024040	3.368115	-2.294837
H	-8.507102	1.708508	-1.966554
H	-8.840677	2.805312	-0.621730
H	-0.575439	-0.058549	2.559512
H	2.770122	-0.959727	3.072200
H	2.709077	-2.189133	1.808733
H	2.531268	-2.655093	3.501702
H	-0.821084	-1.056237	-1.232725
H	1.496623	-0.662276	-1.864060
H	1.431984	-1.981479	-0.677290
H	1.978245	-0.370172	-0.192703
H	-0.217065	1.292373	-1.669746
H	0.186192	1.546409	0.030617
H	-1.487011	1.198465	-0.431298

YT1_NLf.xyz
119

scf done: -2165.555928		
C	-3.772368	-5.649943 1.074096
C	-4.164720	-4.650913 2.003883
C	-5.370318	-4.844012 2.736616
C	-6.145427	-5.970871 2.432872
C	-5.801066	-6.936448 1.479813
C	-4.581936	-6.754832 0.822444
O	-3.385279	-3.589372 2.153778
Y	-2.357152	-2.129002 0.843580
O	-0.926105	-1.994095 2.784515
C	-0.438290	-2.019177 3.913591
O	-0.248252	-3.143594 4.589624
C	-0.653015	-4.370780 3.957529
C	-5.799570	-3.867992 3.846479
C	-4.679041	-3.759202 4.900906
C	-6.674641	-8.159639 1.169974
C	-7.045701	-8.164147 -0.326354
C	-2.410344	-5.560194 0.445691
N	-2.134000	-4.413541 -0.465186
C	-0.748610	-4.557446 -0.940655
O	-3.507374	-0.365205 1.198877
C	-4.452083	0.406658 0.673161
C	-4.564307	1.792061 0.973844
C	-5.588332	2.519823 0.356888
C	-6.510557	1.972068 -0.540957
C	-6.378505	0.609378 -0.814325
C	-5.385899	-0.169344 -0.224021
C	-3.592105	2.471749 1.950092
C	-3.677504	1.788593 3.330051
C	-5.364426	-1.650304 -0.483199
N	-4.089182	-2.204618 -1.026879
C	-3.653765	-1.436312 -2.202312
C	-7.623640	2.791338 -1.207950
C	-7.442003	2.758807 -2.738408
O	-0.743561	-1.520434 -0.308921
C	-0.068882	0.362070 4.049210
C	0.018657	-0.823240 4.666506
C	0.551995	-1.012087 6.058004
C	0.422413	-1.105467 -0.939747
C	1.602147	-1.103564 0.036051
C	0.236425	0.269883 -1.584328
C	-4.328489	-3.617885 -1.373999
C	-3.047901	-4.399402 -1.625969
C	-8.996431	2.189884 -0.847448
C	-7.617349	4.259251 -0.759283
C	-2.157036	2.377180 1.395214
C	-3.904305	3.961888 2.156442
C	-6.088686	-2.471602 3.264011
C	-7.069819	-4.334266 4.576081
C	-5.895560	-9.448187 1.501287
C	-7.977598	-8.168679 1.980935
H	-0.627776	-5.122815 4.745076
H	0.065202	-4.627805 3.173189
H	0.250978	1.273972 4.544172

H	-1.654275	-4.270761	3.531051	H	-9.155734	2.204282	0.235843
H	-4.968726	-3.686152	-2.271103	H	-0.466994	0.444846	3.044440
H	-4.877306	-4.080037	-0.549556	H	0.848107	-0.051499	6.485438
H	-3.312833	-5.426609	-1.923367	H	1.420612	-1.678181	6.064336
H	-2.508762	-3.959651	-2.470445	H	-0.199784	-1.465678	6.711882
H	-2.211601	-6.495455	-0.105287	H	0.677148	-1.815839	-1.754034
H	-1.654418	-5.491622	1.238662	H	2.536620	-0.819974	-0.462009
H	-6.178756	-1.893850	-1.185522	H	1.734249	-2.097668	0.475955
H	-5.564736	-2.201792	0.443863	H	1.414890	-0.395052	0.850692
H	-5.668687	3.573498	0.591798	H	1.136509	0.585359	-2.125024
H	-7.070877	0.122004	-1.499146	H	0.010834	1.018463	-0.817122
H	-7.070120	-6.104523	2.978924	H	-0.599657	0.250055	-2.290179
H	-4.235273	-7.493169	0.100447				
H	-4.400200	-1.490403	-3.011534				
H	-3.521364	-0.390866	-1.920494	YT1_NR.xyz			
H	-2.697097	-1.812108	-2.568058	119			
H	-0.612985	-5.491847	-1.510194	scf done: -2165.526797			
H	-0.480210	-3.702597	-1.561232	C	-5.758824	-4.873064	2.639197
H	-0.065960	-4.575610	-0.086611	C	-4.490258	-4.528411	2.099328
H	-4.980765	-3.076015	5.704114	C	-3.790864	-5.492895	1.331254
H	-4.472546	-4.737682	5.349603	C	-4.379039	-6.715648	1.016476
H	-3.761761	-3.379017	4.448224	C	-5.659941	-7.050273	1.462239
H	-6.399757	-1.785498	4.061330	C	-6.300544	-6.115214	2.283577
H	-5.207729	-2.046454	2.780201	O	-3.926280	-3.342374	2.275969
H	-6.904630	-2.518571	2.533631	Y	-2.582035	-1.886523	1.453067
H	-7.307660	-3.621193	5.372741	N	-1.991723	-4.088440	0.118336
H	-7.938573	-4.378194	3.910034	C	-2.346984	-5.251541	0.991359
H	-6.941962	-5.318215	5.040781	C	-6.283769	-8.398763	1.077624
H	-8.570573	-9.051518	1.718471	C	-7.694103	-8.577056	1.656104
H	-7.787171	-8.209155	3.058694	C	-6.487003	-3.941711	3.622967
H	-8.590935	-7.284868	1.775311	C	-7.796234	-4.553366	4.145660
H	-7.668889	-9.033552	-0.568084	O	-3.778640	-0.145927	1.618173
H	-7.605065	-7.260651	-0.591753	C	-4.641821	0.624841	0.958806
H	-6.156890	-8.206260	-0.964145	C	-5.354479	0.070564	-0.133072
H	-6.501043	-10.335269	1.279555	C	-6.215244	0.860800	-0.891622
H	-4.971479	-9.522405	0.919318	C	-6.427789	2.209873	-0.602202
H	-5.624418	-9.476946	2.561865	C	-5.758465	2.721236	0.514635
H	-1.445479	2.832743	2.095893	C	-4.885646	1.977720	1.318723
H	-1.872081	1.337762	1.222171	C	-5.268749	-1.404903	-0.411738
H	-2.078067	2.914465	0.443515	N	-3.919585	-1.929137	-0.777526
H	-3.185280	4.385573	2.866443	C	-3.400617	-1.190357	-1.934731
H	-3.821090	4.533793	1.225710	C	-4.246556	2.599000	2.571236
H	-4.906186	4.120655	2.570066	C	-4.691931	4.051517	2.801839
H	-2.965262	2.248173	4.027131	C	-7.377716	3.046681	-1.469557
H	-4.681741	1.905433	3.752533	C	-7.439416	4.513452	-1.021302
H	-3.460578	0.722113	3.254615	O	-1.382751	-1.875112	3.378801
H	-8.430331	4.801169	-1.254785	C	-0.423445	-1.130923	3.770402
H	-7.767245	4.354174	0.321527	O	-0.463802	-0.612348	5.007618
H	-6.679528	4.761404	-1.019952	C	-1.605463	-0.928980	5.805185
H	-8.235253	3.330412	-3.235314	H	-1.440030	-0.427505	6.759171
H	-6.478376	3.193357	-3.024878	O	-0.631599	-0.992117	0.563350
H	-7.475075	1.736194	-3.127293	C	0.746977	-1.443776	1.739833
H	-9.804881	2.761296	-1.319342	C	0.680450	-0.780570	2.972571
H	-9.085162	1.151461	-1.181938	C	1.629335	0.310874	3.390872

C	-0.367637	0.049102	-0.367194	H	-4.219353	4.431332	3.714236
C	-4.665133	1.785948	3.813557	H	-4.393191	4.712101	1.980299
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C	-8.800887	2.459790	-1.388084	H	-5.751406	1.824080	3.950366
C	-4.065394	-3.362639	-1.097525	H	-4.369246	0.739927	3.715136
C	-2.738852	-4.103471	-1.159020	H	-8.113340	5.072766	-1.679293
C	-0.554337	-4.211809	-0.179326	H	-7.820960	4.612924	0.000317
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C	-5.402100	-9.547861	1.605745	H	-6.878033	1.998651	-3.334168
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H	-1.691464	-2.008220	5.955038	H	-9.169881	2.475519	-0.357247
H	-4.584293	-3.485068	-2.064348	H	0.408299	-2.473449	1.704040
H	-4.697723	-3.819389	-0.333319	H	2.505617	0.334183	2.735537
H	-2.926203	-5.140006	-1.479389	H	1.172894	1.309474	3.370243
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H	-5.971479	-1.651703	-1.224905	H	-1.344544	0.374879	-0.755542
H	-5.584469	-1.970864	0.472097	H	0.322033	2.095827	-0.447806
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H	-6.740567	0.393018	-1.722834	H	1.309727	1.065017	0.593954
H	-7.276597	-6.367126	2.677483	H	0.606884	0.323995	-2.294433
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H	-0.194264	-3.308105	-0.673858	119			
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H	-8.525358	-4.720615	3.344913	Y	-2.482637	-1.964894	1.600830
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H	-8.100713	-9.545631	1.345840	C	-0.225634	0.184616	-0.163145
H	-7.691399	-8.556896	2.751051	C	0.576482	-0.229979	-1.393120
H	-8.380699	-7.800904	1.301496	C	-5.018360	-1.363271	-0.440368
H	-6.820569	-9.462114	-0.753347	N	-3.685614	-1.966773	-0.736879
H	-7.012400	-7.701754	-0.861808	C	-3.891527	-3.403217	-1.005769
H	-5.399418	-8.424587	-0.933018	C	-2.599475	-4.204614	-1.005113
H	-5.833007	-10.520001	1.337706	N	-1.879103	-4.148250	0.287259
H	-4.390352	-9.507669	1.189722	C	-0.434301	-4.280189	0.036556
H	-5.315232	-9.502627	2.696312	C	-6.821228	3.187868	-1.636949
H	-2.257035	3.039514	3.342516	C	-8.236834	2.601467	-1.805130
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O	-3.917453	-3.347224	2.353269	H	-7.471362	-1.952377	3.465008
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C	-2.259414	-5.278760	1.195768	H	-6.614195	-9.592709	-0.614875
C	-6.163852	-8.465931	1.201093	H	-6.825795	-7.839614	-0.785710
C	-5.288326	-9.585350	1.798487	H	-5.201137	-8.540075	-0.771298
O	-1.153692	-2.031412	3.314254	H	-5.697876	-10.570924	1.546807
C	-0.207350	-1.240590	3.751570	H	-4.262634	-9.546096	1.418067
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C	0.346091	1.431812	0.497792	H	-5.126863	3.675950	-2.928595
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H	-1.349636	-2.481160	5.839769	H	-8.753097	2.545512	-0.841206
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H	-4.559334	-3.800837	-0.238411	H	2.883422	-0.201827	3.204988
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H	-3.666893	-7.484746	0.632980				
H	-3.706141	-1.469279	-2.807194				
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H	-5.525862	-4.527346	5.393889	C	-4.270906	-6.456587	0.958967
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YT1_T1L.xyz
119

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C -0.006328 -3.266339 4.969031
H 1.767503 -0.356687 -1.866791
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H 0.116570 -0.280516 4.358328
H 0.197516 0.380966 -1.422441
H -4.312061 -3.408604 -1.969805
H -4.604379 -3.792118 -0.269165
H -2.672559 -5.028697 -1.199015
H -1.859348 -3.513812 -1.576114
H -1.867318 -5.995084 0.890807
H -1.860444 -4.919325 2.295655
H -5.876953 -1.668268 -1.185063
H -5.611909 -1.977763 0.536094
H -6.080192 3.787439 0.687517
H -6.760711 0.307232 -1.694089
H -7.383910 -6.324092 2.508639
H -3.695235 -7.280767 0.576240
H -3.772121 -1.175405 -2.590607
H -3.244311 -0.012080 -1.349985
H -2.191795 -1.364162 -1.777303
H -0.125704 -4.884962 -0.110607
H -0.129171 -3.104323 -0.225801
H -0.032426 -3.882316 1.357684
H -6.522044 -3.053581 5.582729
H -5.789464 -4.660612 5.419534
H -4.982460 -3.242038 4.718075
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H -6.094168 -2.001751 2.743450
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H -8.619185 -3.886560 4.632347
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H -7.967332 -5.517688 4.449034
H -8.023314 -9.487090 1.062657
H -7.747425 -8.526649 2.519428
H -8.332210 -7.747237 1.036747
H -6.576154 -9.315815 -0.930775
H -6.792724 -7.556166 -0.999572
H -5.165441 -8.248842 -0.957810
H -5.748308 -10.423677 1.204878
H -4.315540 -9.387311 1.203365
H -5.358250 -9.440944 2.629947
H -2.309791 3.246839 3.150774
H -2.422046 1.782163 2.148198
H -2.555687 3.380193 1.399902
H -4.295434 4.673138 3.519640
H -4.550674 4.835433 1.780622
H -5.879006 4.300246 2.831721
H -4.185099 2.535802 4.663757

H	-5.759134	2.062659	4.000308	C	-3.724563	-5.370053	1.483832
H	-4.359780	0.997743	3.786506	C	-6.535201	-3.938716	3.723791
H	-8.318715	4.926427	-1.811418	C	-6.872421	-2.584052	3.071834
H	-8.010580	4.539898	-0.115725	C	-2.288697	-5.071322	1.158123
H	-6.660562	4.930338	-1.198822	C	-6.173249	-8.290096	1.026508
H	-7.710786	3.416176	-3.648063	C	-5.288820	-9.448857	1.528270
H	-6.029469	3.318873	-3.089676	O	-0.901697	-0.800455	0.818266
H	-6.965228	1.840900	-3.351201	C	0.342834	-0.844740	1.220957
H	-9.623025	2.834597	-2.076972	C	0.728152	-0.829932	2.527468
H	-8.902744	1.253462	-1.738430	C	2.160161	-0.897214	2.977009
H	-9.288851	2.345640	-0.403764	C	-7.594362	-8.510402	1.562663
H	-1.063370	0.234570	3.082403	C	-6.233260	-8.329103	-0.513391
H	2.396900	-0.710877	3.758516	C	-7.862102	-4.582632	4.156274
H	2.569784	-1.834065	2.404323	C	-5.700644	-3.701397	4.998467
H	2.880511	-0.117228	2.168980	C	-3.355267	-1.075873	-1.726678
H	-2.107798	-3.422743	4.581438	C	-4.796892	4.216706	2.581860
H	-0.040690	-3.916502	5.849968	C	-4.739916	2.025928	3.740914
H	0.296697	-3.870820	4.108592	C	-7.602286	4.487190	-1.222493
H	0.768594	-2.511337	5.139289	C	-7.023930	2.930711	-3.074904
H	-1.920614	-2.394412	6.809530	O	1.304121	-0.970520	0.247392
H	-1.113032	-0.973910	6.134358	C	1.040158	-0.289856	-0.968699
H	-2.799120	-1.320094	5.705666	C	-0.358796	-0.669776	3.532160
YT1_T1Lb.xyz				C	-0.153682	-3.375454	4.909280
119				H	1.884423	-0.505764	-1.626554
scf done: -2165.543070				H	0.111389	-0.631556	-1.436267
C	-5.064042	2.056924	1.240605	H	0.050492	-0.601655	4.542772
C	-4.846215	0.681255	0.962632	H	0.972023	0.794240	-0.811568
C	-5.515400	0.090080	-0.136628	H	-4.512724	-3.417039	-2.011927
C	-6.356842	0.850127	-0.945987	H	-4.706609	-3.792270	-0.294515
C	-6.582951	2.206831	-0.706680	H	-2.828726	-5.033527	-1.311542
C	-5.923192	2.766498	0.393080	H	-2.047132	-3.526949	-1.773127
O	-4.031119	-0.075908	1.694421	H	-1.840685	-5.962293	0.687848
Y	-2.742725	-1.745872	1.557138	H	-1.738285	-4.890966	2.090991
O	-1.363939	-1.758240	3.513156	H	-6.004141	-1.655478	-1.256717
C	-1.455513	-2.621022	4.675375	H	-5.736058	-1.959762	0.465397
C	-1.936151	-1.855943	5.901945	H	-6.083718	3.815705	0.604807
C	-5.372335	-1.384504	-0.395162	H	-6.850889	0.354399	-1.780067
N	-3.981164	-1.866121	-0.656685	H	-7.245541	-6.333780	2.661580
C	-4.051818	-3.296022	-1.016135	H	-3.690737	-7.253254	0.477222
C	-2.692832	-3.982282	-1.016231	H	-3.887649	-1.206671	-2.682482
N	-1.997432	-3.892747	0.286718	H	-3.381134	-0.018773	-1.457881
C	-0.539036	-3.865217	0.071833	H	-2.312077	-1.368825	-1.857816
C	-7.523464	3.006312	-1.618530	H	-0.192055	-4.778668	-0.437013
C	-8.943523	2.411761	-1.538766	H	-0.259040	-2.991831	-0.516789
C	-4.374161	2.747264	2.427535	H	-0.024641	-3.790145	1.033519
C	-2.846492	2.727998	2.219277	H	-6.251935	-3.061831	5.698303
O	-3.888165	-3.283910	2.567566	H	-5.486727	-4.650071	5.503608
C	-4.450494	-4.455414	2.288254	H	-4.755030	-3.214294	4.755117
C	-5.740952	-4.829314	2.752802	H	-7.453226	-1.964709	3.766094
C	-6.256550	-6.058092	2.319815	H	-5.970300	-2.032048	2.803494
C	-5.577371	-6.951741	1.483899	H	-7.480515	-2.729760	2.171407
C	-4.288788	-6.581683	1.091611	H	-8.367122	-3.919611	4.866912
				H	-8.543868	-4.734260	3.312152
				H	-7.710680	-5.545825	4.655719

H	-7.979123	-9.472098	1.206502	C	-5.263061	-1.385744	-0.262854
H	-7.618065	-8.531559	2.657366	N	-3.923689	-1.983070	-0.534626
H	-8.284306	-7.731498	1.220758	C	-4.092546	-3.410892	-0.852935
H	-6.649944	-9.282264	-0.860133	C	-2.783605	-4.189905	-0.787721
H	-6.864686	-7.521832	-0.899788	N	-2.130440	-4.104078	0.536661
H	-5.240034	-8.219144	-0.960510	C	-0.666005	-4.126085	0.392804
H	-5.698918	-10.414217	1.208327	C	-6.963517	3.162845	-1.602399
H	-4.267503	-9.377562	1.140886	C	-8.425709	2.674474	-1.612282
H	-5.230617	-9.449036	2.621712	C	-4.088610	2.667849	2.620198
H	-2.338696	3.180365	3.080279	C	-2.556325	2.517514	2.549693
H	-2.476432	1.709618	2.091076	O	-4.346245	-3.389064	2.460382
H	-2.571844	3.302806	1.327608	C	-4.808609	-4.613430	2.254526
H	-4.283198	4.648741	3.447612	C	-6.115739	-5.018958	2.641709
H	-4.527449	4.820215	1.708166	C	-6.536866	-6.301814	2.269375
H	-5.873973	4.320290	2.753526	C	-5.745808	-7.221812	1.571703
H	-4.233586	2.504487	4.588351	C	-4.440854	-6.822575	1.274386
H	-5.819462	2.079455	3.920459	C	-3.964904	-5.557833	1.613432
H	-4.451335	0.974443	3.706336	C	-7.015282	-4.105987	3.492544
H	-8.275007	5.016889	-1.905717	C	-7.329505	-2.790088	2.755977
H	-7.993332	4.618998	-0.208102	C	-2.504857	-5.246930	1.428468
H	-6.623326	4.975489	-1.277838	C	-6.238919	-8.617699	1.167595
H	-7.688621	3.494562	-3.740271	C	-5.366353	-9.692752	1.845552
H	-6.016463	3.350706	-3.164800	O	-0.814389	-0.857734	0.847245
H	-6.989013	1.899120	-3.439292	C	0.149407	-0.087899	0.886578
H	-9.632009	2.963848	-2.189802	C	0.852410	0.410392	2.092251
H	-8.959967	1.362392	-1.849804	C	1.908003	1.467267	1.907968
H	-9.329020	2.460422	-0.515018	C	-7.697845	-8.863235	1.575995
H	-0.954620	0.234606	3.355615	C	-6.138177	-8.776297	-0.362623
H	2.423039	-0.063282	3.642899	C	-8.356377	-4.769641	3.841898
H	2.388307	-1.822871	3.526783	C	-6.293386	-3.786717	4.818177
H	2.833045	-0.855221	2.118323	C	-3.278820	-1.278543	-1.642641
H	-2.235941	-3.329222	4.379927	C	-4.394811	4.168558	2.744695
H	-0.292469	-4.110552	5.708691	C	-4.623213	1.981926	3.894128
H	0.159000	-3.905328	4.005198	C	-6.959441	4.644673	-1.202243
H	0.659211	-2.707452	5.210543	C	-6.384385	3.053038	-3.026749
H	-2.126662	-2.557947	6.719999	O	0.701812	0.401001	-0.224899
H	-1.195515	-1.131808	6.256863	C	0.129704	0.032876	-1.480205
H	-2.867077	-1.324568	5.686932	C	0.523118	-0.112383	3.282561
YT1_T1Lf.xyz				C	-0.207944	-3.675411	5.006867
119				H	0.740978	0.526570	-2.234927
scf done: -2165.551265				H	0.165525	-1.050780	-1.617090
C	-4.737881	2.033476	1.379629	H	1.030910	0.238293	4.177990
C	-4.603315	0.642379	1.111389	H	-0.904027	0.375932	-1.543903
C	-5.275637	0.099747	-0.015052	H	-4.531766	-3.535749	-1.858971
C	-6.013959	0.923228	-0.862834	H	-4.798700	-3.838194	-0.137884
C	-6.138602	2.296037	-0.641592	H	-2.981981	-5.238503	-1.052672
C	-5.493076	2.806396	0.489981	H	-2.082756	-3.805211	-1.535731
O	-3.875981	-0.158325	1.881338	H	-2.005237	-6.152271	1.046038
Y	-2.811178	-2.013878	1.862410	H	-2.055736	-5.015980	2.403285
O	-1.622190	-2.371867	3.553720	H	-5.928543	-1.605360	-1.114950
C	-1.577725	-3.027445	4.790434	H	-5.662190	-1.919901	0.606584
C	-1.920253	-2.064122	5.928553	H	-5.585357	3.865084	0.695991
				H	-6.513399	0.462792	-1.714095
				H	-7.539433	-6.601581	2.546548

H	-3.758230	-7.513644	0.781438
H	-3.861453	-1.374262	-2.574835
H	-3.200168	-0.217930	-1.397628
H	-2.277854	-1.677825	-1.816643
H	-0.318652	-5.050300	-0.096707
H	-0.334247	-3.266762	-0.194550
H	-0.204216	-4.061227	1.381673
H	-6.908494	-3.118949	5.433542
H	-6.112997	-4.703492	5.390594
H	-5.334550	-3.299342	4.630826
H	-8.015246	-2.177885	3.353992
H	-6.420869	-2.211457	2.586366
H	-7.812986	-2.986824	1.792015
H	-8.941255	-4.088357	4.469115
H	-8.954882	-4.988592	2.950373
H	-8.222219	-5.699873	4.404627
H	-8.007898	-9.864717	1.258281
H	-7.831191	-8.806377	2.661500
H	-8.378149	-8.142621	1.109612
H	-6.473294	-9.773496	-0.672303
H	-6.761209	-8.034020	-0.873060
H	-5.109653	-8.647693	-0.714827
H	-5.700188	-10.697885	1.560853
H	-4.313646	-9.599472	1.560527
H	-5.423852	-9.610472	2.935932
H	-2.090111	2.955278	3.441055
H	-2.269657	1.467010	2.491299
H	-2.159080	3.040460	1.671373
H	-3.916468	4.558303	3.649936
H	-4.006816	4.743322	1.896194
H	-5.469013	4.364817	2.831719
H	-4.149310	2.413486	4.784508
H	-5.705255	2.129600	3.983335
H	-4.422412	0.909853	3.875783
H	-7.551790	5.223628	-1.919194
H	-7.398221	4.800085	-0.210992
H	-5.946483	5.061590	-1.196314
H	-6.967615	3.659888	-3.729784
H	-5.347068	3.403812	-3.053747
H	-6.396959	2.020699	-3.390671
H	-9.030418	3.276029	-2.301797
H	-8.501182	1.629246	-1.928301
H	-8.868651	2.751240	-0.613860
H	-0.233434	-0.891772	3.400242
H	2.325214	1.751808	2.876566
H	2.724143	1.113457	1.270055
H	1.498013	2.364099	1.432598
H	-2.333964	-3.834303	4.802811
H	-0.173582	-4.234219	5.949155
H	0.021943	-4.369425	4.191200
H	0.579300	-2.912894	5.032263
H	-1.934847	-2.578053	6.896753
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H	-2.904594	-1.615801	5.763134

YT1_T1R.xyz			
119			
scf done: -2165.533535			
C	-3.835593	-5.515257	1.533409
C	-4.634237	-4.596001	2.259552
C	-5.921797	-5.009741	2.699142
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C	-4.326555	-6.772730	1.189614
O	-4.144310	-3.382434	2.485726
Y	-2.824795	-1.878165	1.696265
O	-1.091319	-0.846522	0.517822
C	-0.217661	-0.049368	0.992036
O	0.017524	1.120174	0.375429
C	-0.802543	1.447383	-0.743675
C	-6.784432	-4.118849	3.608787
C	-6.019127	-3.868128	4.923626
C	-6.121112	-8.575509	1.154643
C	-6.135738	-8.693482	-0.382318
C	-2.403535	-5.172144	1.235330
N	-2.139052	-4.011902	0.326367
C	-0.703276	-4.036129	-0.000182
O	-4.048545	-0.148962	1.851588
C	-4.738101	0.691369	1.083199
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C	-5.568286	2.881399	0.482520
C	-6.183021	2.408026	-0.681679
C	-6.080910	1.037191	-0.926603
C	-5.384659	0.185333	-0.072236
C	-4.277328	2.666311	2.677610
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C	-5.384348	-1.295032	-0.336974
N	-4.044712	-1.899587	-0.590901
C	-3.388013	-1.219543	-1.713953
C	-6.961654	3.310356	-1.648452
C	-6.354675	3.204425	-3.061319
O	-1.372330	-1.821025	3.417143
C	-1.415356	-1.861147	4.836042
C	-1.293715	-3.300436	5.331724
C	-2.678474	-1.178912	5.348751
C	-4.231524	-3.331723	-0.882420
C	-2.921310	-4.103809	-0.929202
C	-8.435612	2.860686	-1.696172
C	-6.926886	4.785867	-1.227142
C	-2.748662	2.476895	2.722779
C	-4.551065	4.172267	2.814267
C	-7.100121	-2.772117	2.930751
C	-8.126530	-4.773537	3.971504
C	-5.191919	-9.659511	1.736238
C	-7.543080	-8.844362	1.666069
C	0.517936	-0.281802	2.173389
C	0.362097	-1.555359	2.720850

C	1.259699	0.835725	2.859914	H	-5.308727	3.529487	-3.062014
H	-0.453285	2.422136	-1.085716	H	-6.385252	2.178013	-3.440399
H	-1.854388	1.509348	-0.451552	H	-9.008980	3.486913	-2.390305
H	0.921617	-1.804753	3.619119	H	-8.531189	1.821892	-2.027668
H	-0.689756	0.709796	-1.542864	H	-8.898363	2.936568	-0.706656
H	-4.749677	-3.461158	-1.849430	H	0.222409	-2.390011	2.044293
H	-4.878293	-3.755762	-0.110480	H	1.773785	0.460527	3.750072
H	-3.139603	-5.154586	-1.167517	H	0.597073	1.650768	3.175859
H	-2.297528	-3.720733	-1.742392	H	2.017970	1.278442	2.204860
H	-1.917048	-6.062012	0.803385	H	-0.552362	-1.286417	5.212165
H	-1.880876	-4.942077	2.173803	H	-1.273148	-3.343107	6.426476
H	-6.037126	-1.502667	-1.201414	H	-0.374380	-3.763287	4.957203
H	-5.803818	-1.830103	0.523029	H	-2.144424	-3.892872	4.978628
H	-5.649443	3.936730	0.708823	H	-2.696262	-1.168765	6.444404
H	-6.562250	0.602867	-1.801485	H	-3.574575	-1.705894	5.004449
H	-7.347245	-6.591662	2.641189	H	-2.727902	-0.146148	4.994183
H	-3.674925	-7.444544	0.632821				
H	-3.919541	-1.413673	-2.660579				
H	-3.391507	-0.144952	-1.531151	YT1_T1Rb.xyz			
H	-2.350633	-1.543294	-1.809292	119			
H	-0.445835	-4.914767	-0.612862	scf done: -2165.541648			
H	-0.420667	-3.124400	-0.530737	C	-3.771070	-5.481898	1.512642
H	-0.118350	-4.094415	0.921572	C	-4.538599	-4.584101	2.296750
H	-6.591222	-3.199641	5.578237	C	-5.819512	-5.003307	2.752212
H	-5.854504	-4.809219	5.460207	C	-6.278798	-6.260800	2.338776
H	-5.048582	-3.410740	4.724008	C	-5.553984	-7.142241	1.529203
H	-7.742221	-2.165090	3.580204	C	-4.279866	-6.723842	1.139947
H	-6.189770	-2.206205	2.729467	O	-4.027220	-3.383955	2.555740
H	-7.637244	-2.929731	1.988054	Y	-2.858400	-1.819342	1.620239
H	-8.685908	-4.101621	4.631251	O	-1.060048	-0.965241	0.664084
H	-8.748419	-4.957876	3.088328	C	-0.083504	-0.246747	1.155604
H	-7.994645	-5.720790	4.505494	O	0.341864	0.821151	0.423013
H	-7.866992	-9.842410	1.351604	C	-0.433174	1.187416	-0.704281
H	-7.595611	-8.810297	2.759460	C	-6.659520	-4.135431	3.704018
H	-8.263335	-8.122392	1.266574	C	-5.868841	-3.926685	5.010688
H	-6.489037	-9.684580	-0.691058	C	-6.087618	-8.513491	1.093401
H	-6.799284	-7.942878	-0.824899	C	-6.130616	-8.585604	-0.445934
H	-5.137483	-8.549224	-0.807914	C	-2.357089	-5.120757	1.160423
H	-5.542638	-10.659679	1.455115	N	-2.157284	-3.953854	0.246638
H	-4.165537	-9.553463	1.370895	C	-0.731363	-3.928886	-0.124663
H	-5.163341	-9.603188	2.829382	O	-4.121794	-0.125876	1.816903
H	-2.344344	2.896074	3.652456	C	-4.823670	0.712500	1.053169
H	-2.477472	1.421530	2.675830	C	-4.947889	2.097967	1.344633
H	-2.267716	2.997155	1.886923	C	-5.669088	2.892861	0.445028
H	-4.123445	4.530441	3.757024	C	-6.292700	2.408987	-0.710006
H	-4.091418	4.751459	2.005554	C	-6.186495	1.037321	-0.946763
H	-5.622691	4.398462	2.834601	C	-5.478567	0.195995	-0.091563
H	-4.510011	2.354170	4.823774	C	-4.347970	2.703961	2.623035
H	-6.009373	2.150744	3.900135	C	-4.980586	2.012164	3.847636
H	-4.766276	0.887883	3.850826	C	-5.463568	-1.284522	-0.349977
H	-7.483622	5.390794	-1.951041	N	-4.114694	-1.877118	-0.592683
H	-7.387621	4.940857	-0.245871	C	-3.439566	-1.174864	-1.693878
H	-5.903159	5.173743	-1.189095	C	-7.078058	3.302885	-1.679078
H	-6.907494	3.835252	-3.767610	C	-6.471681	3.193389	-3.091992

N	-2.169113	-3.973647	0.678430	H	-0.263275	-3.859312	1.557853
C	-0.703220	-3.922902	0.559625	H	-7.157081	-3.150132	5.390832
O	-4.212488	-0.157077	2.032031	H	-6.340475	-4.724610	5.392629
C	-4.827646	0.676611	1.206431	H	-5.534401	-3.308688	4.685812
C	-5.014637	2.053208	1.521192	H	-8.151739	-2.220513	3.247743
C	-5.626647	2.869835	0.562108	H	-6.514574	-2.225709	2.573298
C	-6.088779	2.415712	-0.678273	H	-7.845150	-3.025275	1.700856
C	-5.935444	1.051930	-0.938865	H	-9.113720	-4.149443	4.299775
C	-5.331112	0.186470	-0.029017	H	-9.018249	-5.045382	2.781351
C	-4.606819	2.614214	2.894943	H	-8.365936	-5.748896	4.276897
C	-5.358908	1.846165	4.001607	H	-7.868966	-9.899420	1.112975
C	-5.308477	-1.292693	-0.314748	H	-7.798356	-8.853771	2.534468
N	-3.957136	-1.899340	-0.482058	H	-8.270251	-8.184680	0.960181
C	-3.246808	-1.235083	-1.577169	H	-6.233121	-9.759603	-0.720459
C	-6.762649	3.330447	-1.710136	H	-6.548711	-8.025864	-0.927873
C	-5.956707	3.310232	-3.024120	H	-4.895168	-8.604229	-0.683330
O	-1.617756	-2.055021	3.559448	H	-5.559327	-10.680776	1.545831
C	-1.223208	-2.152512	4.895531	H	-4.204144	-9.546808	1.634489
C	-1.085699	-3.618016	5.312926	H	-5.392672	-9.597360	2.941745
C	-2.194193	-1.404147	5.809732	H	-2.811060	2.846106	4.106598
C	-4.109253	-3.337160	-0.764084	H	-2.772042	1.434547	3.032692
C	-2.792968	-4.097677	-0.657518	H	-2.534173	3.071049	2.373988
C	-8.194262	2.830353	-1.988505	H	-4.659265	4.440408	4.047107
C	-6.853423	4.785943	-1.231099	H	-4.431118	4.730474	2.320280
C	-3.086561	2.476360	3.111373	H	-6.032053	4.283990	2.947420
C	-4.956710	4.102237	3.048540	H	-5.066806	2.222790	4.989585
C	-7.421483	-2.820240	2.691122	H	-6.440705	1.982826	3.894957
C	-8.479916	-4.819245	3.708796	H	-5.139804	0.778337	3.955313
C	-5.268970	-9.669693	1.856148	H	-7.333843	5.399455	-2.001012
C	-7.601297	-8.894811	1.457967	H	-7.450051	4.877035	-0.317276
C	1.087786	-0.098932	1.422438	H	-5.864166	5.214511	-1.037380
C	1.135666	-1.053829	2.362061	H	-6.435998	3.940326	-3.782969
C	2.273186	0.715731	0.983743	H	-4.940499	3.687099	-2.863788
H	-1.332092	2.913899	-0.528893	H	-5.877279	2.298303	-3.433871
H	-2.318553	1.618867	0.222794	H	-8.692524	3.474100	-2.723361
H	2.079265	-1.290396	2.847299	H	-8.197707	1.810126	-2.384847
H	-1.564650	1.361969	-1.380013	H	-8.792528	2.832240	-1.071553
H	-4.528253	-3.491591	-1.774724	H	0.233876	-1.571202	2.694510
H	-4.824791	-3.753200	-0.050999	H	3.180509	0.357987	1.475953
H	-2.974177	-5.154031	-0.900906	H	2.138716	1.773371	1.231244
H	-2.084027	-3.720658	-1.401423	H	2.422644	0.660822	-0.099809
H	-1.959385	-6.013013	1.201058	H	-0.228511	-1.678466	5.012840
H	-2.095973	-4.874910	2.552683	H	-0.732080	-3.710888	6.346341
H	-5.901894	-1.487088	-1.224473	H	-0.373308	-4.136558	4.661786
H	-5.788924	-1.836031	0.506750	H	-2.054564	-4.123789	5.232616
H	-5.759223	3.916815	0.803394	H	-1.861256	-1.426696	6.853992
H	-6.308438	0.631784	-1.871841	H	-3.190067	-1.858957	5.756826
H	-7.546221	-6.641427	2.465954	H	-2.279804	-0.358468	5.498429
H	-3.665880	-7.438494	0.866559				
H	-3.721003	-1.451321	-2.549828				
H	-3.276117	-0.158321	-1.414976				
H	-2.202568	-1.552124	-1.616214				
H	-0.303600	-4.819050	0.058002				
H	-0.401756	-3.035921	-0.003272				
				YT2R_NRB.xyz			
				134			
				scf done: -2511.187674			
				C	-5.713024	-4.883307	4.828228

C	-5.550365	-3.499471	4.541745	C	-1.982254	-3.792069	10.601032
C	-6.650786	-2.631198	4.750830	C	-0.303068	-3.354647	5.149941
C	-7.839540	-3.110666	5.296215	H	-6.594068	1.472235	4.844610
C	-8.014188	-4.454901	5.627844	H	-6.078178	0.952852	3.236105
C	-6.935763	-5.304857	5.365267	H	-4.840220	2.943732	4.035224
O	-4.408485	-2.990642	4.078853	H	-4.244889	2.033466	5.420841
Y	-3.348936	-1.193700	3.676454	H	-3.319618	2.995239	2.173961
O	-2.208540	-0.881729	5.609606	H	-2.486511	1.496096	1.743024
C	-1.000613	-0.938120	6.038625	H	-7.566005	-0.726983	4.526402
C	-0.525134	-1.901526	6.927712	H	-6.532470	-1.191823	3.171213
C	0.884812	-1.968376	7.455872	H	-7.050027	-6.357492	5.589388
C	-6.608903	-1.208101	4.265532	H	-8.653870	-2.403597	5.446169
N	-5.499039	-0.347253	4.765793	H	-7.168782	0.544146	-1.339662
C	-5.760226	1.021067	4.279156	H	-5.146422	3.526125	0.956791
C	-4.551603	1.935827	4.374612	H	-6.355654	0.007799	6.685444
N	-3.383652	1.448269	3.611940	H	-5.305160	-1.423786	6.556899
C	-2.166566	2.021354	4.211455	H	-4.576665	0.184691	6.593647
C	-9.340745	-4.936783	6.230337	H	-2.193679	3.123216	4.184849
C	-9.333969	-6.442009	6.530244	H	-2.067060	1.677533	5.240496
C	-4.589543	-5.896620	4.556446	H	-1.285958	1.680781	3.662595
C	-5.016355	-7.345966	4.837029	H	-4.556946	-3.226490	-1.308577
O	-4.070576	-0.767461	1.699551	H	-4.113913	-1.585289	-1.813684
C	-4.767970	0.130402	1.015868	H	-3.733509	-2.140777	-0.168686
C	-5.697421	-0.220492	-0.000493	H	-6.477943	-3.608714	0.282940
C	-6.445701	0.812810	-0.580198	H	-5.666608	-2.605045	1.492098
C	-6.313171	2.166321	-0.249057	H	-7.338274	-2.242554	1.005750
C	-5.335779	2.485384	0.697068	H	-6.861934	-2.845765	-1.984151
C	-4.567249	1.501528	1.314846	H	-7.846480	-1.512709	-1.378982
C	-5.844070	-1.673382	-0.483203	H	-6.520558	-1.196779	-2.518869
C	-6.826721	-1.800885	-1.657764	H	-8.765822	3.552011	-2.314449
C	-3.408305	1.895733	2.187309	H	-7.712860	2.194399	-2.722347
C	-7.150381	3.276360	-0.899263	H	-8.889443	2.042034	-1.403208
C	-8.185595	2.725872	-1.889584	H	-8.498138	4.868893	-0.253183
O	-1.351584	-1.968918	2.909258	H	-8.587620	3.402835	0.742201
C	-0.137008	-2.288701	3.001217	H	-7.220400	4.512104	0.915643
C	0.492599	-2.947890	4.102286	H	-6.801508	5.048736	-2.128452
C	1.977931	-3.197347	4.062704	H	-5.482637	4.701469	-1.001568
O	0.680737	-2.043624	1.968367	H	-5.678011	3.713902	-2.454406
C	0.091340	-1.473987	0.798999	H	-2.550195	-6.249886	5.249709
C	-7.906156	4.060218	0.191777	H	-3.067924	-4.551664	5.331529
C	-6.222438	4.241410	-1.664170	H	-3.665491	-5.717886	6.524034
C	-4.472980	-2.186524	-0.970535	H	-4.180735	-8.015926	4.606495
C	-6.358845	-2.581940	0.649328	H	-5.281120	-7.506273	5.887908
C	-5.432296	-0.389195	6.233637	H	-5.865415	-7.652620	4.216457
C	-4.160473	-5.827587	3.076888	H	-3.344318	-6.535384	2.886794
C	-3.392389	-5.582767	5.471372	H	-4.997793	-6.096013	2.423269
C	-9.608207	-4.188734	7.551502	H	-3.824328	-4.825618	2.808117
C	-10.491139	-4.651150	5.244754	H	-10.295269	-6.737004	6.964922
O	-0.155057	-0.079846	5.389176	H	-9.185906	-7.037672	5.623213
C	0.786363	0.700231	6.119160	H	-8.550845	-6.710180	7.247497
C	-1.540152	-2.639554	7.745143	H	-10.558820	-4.511973	7.992485
O	-1.663232	-1.980030	8.999475	H	-8.812038	-4.383412	8.277903
C	-2.588335	-2.579108	9.896944	H	-9.663184	-3.106170	7.399617
C	-2.994267	-1.491729	10.880277	H	-11.449745	-4.979010	5.664572

H	-10.575376	-3.583712	5.017796	C	-5.776045	-0.282978	-0.121019
H	-10.334071	-5.180240	4.298979	C	-6.473639	0.777788	-0.713661
H	0.106921	-4.037752	5.888026	C	-6.240282	2.129719	-0.436509
H	-1.380721	-3.362524	5.037577	C	-5.213356	2.414564	0.467043
H	0.898189	-1.410097	0.068831	C	-4.488434	1.403011	1.092718
H	-0.307149	-0.477390	1.007067	C	-6.043985	-1.739697	-0.533960
H	-0.716207	-2.105374	0.421570	C	-7.082374	-1.845203	-1.662057
H	2.265989	-3.776288	3.178247	C	-3.278470	1.747668	1.915696
H	2.289950	-3.757724	4.948150	C	-7.030652	3.269890	-1.092762
H	2.557940	-2.267709	4.031422	C	-8.101659	2.756246	-2.064720
H	1.630635	-1.701234	6.704229	O	-1.244775	-1.592962	3.069851
H	1.102392	-2.996053	7.771636	C	0.031648	-1.553717	3.344658
H	1.037781	-1.340348	8.341671	C	0.657029	-2.178632	4.385256
H	-1.207006	-3.681117	7.894402	C	2.159549	-2.225286	4.487195
H	-2.511780	-2.666218	7.234227	O	0.799983	-0.774154	2.507520
H	1.807037	0.346646	5.947617	C	0.442997	-0.812635	1.132361
H	0.572447	0.688693	7.190368	C	-7.734902	4.101596	-0.002577
H	0.705235	1.728454	5.751591	C	-6.069151	4.181007	-1.881748
H	-3.479934	-2.901219	9.330774	C	-4.734994	-2.372637	-1.049803
H	-2.702719	-4.238932	11.294209	C	-6.576347	-2.555011	0.660074
H	-1.096037	-3.491384	11.169660	C	-5.258488	-0.196410	6.195335
H	-1.685276	-4.568083	9.889266	C	-4.631643	-5.895919	2.835904
H	-3.721453	-1.869525	11.605846	C	-3.226948	-5.701334	4.913912
H	-3.436219	-0.643434	10.350266	C	-8.901775	-3.953672	8.294572
H	-2.115921	-1.132407	11.426684	C	-10.218933	-4.456046	6.214411
YT2R_NRBf.xyz				O	-0.759005	0.222842	6.557674
134				C	0.620129	0.544283	6.779877
scf done: -2511.215614				C	-1.740196	-3.146774	7.301789
C	-5.619631	-4.870467	4.904320	O	-2.134443	-2.518968	8.501927
C	-5.458051	-3.496773	4.570768	C	-3.267892	-3.106280	9.141918
C	-6.484519	-2.585574	4.931257	C	-3.784824	-2.072695	10.130136
C	-7.567611	-3.007411	5.699681	C	-2.909022	-4.422797	9.826673
C	-7.709187	-4.332474	6.116066	C	-0.173412	-3.008697	5.333693
C	-6.728805	-5.229924	5.680086	H	-6.420599	1.543980	4.661657
O	-4.393761	-3.041723	3.915978	H	-5.939274	0.872714	3.098863
Y	-3.328649	-1.240935	3.484166	H	-4.650581	2.906440	3.716207
O	-2.318638	-0.978780	5.669499	H	-4.028618	2.087479	5.146239
C	-1.240057	-0.983229	6.264775	H	-3.119431	2.837893	1.866057
C	-0.605793	-2.321762	6.666423	H	-2.397971	1.274446	1.462271
C	0.548874	-2.272033	7.674615	H	-7.435187	-0.699616	4.660415
C	-6.494475	-1.191452	4.361956	H	-6.495255	-1.245221	3.266283
N	-5.358259	-0.298200	4.733556	H	-6.837490	-6.272826	5.948776
C	-5.604504	1.026862	4.127935	H	-8.327878	-2.271772	5.958114
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134

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C	-0.139717	-1.823115	6.472063	H	-4.665203	4.311856	-1.351770
C	-0.416677	-3.321894	6.664101	H	-4.971419	3.282752	-2.756416

H	-2.942890	-6.555308	5.275614	O	-1.698908	-0.857774	1.541536
H	-3.233977	-4.808655	5.130822	C	-1.069957	-1.950735	1.499677
H	-3.731621	-5.673400	6.600052	C	0.322789	-2.116219	1.456782
H	-4.769014	-8.162063	5.147814	C	0.960243	-3.479424	1.415960
H	-5.581974	-7.395984	6.515965	C	-6.648814	-1.459455	4.213513
H	-6.463370	-7.686456	5.001129	N	-5.477704	-0.551992	4.393817
H	-4.162505	-6.960606	3.107879	C	-5.848671	0.773423	3.862343
H	-5.843127	-6.433479	2.901681	C	-4.663764	1.719805	3.768721
H	-4.536420	-5.234565	2.907663	N	-3.572806	1.174302	2.933576
H	-10.403470	-6.062487	8.078812	C	-2.271324	1.617370	3.462701
H	-9.491226	-6.620289	6.672892	C	-8.269106	-5.064006	7.338526
H	-8.639645	-6.154119	8.157912	C	-8.091250	-6.544793	7.701494
H	-10.386660	-3.720613	8.827530	C	-4.650947	-6.134092	3.862817
H	-8.613456	-3.703003	8.900607	C	-4.843272	-7.552954	4.420468
H	-9.474955	-2.475779	7.962635	O	-4.839352	-0.874937	1.112300
H	-11.576696	-4.384726	6.683288	C	-5.439754	0.150587	0.519222
H	-10.683600	-3.156511	5.775181	C	-6.544329	-0.013264	-0.359175
H	-10.642852	-4.841507	5.244703	C	-7.175759	1.142854	-0.836340
H	1.312066	-0.974077	5.102910	C	-6.772631	2.445432	-0.524082
H	-0.334763	-0.865703	4.506317	C	-5.639754	2.571636	0.284104
H	-0.610198	-5.113355	0.686192	C	-4.968744	1.460950	0.790755
H	-0.988509	-3.370195	0.605049	C	-7.006516	-1.409940	-0.807421
H	-2.022999	-4.460603	1.557468	C	-8.174882	-1.347346	-1.803639
H	2.150260	-4.006140	4.956624	C	-3.665085	1.654698	1.518739
H	2.782087	-2.626652	4.064109	C	-7.494394	3.695711	-1.044666
H	2.089505	-4.007042	3.196890	C	-8.725764	3.349341	-1.892712
H	1.082276	-0.285927	7.447527	O	-2.154108	-1.627434	4.566508
H	1.904391	-1.802820	7.099724	C	-1.200494	-2.334801	5.017917
H	0.802877	-1.722233	8.466894	C	0.124820	-2.403838	4.514370
H	-1.113118	-3.680357	5.896567	C	1.090270	-3.394605	5.116783
H	0.529271	-3.863981	6.538548	O	-1.394312	-3.093600	6.112625
H	-0.517615	0.095136	9.185976	C	-2.673846	-3.061688	6.735384
H	-1.198757	-1.571667	9.231999	C	-7.964320	4.552896	0.147338
H	-2.222343	-0.162958	9.631571	C	-6.531126	4.525375	-1.916509
H	-1.438744	-5.449650	7.477805	C	-5.836159	-2.126948	-1.511652
H	0.080362	-6.494080	9.158458	C	-7.472144	-2.249732	0.397592
H	0.533905	-4.887220	9.761002	C	-5.125451	-0.458748	5.816370
H	0.994619	-5.394270	8.124136	C	-5.026422	-6.174471	2.367093
H	-2.404205	-5.934053	9.727702	C	-3.160865	-5.779291	4.025546
H	-3.139377	-4.488743	9.004689	C	-8.004159	-4.226935	8.605544
H	-1.919289	-4.323647	10.285414	C	-9.729522	-4.854679	6.890782
				O	-1.885734	-3.048489	1.795142
YT2R_TRB.xyz				C	-2.140356	-3.958997	0.710635
134				C	1.095931	-1.004271	0.800826
scf done: -2511.191445				O	1.105654	-1.222312	-0.600836
C	-5.540615	-5.095197	4.565187	C	1.724920	-0.189479	-1.361074
C	-5.540453	-3.728675	4.162604	C	1.204904	-0.332380	-2.783408
C	-6.489303	-2.853468	4.752537	C	3.249180	-0.274320	-1.297064
C	-7.341083	-3.299443	5.760766	C	0.510937	-1.514558	3.511563
C	-7.318947	-4.617926	6.219485	H	-6.627191	1.232304	4.496741
C	-6.418378	-5.480948	5.586241	H	-6.279566	0.631586	2.868380
O	-4.700116	-3.248145	3.252210	H	-5.010150	2.685116	3.371868
Y	-3.647106	-1.422059	2.797888	H	-4.264226	1.917926	4.768191
				H	-3.425395	2.730936	1.513194

H	-2.864811	1.136150	0.979592
H	-7.529329	-0.994083	4.686757
H	-6.838556	-1.495987	3.134962
H	-6.402612	-6.517505	5.897437
H	-8.049067	-2.588083	6.183363
H	-8.029139	1.016875	-1.490284
H	-5.246972	3.559766	0.520004
H	-5.905545	0.074893	6.383845
H	-5.033019	-1.464674	6.224848
H	-4.172453	0.057167	5.948072
H	-2.213643	2.716392	3.519249
H	-2.109297	1.197992	4.459057
H	-1.478912	1.257094	2.804399
H	-6.139344	-3.134839	-1.820601
H	-5.528299	-1.576212	-2.407409
H	-4.975967	-2.210893	-0.844611
H	-7.838705	-3.226007	0.057710
H	-6.654624	-2.420154	1.099549
H	-8.295036	-1.751320	0.923412
H	-8.441771	-2.364860	-2.108891
H	-9.070182	-0.893320	-1.364312
H	-7.915275	-0.789991	-2.710289
H	-9.213546	4.270367	-2.229564
H	-8.457728	2.773844	-2.785063
H	-9.462948	2.773714	-1.322726
H	-8.473712	5.458095	-0.204308
H	-8.662802	3.992835	0.778258
H	-7.125188	4.867799	0.775874
H	-7.027015	5.430390	-2.287633
H	-5.644893	4.838452	-1.355658
H	-6.189898	3.944927	-2.780061
H	-2.537455	-6.516781	3.504153
H	-2.941211	-4.790530	3.621888
H	-2.872313	-5.793113	5.082193
H	-4.200136	-8.246212	3.867303
H	-4.565182	-7.622985	5.478039
H	-5.874519	-7.905088	4.310725
H	-4.374610	-6.872985	1.826775
H	-6.059699	-6.515769	2.240372
H	-4.941791	-5.184270	1.914862
H	-8.782876	-6.813922	8.507193
H	-8.305628	-7.201057	6.851302
H	-7.076038	-6.760029	8.051967
H	-8.683957	-4.522483	9.413636
H	-6.976483	-4.367135	8.957815
H	-8.150979	-3.157728	8.422440
H	-10.424017	-5.159603	7.682794
H	-9.934592	-3.805777	6.654836
H	-9.951196	-5.445807	5.996123
H	1.580509	-1.388925	3.355272
H	-0.093288	-0.627597	3.343695
H	-2.620598	-3.788296	7.546837
H	-3.464467	-3.345009	6.036757
H	-2.880343	-2.068549	7.144733

H	1.204829	-3.244609	6.196450
H	2.077563	-3.288481	4.657708
H	0.768422	-4.433229	4.977901
H	0.420983	-4.193744	2.043331
H	1.986793	-3.417026	1.794978
H	1.026859	-3.874891	0.395321
H	2.125243	-0.992668	1.196595
H	0.634487	-0.031466	1.027834
H	-1.214138	-4.430516	0.376948
H	-2.612371	-3.430764	-0.123384
H	-2.820835	-4.711516	1.105333
H	1.403130	0.787424	-0.958849
H	3.704672	0.519289	-1.898562
H	3.588805	-1.239759	-1.686152
H	3.622642	-0.167071	-0.274146
H	1.619816	0.447072	-3.430025
H	0.114284	-0.258353	-2.800392
H	1.489192	-1.307464	-3.192349

YT2R_TRBb.xyz

134

scf done: -2511.213664

C	-5.690980	-5.175340	4.499459
C	-5.648531	-3.794052	4.170040
C	-6.678214	-2.946758	4.646776
C	-7.680803	-3.444902	5.475696
C	-7.729125	-4.789488	5.848656
C	-6.726463	-5.617154	5.331824
O	-4.680917	-3.267844	3.426086
Y	-3.652530	-1.464866	3.001319
O	-1.888973	-2.203007	1.629872
C	-0.813045	-2.793562	1.756724
C	0.475566	-1.969374	1.635806
C	1.803081	-2.721069	1.487283
C	-6.749553	-1.521162	4.175849
N	-5.569505	-0.662493	4.492073
C	-5.882593	0.708519	4.045029
C	-4.686973	1.643635	4.106347
N	-3.530849	1.163559	3.318876
C	-2.289817	1.586198	3.991579
C	-8.844865	-5.298127	6.770900
C	-8.730785	-6.802766	7.051354
C	-4.645014	-6.159162	3.951081
C	-4.921274	-7.608968	4.379732
O	-4.597278	-0.717999	1.226759
C	-5.168406	0.344165	0.677806
C	-6.196466	0.247563	-0.297953
C	-6.790934	1.437641	-0.737108
C	-6.419559	2.713931	-0.297129
C	-5.364248	2.777817	0.615020
C	-4.736449	1.629514	1.091402
C	-6.613265	-1.113390	-0.879278
C	-7.693043	-0.978262	-1.963507

C	-3.506653	1.755044	1.945914	H	-7.877999	3.219132	-2.677750
C	-7.093531	4.002568	-0.786882	H	-9.022746	3.112422	-1.326530
C	-8.234704	3.726598	-1.775174	H	-8.157003	5.698556	0.087842
O	-1.990239	-1.475944	4.426595	H	-8.431650	4.163565	0.934241
C	-0.826106	-1.887574	4.854927	H	-6.904941	5.031518	1.143970
C	0.385527	-1.744407	4.233020	H	-6.516379	5.824914	-1.844315
C	1.661425	-2.150197	4.929094	H	-5.228412	5.163566	-0.828566
O	-0.811115	-2.541218	6.064300	H	-5.626316	4.379639	-2.362446
C	-1.989739	-2.501741	6.844007	H	-2.501724	-6.500566	4.102511
C	-7.679175	4.767874	0.416388	H	-2.957259	-4.783884	4.152880
C	-6.053768	4.893918	-1.495326	H	-3.219605	-5.820243	5.570919
C	-5.385421	-1.786425	-1.527229	H	-4.159526	-8.263903	3.942572
C	-7.178588	-2.029650	0.223354	H	-4.876260	-7.736629	5.467120
C	-5.281393	-0.703290	5.931477	H	-5.897425	-7.963688	4.031324
C	-4.653754	-6.124762	2.409305	H	-3.901042	-6.816517	2.011213
C	-3.245311	-5.784983	4.475911	H	-5.631774	-6.434406	2.024151
C	-8.776437	-4.554454	8.119875	H	-4.437239	-5.122924	2.035845
C	-10.217211	-5.037670	6.119029	H	-9.544546	-7.118270	7.713309
O	-0.906772	-4.090828	1.985264	H	-8.804746	-7.393889	6.132353
C	0.124106	-4.931457	2.519498	H	-7.786310	-7.055359	7.545386
C	0.300826	-1.090503	0.383826	H	-9.573799	-4.895842	8.791086
O	0.260190	-1.930486	-0.745355	H	-7.815646	-4.731775	8.615216
C	-0.147880	-1.299965	-1.959040	H	-8.890332	-3.473178	7.992011
C	-0.523529	-2.419098	-2.916322	H	-11.026389	-5.392303	6.768834
C	0.951136	-0.402065	-2.521844	H	-10.383600	-3.971741	5.934314
C	0.470492	-1.052451	2.898052	H	-10.297391	-5.558060	5.158993
H	-6.695355	1.133058	4.660605	H	1.386427	-0.445305	2.845820
H	-6.250220	0.650695	3.017345	H	-0.374729	-0.364335	2.786981
H	-5.000153	2.641232	3.764899	H	-1.761901	-3.067473	7.750185
H	-4.363233	1.757758	5.145562	H	-2.837646	-2.967444	6.332457
H	-3.258617	2.825495	2.039281	H	-2.261260	-1.475687	7.122293
H	-2.661462	1.275237	1.432681	H	1.521358	-2.188951	6.012086
H	-7.649539	-1.051840	4.606685	H	2.461175	-1.427080	4.718539
H	-6.862139	-1.491372	3.085181	H	2.056829	-3.135833	4.634208
H	-6.750746	-6.668134	5.588937	H	2.099037	-3.254820	2.389014
H	-8.447580	-2.754484	5.823637	H	2.583573	-1.979331	1.286894
H	-7.586586	1.362089	-1.467326	H	1.786743	-3.406418	0.637011
H	-4.999984	3.744638	0.959853	H	1.151550	-0.390655	0.343524
H	-6.097478	-0.248752	6.516659	H	-0.624782	-0.503405	0.462217
H	-5.173184	-1.743015	6.244414	H	0.582358	-4.459251	3.389126
H	-4.350019	-0.178179	6.152961	H	0.867410	-5.177923	1.760733
H	-2.276001	2.676057	4.153888	H	-0.397781	-5.836246	2.828809
H	-2.181919	1.068492	4.945781	H	-1.042764	-0.689884	-1.750369
H	-1.427728	1.323981	3.375564	H	0.626987	0.056070	-3.461630
H	-5.661990	-2.767154	-1.933040	H	1.855166	-0.988132	-2.717625
H	-5.003891	-1.175074	-2.352893	H	1.209559	0.408342	-1.833416
H	-4.584769	-1.926361	-0.798404	H	-0.880779	-2.009900	-3.866015
H	-7.500915	-2.985106	-0.207870	H	-1.312956	-3.040436	-2.485574
H	-6.427155	-2.241122	0.985566	H	0.345541	-3.053603	-3.119047
H	-8.051343	-1.569625	0.701775				
H	-7.932486	-1.971432	-2.357991				
H	-8.622234	-0.549437	-1.571771				
H	-7.356840	-0.362904	-2.805228				
H	-8.690041	4.672598	-2.087390				

YT2R_TRBf.xyz
134
scf done: -2511.202400

C	-5.439966	-5.169093	4.663699	C	1.254633	0.677166	-2.770972
C	-5.496120	-3.821970	4.198846	C	3.211309	-0.257852	-1.472822
C	-6.451982	-2.947182	4.781871	C	0.415262	-1.589739	4.217847
C	-7.262951	-3.374552	5.831052	H	-6.691312	1.132611	4.354914
C	-7.188852	-4.671427	6.344447	H	-6.273779	0.477052	2.764547
C	-6.277238	-5.534427	5.725826	H	-5.050874	2.561027	3.216129
O	-4.702044	-3.364289	3.242432	H	-4.363427	1.886792	4.687682
Y	-3.651656	-1.528703	2.760429	H	-3.257883	2.571328	1.490528
O	-1.622934	-1.025570	1.886632	H	-2.755375	0.935733	1.021908
C	-1.214386	-2.101594	1.269579	H	-7.549768	-1.122032	4.649380
C	-0.048861	-2.317044	0.616712	H	-6.831179	-1.651838	3.119435
C	0.417166	-3.655086	0.110573	H	-6.221794	-6.555378	6.081409
C	-6.651703	-1.575693	4.197460	H	-7.981076	-2.666585	6.242540
N	-5.506378	-0.633209	4.361286	H	-7.882382	1.055920	-1.592593
C	-5.882325	0.663504	3.767331	H	-4.997546	3.476233	0.422735
C	-4.707928	1.626820	3.681776	H	-6.004537	0.061774	6.311162
N	-3.568759	1.055537	2.931598	H	-5.087506	-1.458582	6.233699
C	-2.294173	1.476427	3.537490	H	-4.262318	0.077355	5.923706
C	-8.103378	-5.099938	7.499766	H	-2.207213	2.574392	3.571174
C	-7.862057	-6.553849	7.929096	H	-2.215487	1.086701	4.556639
C	-4.539148	-6.211423	3.978849	H	-1.471253	1.070307	2.947091
C	-4.656313	-7.603717	4.618194	H	-6.230522	-3.178812	-1.873026
O	-4.820856	-0.967658	1.069679	H	-5.554253	-1.653413	-2.475768
C	-5.365737	0.082087	0.460132	H	-5.017767	-2.301433	-0.914468
C	-6.469519	-0.034992	-0.427458	H	-7.923807	-3.175727	0.016360
C	-7.030696	1.146209	-0.930771	H	-6.687531	-2.430107	1.042597
C	-6.560599	2.429713	-0.635710	H	-8.292436	-1.676995	0.882677
C	-5.437377	2.507172	0.191239	H	-8.505309	-2.299544	-2.137533
C	-4.835689	1.370362	0.726186	H	-9.044376	-0.785022	-1.407454
C	-7.006615	-1.408508	-0.863581	H	-7.900132	-0.765170	-2.766401
C	-8.180310	-1.294117	-1.848968	H	-8.870713	4.353972	-2.412267
C	-3.555052	1.509842	1.504307	H	-8.195285	2.804829	-2.925012
C	-7.202835	3.707886	-1.190875	H	-9.217596	2.894480	-1.477476
C	-8.441030	3.414262	-2.048922	H	-8.095630	5.538119	-0.400876
O	-2.353509	-1.873030	4.860580	H	-8.371666	4.107662	0.611730
C	-1.456145	-2.364683	5.552524	H	-6.790112	4.900627	0.607084
C	0.003713	-2.251470	5.308953	H	-6.620560	5.385212	-2.463624
C	0.939271	-2.889987	6.298863	H	-5.286574	4.736330	-1.499810
O	-1.706866	-3.061524	6.654596	H	-5.862945	3.844437	-2.912386
C	-3.069900	-3.253048	7.058293	H	-2.432203	-6.553429	3.554698
C	-7.638253	4.615676	-0.023649	H	-2.886594	-4.840039	3.561321
C	-6.182068	4.461876	-2.066220	H	-2.721327	-5.731821	5.092947
C	-5.878981	-2.183692	-1.573808	H	-4.006998	-8.301932	4.078992
C	-7.502769	-2.219217	0.349152	H	-4.339827	-7.605969	5.667452
C	-5.195429	-0.472355	5.785502	H	-5.676257	-7.999401	4.565584
C	-4.970363	-6.341053	2.503783	H	-4.318111	-7.046691	1.974674
C	-3.055658	-5.799392	4.050847	H	-5.998473	-6.712999	2.435221
C	-7.855786	-4.195093	8.722969	H	-4.921704	-5.373097	2.002465
C	-9.577093	-4.968889	7.065639	H	-8.528468	-6.809825	8.759895
O	-2.186548	-3.118105	1.455661	H	-8.065672	-7.257710	7.115270
C	-2.656023	-3.827879	0.301953	H	-6.833154	-6.713726	8.269492
C	0.846745	-1.148981	0.356335	H	-8.517523	-4.474988	9.551316
O	0.893493	-0.893934	-1.046875	H	-6.821116	-4.284116	9.072061
C	1.746378	0.177635	-1.419958	H	-8.040989	-3.141247	8.492078

H	-10.248538	-5.261956	7.881655
H	-9.825638	-3.941204	6.782901
H	-9.787074	-5.610377	6.203558
H	1.477618	-1.490274	4.012932
H	-0.283245	-1.161827	3.502213
H	-3.038675	-4.031671	7.819248
H	-3.692435	-3.565555	6.218299
H	-3.454857	-2.326868	7.490981
H	0.796837	-2.485802	7.306205
H	1.976274	-2.719699	6.000514
H	0.771680	-3.969716	6.364382
H	-0.019127	-4.486611	0.670878
H	1.505678	-3.729689	0.226940
H	0.210943	-3.812803	-0.956108
H	1.865882	-1.366945	0.724480
H	0.480533	-0.257761	0.885500
H	-2.090464	-4.750408	0.153954
H	-2.569417	-3.196726	-0.586472
H	-3.702909	-4.072455	0.487054
H	1.643832	0.993313	-0.681224
H	3.857018	0.579061	-1.760182
H	3.336924	-1.059731	-2.207812
H	3.559601	-0.627633	-0.503628
H	1.860136	1.518819	-3.122637
H	0.211760	0.998415	-2.702175
H	1.314882	-0.125750	-3.513032

YT2R_TRF.xyz
134

C	-5.037179	0.735765	0.652754
C	-4.566196	0.830598	1.990737
C	-4.717382	2.059401	2.682469
C	-5.409385	3.120175	2.102753
C	-5.956272	3.029225	0.820366
C	-5.730221	1.834685	0.127987
O	-3.995370	-0.182430	2.628902
Y	-3.543611	-0.975750	4.565086
O	-3.057373	-1.333847	6.859090
C	-2.313196	-1.441367	7.869617
O	-2.832830	-1.287163	9.104211
C	-4.237255	-1.113218	9.225817
C	-3.997017	2.270936	3.986212
N	-4.352399	1.403912	5.156099
C	-3.624138	1.953034	6.316269
C	-6.720466	4.217019	0.220313
C	-5.775887	5.429856	0.100951
C	-4.742268	-0.499184	-0.216058
C	-5.364155	-1.772407	0.387556
O	-4.016416	-3.017265	4.241804
C	-5.009626	-3.902001	4.317622
C	-6.347027	-3.436925	4.259246
C	-7.412348	-4.328050	4.366804

C	-7.216398	-5.701543	4.521710
C	-5.889539	-6.142350	4.555143
C	-4.777445	-5.297711	4.454814
C	-6.630592	-1.980548	4.009408
N	-6.091579	-1.034685	5.030011
C	-6.542137	-1.436699	6.366124
C	-3.350917	-5.868186	4.486920
C	-2.598221	-5.317886	5.714003
C	-8.420247	-6.646152	4.639084
C	-9.275412	-6.553770	3.359681
O	-1.381556	-0.701324	4.199946
C	-0.119848	-0.801902	4.370577
O	0.595403	-1.506468	3.464287
C	-0.113621	-2.082844	2.369971
C	0.599202	-0.311228	5.464716
C	2.092640	-0.510639	5.525215
C	-0.020090	0.785070	6.281859
O	-0.311686	2.015545	5.614611
C	0.811813	2.802980	5.219131
C	1.086695	2.642071	3.726745
C	-3.327138	-7.401626	4.586303
C	-2.608499	-5.482727	3.191656
C	-7.998383	-8.109863	4.825664
C	-9.279548	-6.240148	5.852837
C	-6.569190	0.322201	4.701670
C	-5.804797	1.414376	5.436416
C	-5.287627	-0.353472	-1.645078
C	-3.213609	-0.680282	-0.316452
C	-7.278204	3.907581	-1.175758
C	-7.905333	4.586687	1.134128
C	-0.910130	-1.732726	7.901635
C	-0.169339	-1.605224	9.209605
C	-0.281131	-2.141582	6.746993
C	0.508620	4.249466	5.590252
H	-7.643770	0.419019	4.936192
H	-6.459113	0.468397	3.625231
H	-6.238670	2.391071	5.173533
H	-5.935532	1.296453	6.517044
H	-4.142984	3.319493	4.293207
H	-2.918966	2.130211	3.835174
H	-7.722632	-1.841281	3.944940
H	-6.205435	-1.666518	3.050288
H	-5.706938	-7.203609	4.663859
H	-8.422742	-3.925199	4.317316
H	-6.108793	1.753320	-0.882814
H	-5.501925	4.045176	2.670153
H	-7.642776	-1.448660	6.427264
H	-6.173240	-2.439229	6.588549
H	-6.158176	-0.747356	7.118659
H	-4.005819	2.950882	6.586229
H	-3.736182	1.289870	7.176962
H	-2.561390	2.051416	6.077608
H	-2.973973	-1.567603	-0.915216
H	-2.750810	0.188816	-0.796942

H	-2.777337	-0.801459	0.676960
H	-5.184506	-2.629276	-0.273009
H	-4.927461	-1.999799	1.360730
H	-6.448933	-1.662096	0.500049
H	-5.023788	-1.246116	-2.222242
H	-6.379536	-0.262752	-1.664299
H	-4.860758	0.511051	-2.164948
H	-7.830297	4.774709	-1.554303
H	-6.481788	3.686516	-1.894112
H	-7.968586	3.057447	-1.157513
H	-8.456101	5.441464	0.724001
H	-8.601642	3.746600	1.228791
H	-7.571843	4.859507	2.140364
H	-6.306403	6.293925	-0.316926
H	-5.372155	5.726337	1.074341
H	-4.928559	5.200639	-0.553755
H	-1.565769	-5.688655	5.726947
H	-2.577527	-4.227556	5.706055
H	-3.083863	-5.644356	6.640708
H	-2.286534	-7.744124	4.589170
H	-3.792952	-7.764633	5.509058
H	-3.827545	-7.878226	3.736318
H	-1.575353	-5.850455	3.222341
H	-3.099622	-5.929252	2.319959
H	-2.595857	-4.399926	3.057807
H	-8.887889	-8.743416	4.911520
H	-7.413212	-8.476892	3.975814
H	-7.404627	-8.249064	5.735487
H	-10.150305	-6.899994	5.947195
H	-8.700428	-6.306346	6.780141
H	-9.649496	-5.213938	5.762734
H	-10.147910	-7.214522	3.429210
H	-9.641289	-5.536283	3.189833
H	-8.693528	-6.848413	2.480113
H	-0.876536	-2.453082	5.898301
H	0.726102	-2.541121	6.800622
H	-4.435506	-1.067535	10.297166
H	-4.775441	-1.953320	8.780323
H	-4.565568	-0.182744	8.753082
H	-0.218348	-0.590317	9.620517
H	0.884528	-1.860365	9.069764
H	-0.579825	-2.275186	9.972891
H	2.448951	-0.393832	6.555327
H	2.651711	0.209312	4.909809
H	2.382374	-1.506838	5.179034
H	0.629276	0.987070	7.148531
H	-0.988562	0.467211	6.679250
H	1.694197	2.469719	5.787692
H	0.647473	-2.559222	1.750570
H	-0.639354	-1.317357	1.794202
H	-0.833166	-2.833344	2.708166
H	1.338045	4.908222	5.312740
H	0.333994	4.344977	6.665897
H	-0.389366	4.592967	5.065664

H	1.947169	3.247654	3.421323
H	0.216430	2.968408	3.147502
H	1.290546	1.599020	3.472419

YT2R_TRFb.xyz
134

C	-4.880933	0.664954	0.660279
C	-4.413354	0.758504	1.999230
C	-4.535629	1.995664	2.681680
C	-5.197915	3.068961	2.090056
C	-5.742500	2.981894	0.806618
C	-5.544620	1.776745	0.124610
O	-3.872885	-0.267168	2.647973
Y	-3.451187	-1.024925	4.594323
O	-3.083268	-1.354229	7.063993
C	-2.505701	-1.777498	8.069947
O	-3.064461	-1.718233	9.278740
C	-4.381270	-1.177650	9.394453
C	-3.824013	2.199670	3.991733
N	-4.228347	1.356115	5.163240
C	-3.502965	1.886421	6.334547
C	-6.476877	4.183041	0.196059
C	-5.506278	5.375207	0.077816
C	-4.607178	-0.579627	-0.201774
C	-5.233535	-1.844075	0.415576
O	-3.969085	-3.077461	4.362298
C	-4.986518	-3.935117	4.417180
C	-6.310619	-3.438193	4.315692
C	-7.401312	-4.299954	4.407967
C	-7.245686	-5.675604	4.586669
C	-5.931869	-6.149833	4.655169
C	-4.795483	-5.336097	4.570482
C	-6.552804	-1.981129	4.028403
N	-6.025278	-1.027008	5.045777
C	-6.521521	-1.394451	6.374115
C	-3.386851	-5.948975	4.621670
C	-2.620076	-5.403336	5.841216
C	-8.475926	-6.587228	4.686349
C	-9.300002	-6.485989	3.387387
O	-1.325438	-0.815900	4.444225
C	-0.100765	-0.557635	4.047760
O	0.310113	-1.161465	2.889240
C	-0.353741	-2.350684	2.501700
C	0.789627	0.250487	4.689460
C	2.201053	0.411145	4.188673
C	0.345879	1.013187	5.896328
O	-0.291708	2.288471	5.677189
C	0.546871	3.323317	5.168585
C	0.287219	3.543751	3.681197
C	-3.410722	-7.480605	4.745150
C	-2.626910	-5.604249	3.325043
C	-8.097156	-8.059601	4.896392

C	-9.350313	-6.146207	5.876889	H	-3.134627	-6.037189	2.456118
C	-6.464655	0.333204	4.683052	H	-2.565915	-4.524325	3.183514
C	-5.684546	1.417053	5.413107	H	-9.004751	-8.668588	4.969488
C	-5.167317	-0.440333	-1.625793	H	-7.504232	-8.450626	4.062795
C	-3.080785	-0.769677	-0.317498	H	-7.526490	-8.205172	5.819938
C	-7.032073	3.879398	-1.202272	H	-10.239940	-6.782028	5.959322
C	-7.659522	4.581441	1.100739	H	-8.792954	-6.217554	6.817151
C	-1.160607	-2.396293	8.138642	H	-9.690864	-5.111643	5.768230
C	-0.696164	-2.938053	9.463182	H	-10.190912	-7.123069	3.443337
C	-0.421068	-2.437229	7.021181	H	-9.635326	-5.461252	3.199163
C	0.285026	4.580593	5.990374	H	-8.706505	-6.804667	2.524116
H	-7.540957	0.460719	4.894170	H	-0.770890	-2.017475	6.082265
H	-6.330191	0.457557	3.606537	H	0.568851	-2.883683	7.037838
H	-6.082212	2.401074	5.122653	H	-4.591521	-1.149488	10.463044
H	-5.841433	1.325172	6.493013	H	-5.100396	-1.821202	8.884538
H	-3.942262	3.255019	4.286431	H	-4.425191	-0.170270	8.974614
H	-2.748671	2.025712	3.860179	H	-0.647891	-2.151759	10.223175
H	-7.638843	-1.820007	3.924865	H	0.297896	-3.378493	9.359084
H	-6.090576	-1.697449	3.076734	H	-1.376594	-3.706890	9.842860
H	-5.780019	-7.214526	4.777075	H	2.907473	0.462516	5.028436
H	-8.399056	-3.871434	4.325111	H	2.356484	1.324183	3.594286
H	-5.921741	1.696832	-0.886772	H	2.492369	-0.429419	3.554486
H	-5.269255	4.000470	2.649717	H	1.206562	1.174324	6.566599
H	-7.623804	-1.396051	6.402550	H	-0.408609	0.448575	6.451814
H	-6.170793	-2.396019	6.630270	H	1.597860	3.026973	5.307985
H	-6.157016	-0.688251	7.121642	H	0.153175	-2.692345	1.597023
H	-3.867673	2.891157	6.602240	H	-1.410030	-2.180188	2.272165
H	-3.645308	1.222086	7.190400	H	-0.277469	-3.129172	3.270837
H	-2.434549	1.965269	6.112474	H	0.908831	5.412705	5.646710
H	-2.851622	-1.669298	-0.901782	H	0.496481	4.401453	7.048727
H	-2.620919	0.087694	-0.820920	H	-0.764124	4.882258	5.898313
H	-2.625841	-0.871158	0.669408	H	0.957263	4.309065	3.273519
H	-5.065902	-2.705939	-0.241561	H	-0.744003	3.877820	3.522181
H	-4.791201	-2.068887	1.386605	H	0.432855	2.615524	3.123625
H	-6.316597	-1.725098	0.536380				
H	-4.922590	-1.342380	-2.196705				
H	-6.258027	-0.333889	-1.633005	YT2R_TRFf.xyz			
H	-4.733896	0.412077	-2.159865	134			
H	-7.561681	4.757013	-1.588723	scf done: -2511.228813			
H	-6.236040	3.636532	-1.913947	C	-5.017306	0.788745	0.693359
H	-7.741918	3.045395	-1.184836	C	-4.567310	0.930433	2.035074
H	-8.189227	5.446254	0.683897	C	-4.856002	2.135867	2.724191
H	-8.374365	3.756854	1.193992	C	-5.644933	3.122717	2.138214
H	-7.326473	4.850828	2.108053	C	-6.162426	2.979895	0.848393
H	-6.016106	6.248183	-0.347201	C	-5.810075	1.813308	0.159984
H	-5.102689	5.667670	1.052434	O	-3.889828	-0.012280	2.674886
H	-4.659627	5.125557	-0.570164	Y	-3.647574	-0.904872	4.631121
H	-1.606944	-5.823037	5.873276	O	-3.027674	-0.967894	6.706212
H	-2.544184	-4.316565	5.799850	C	-2.273420	-0.805387	7.765783
H	-3.128775	-5.682326	6.771573	O	-2.895260	-0.173369	8.835357
H	-2.381207	-7.854586	4.764215	C	-3.861143	-0.985551	9.485470
H	-3.897012	-7.815020	5.668359	C	-4.183938	2.399905	4.041736
H	-3.916288	-7.955801	3.897524	N	-4.498691	1.505235	5.195485
H	-1.610065	-6.014529	3.360323	C	-3.784321	2.047506	6.365580

C	-7.044827	4.079202	0.242058	H	-7.632994	-1.415468	6.521025
C	-6.264316	5.407883	0.199664	H	-6.159695	-2.413176	6.579706
C	-4.608866	-0.422598	-0.161117	H	-6.101299	-0.733495	7.134856
C	-5.155973	-1.730945	0.440705	H	-4.143241	3.058974	6.616828
O	-4.111301	-2.936715	4.235374	H	-3.897610	1.387911	7.226629
C	-5.089965	-3.836149	4.293419	H	-2.717269	2.117722	6.138659
C	-6.432149	-3.385759	4.252394	H	-2.755318	-1.366746	-0.812793
C	-7.486656	-4.290803	4.346150	H	-2.662358	0.402075	-0.710889
C	-7.272742	-5.665208	4.467554	H	-2.647836	-0.570705	0.776231
C	-5.940459	-6.091321	4.481370	H	-4.877040	-2.583718	-0.190373
C	-4.839178	-5.231263	4.395627	H	-4.756829	-1.905814	1.440814
C	-6.728386	-1.928188	4.029050	H	-6.250512	-1.704451	0.494845
N	-6.163579	-0.984965	5.039489	H	-4.778438	-1.195837	-2.170491
C	-6.538120	-1.406428	6.395667	H	-6.223978	-0.327788	-1.650880
C	-3.404441	-5.781081	4.414842	H	-4.762903	0.569548	-2.116078
C	-2.666942	-5.256547	5.662525	H	-8.125075	4.553572	-1.574434
C	-8.464553	-6.626335	4.573914	H	-6.640936	3.640929	-1.867003
C	-9.334627	-6.513226	3.306308	H	-8.078255	2.821298	-1.226836
O	-1.339668	-1.030336	4.080761	H	-8.947211	5.052293	0.701596
C	-0.149962	-1.256606	4.319710	H	-8.891109	3.335725	1.146433
O	0.648815	-1.750932	3.395365	H	-8.052645	4.536363	2.138246
C	0.075682	-1.987398	2.096320	H	-6.882060	6.205859	-0.229434
C	0.496070	-1.016814	5.671519	H	-5.955484	5.729316	1.199321
C	1.979847	-1.397900	5.674190	H	-5.361473	5.309363	-0.412032
C	0.349384	0.489965	5.949358	H	-1.628407	-5.610935	5.669828
O	0.967991	1.194687	4.892387	H	-2.665592	-4.165899	5.687250
C	1.396910	2.517303	5.201871	H	-3.151634	-5.617814	6.576442
C	2.269280	2.967185	4.041142	H	-2.314302	-7.644926	4.460213
C	-3.359422	-7.316225	4.465864	H	-3.821727	-7.714083	5.375782
C	-2.658927	-5.344082	3.137383	H	-3.852743	-7.772014	3.600403
C	-8.024082	-8.089188	4.720410	H	-1.624035	-5.708443	3.160565
C	-9.315134	-6.259596	5.806170	H	-3.143174	-5.761739	2.247632
C	-6.682285	0.364051	4.740118	H	-2.652280	-4.256672	3.044931
C	-5.947700	1.467593	5.487009	H	-8.905398	-8.735016	4.799075
C	-5.129261	-0.326669	-1.603573	H	-7.442931	-8.428425	3.856308
C	-3.069427	-0.493335	-0.227789	H	-7.420064	-8.243503	5.620965
C	-7.493513	3.746517	-1.187610	H	-10.177290	-6.931582	5.894373
C	-8.306423	4.261236	1.109391	H	-8.724984	-6.340443	6.725242
C	-0.969168	-1.163145	7.882933	H	-9.697598	-5.235854	5.744540
C	-0.183355	-0.959989	9.148751	H	-10.198068	-7.186507	3.368546
C	-0.302443	-1.877618	6.738601	H	-9.715210	-5.496628	3.165905
C	0.225387	3.465548	5.442295	H	-8.758795	-6.778426	2.413460
H	-7.757334	0.422078	4.984900	H	-1.058671	-2.468604	6.213857
H	-6.585306	0.530784	3.664570	H	0.416788	-2.598139	7.146786
H	-6.416565	2.432990	5.241260	H	-4.357319	-0.360356	10.231810
H	-6.066322	1.329568	6.565951	H	-3.382722	-1.836239	9.989464
H	-4.403646	3.437102	4.345476	H	-4.605310	-1.369487	8.778815
H	-3.096158	2.331483	3.903638	H	0.715817	-0.346299	8.990045
H	-7.822145	-1.792715	3.997689	H	0.170295	-1.916344	9.560982
H	-6.334783	-1.604136	3.058161	H	-0.786170	-0.463461	9.911176
H	-5.745153	-7.152690	4.564317	H	2.387327	-1.224985	6.675484
H	-8.502118	-3.899188	4.313319	H	2.546645	-0.798841	4.959131
H	-6.166521	1.695024	-0.855302	H	2.119074	-2.454744	5.431340
H	-5.840473	4.029907	2.708456	H	0.835189	0.717480	6.909423

H	-0.712322	0.746810	6.043837	O	0.231047	-3.125713	2.669531
H	2.010205	2.474408	6.119296	C	-0.607998	-3.307309	1.525366
H	0.895502	-2.363851	1.486431	C	-3.608405	-1.542432	-0.936151
H	-0.319484	-1.056858	1.685905	C	-5.654500	-2.187499	0.382821
H	-0.725670	-2.725267	2.164575	C	-7.720179	4.301930	0.064256
H	0.589354	4.477605	5.647019	C	-5.802577	4.770637	-1.489570
H	-0.378888	3.154788	6.300099	C	-3.726811	-5.543229	2.476965
H	-0.418360	3.505161	4.556995	C	-2.405423	-5.299949	4.610586
H	2.689789	3.958191	4.236222	C	-5.621209	-0.344509	6.238204
H	1.680203	3.017439	3.119703	C	-8.596503	-4.854114	7.674252
H	3.091575	2.263866	3.885092	C	-9.598945	-5.464440	5.452579
YT2S_NLB.xyz				O	-1.586681	-2.242872	7.255088
134				C	-2.876836	-2.836274	7.206188
scf done: -2511.190623				C	-0.181706	1.150527	7.105186
C	-6.204561	-2.808704	4.671264	O	-0.914304	1.784252	8.156620
C	-4.996764	-3.479874	4.356193	C	-0.639444	3.172273	8.311809
C	-4.924237	-4.885349	4.562135	C	-1.849312	3.785035	9.002320
C	-6.004086	-5.506222	5.204045	C	0.559873	-0.970169	8.296105
C	-7.167470	-4.843985	5.608388	C	0.643341	3.400792	9.110163
C	-7.250125	-3.485867	5.294662	H	-6.919431	1.229568	4.598921
O	-3.979424	-2.770137	3.865037	H	-6.031613	0.827140	3.123671
Y	-3.153534	-0.799599	3.857176	H	-5.345475	3.003446	4.086193
O	-2.320954	-0.524588	5.959695	H	-4.866439	2.208809	5.582603
C	-1.446157	-0.978199	6.785401	H	-3.416001	3.470417	2.687017
C	-0.286043	-0.333742	7.221742	H	-2.380976	2.086704	2.306206
C	0.904223	-0.702039	5.191622	H	-7.461154	-1.108451	4.412693
C	0.909000	-1.907858	4.529240	H	-6.284078	-1.350734	3.114558
C	1.919443	-2.988817	4.810724	H	-5.934914	-6.570441	5.388149
C	-3.757367	-5.723211	4.008741	H	-8.156276	-2.927348	5.523775
C	-3.924859	-7.224869	4.289472	H	-6.441971	0.986334	-1.542688
C	-8.329297	-5.546609	6.323097	H	-5.062471	3.947240	1.211382
C	-8.035268	-7.027444	6.599828	H	-6.618951	-0.003576	6.559666
C	-6.417479	-1.395720	4.201774	H	-5.468696	-1.358034	6.610503
N	-5.515690	-0.355092	4.771840	H	-4.857394	0.298067	6.679260
C	-5.928045	0.944277	4.205244	H	-2.805287	3.560437	4.907274
C	-4.946590	2.065339	4.500832	H	-2.633285	2.044064	5.847069
N	-3.587665	1.805448	3.976782	H	-1.606539	2.342920	4.432673
C	-2.609816	2.477433	4.846259	H	-3.551715	-2.565996	-1.326653
O	-3.712559	-0.282135	1.851993	H	-3.195587	-0.868264	-1.694958
C	-4.382077	0.600519	1.120052	H	-2.990799	-1.473190	-0.038738
C	-4.357466	1.956690	1.527587	H	-5.641112	-3.196070	-0.047838
C	-5.113669	2.917336	0.861314	H	-5.077294	-2.206874	1.308468
C	-5.905319	2.590639	-0.242301	H	-6.696621	-1.942826	0.619788
C	-5.864440	1.258324	-0.668587	H	-5.778253	-2.327613	-2.304100
C	-5.119521	0.249842	-0.042847	H	-6.941641	-1.109663	-1.777461
C	-3.399271	2.370839	2.606153	H	-5.504942	-0.629246	-2.705349
C	-5.072628	-1.173908	-0.620435	H	-8.138669	3.918686	-2.576312
C	-5.873480	-1.304266	-1.925183	H	-6.910601	2.690011	-2.895500
C	-6.737323	3.673062	-0.943140	H	-8.255520	2.338833	-1.793110
C	-7.553413	3.114635	-2.117109	H	-8.316710	5.086063	-0.416991
O	-1.031386	-1.349632	3.221095	H	-8.407407	3.547530	0.461995
C	-0.038072	-2.089938	3.470564	H	-7.196615	4.756246	0.911500
				H	-6.381519	5.559094	-1.985016
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H	-5.097924	4.355764	-2.217792	Y	-3.152334	-0.782929	3.529568
H	-1.595032	-5.888952	4.164641	O	-2.265699	-0.510335	5.798160
H	-2.202509	-4.244311	4.430105	C	-1.376412	-0.950974	6.536748
H	-2.387157	-5.476354	5.691157	C	0.017769	-0.348668	6.651232
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H	-3.933912	-7.445851	5.362571	C	0.967294	-1.205848	4.353883
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H	-2.883870	-6.094643	2.042221	C	-3.701696	-5.619171	4.304247
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H	-3.635234	-4.488551	2.209393	C	-8.255085	-5.250195	6.649901
H	-8.882087	-7.480198	7.126755	C	-7.973288	-6.714192	7.015161
H	-7.883182	-7.593898	5.674946	C	-6.381516	-1.294436	4.148918
H	-7.147565	-7.154672	7.228788	N	-5.457313	-0.217078	4.607385
H	-9.432167	-5.335583	8.196036	C	-5.850324	1.035777	3.934336
H	-7.714966	-4.908045	8.321994	C	-4.826305	2.150274	4.093353
H	-8.851003	-3.797411	7.544979	N	-3.492829	1.797169	3.555583
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H	-9.442854	-5.958164	4.487732	C	-4.507600	0.478773	0.804704
H	1.752474	-0.438109	5.814332	C	-4.355924	1.849600	1.131555
H	0.311281	0.111973	4.792375	C	-5.065747	2.829446	0.441082
H	-0.195940	-4.168849	1.000314	C	-5.928525	2.507656	-0.608992
H	-1.637887	-3.507671	1.824870	C	-6.012738	1.154614	-0.957291
H	-0.581951	-2.422951	0.884234	C	-5.323804	0.125075	-0.303219
H	2.528272	-3.212605	3.927816	C	-3.317257	2.252396	2.139659
H	2.589569	-2.676931	5.616201	C	-5.415226	-1.328811	-0.795282
H	1.443778	-3.927209	5.116055	C	-6.290540	-1.467132	-2.050419
H	1.576113	-0.556193	8.273390	C	-6.707817	3.613132	-1.334399
H	0.161380	-0.774502	9.300508	C	-7.586031	3.062578	-2.466568
H	0.633129	-2.052319	8.173257	O	-1.085455	-1.106603	3.148377
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H	-2.761874	-3.826625	7.647628	C	-4.002606	-1.831781	-1.157141
H	-3.587226	-2.255879	7.805152	C	-6.020823	-2.235918	0.293118
H	-3.251026	-2.938486	6.187060	C	-7.623253	4.339796	-0.329171
H	-1.709023	4.859263	9.159163	C	-5.721900	4.627695	-1.946988
H	-2.753169	3.634444	8.405241	C	-3.616942	-5.561603	2.764871
H	-2.003796	3.311108	9.977068	C	-2.373096	-5.129191	4.910641
H	0.849603	4.471003	9.217889	C	-5.538520	-0.077703	6.065314
H	0.543921	2.964504	10.109268	C	-8.470881	-4.464738	7.958731
H	1.511125	2.943862	8.625217	C	-9.549887	-5.206822	5.814434
YT2S_NLBb.xyz				O	-1.581163	-1.965765	7.349428
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C	-6.162752	-2.667412	4.727444	O	-0.868652	0.804724	8.578047
C	-4.967554	-3.373037	4.435346	C	-1.033133	1.976241	9.376631
C	-4.885021	-4.752411	4.771559	C	-2.219629	1.713731	10.290900
C	-5.951501	-5.313377	5.485968	C	0.955961	-1.239918	7.469445
C	-7.106200	-4.614453	5.855284	C	0.235716	2.297161	10.162255
C	-7.192385	-3.285510	5.434233	H	-6.821513	1.390825	4.322444
O	-3.966701	-2.726380	3.846404	H	-5.986925	0.822410	2.871183
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H	-3.245396	3.352407	2.144755
H	-2.338240	1.866894	1.823077
H	-7.418123	-0.983583	4.362747
H	-6.277567	-1.339233	3.058323
H	-5.878980	-6.358124	5.759333
H	-8.090674	-2.705549	5.640946
H	-6.647324	0.882623	-1.790850
H	-4.919428	3.869963	0.727207
H	-6.527451	0.300049	6.374511
H	-5.388877	-1.056486	6.522225
H	-4.766440	0.597887	6.438164
H	-2.581988	3.557861	4.354196
H	-2.475835	2.095971	5.379242
H	-1.467853	2.239626	3.929446
H	-4.047354	-2.875502	-1.490959
H	-3.577242	-1.234650	-1.971481
H	-3.333813	-1.770409	-0.296836
H	-6.116418	-3.262315	-0.080954
H	-5.391285	-2.259544	1.183826
H	-7.022647	-1.889915	0.573689
H	-6.292512	-2.513883	-2.372864
H	-7.332007	-1.181215	-1.864550
H	-5.912047	-0.867345	-2.885343
H	-8.125621	3.884823	-2.948812
H	-6.989327	2.562886	-3.237031
H	-8.331879	2.351132	-2.096250
H	-8.182348	5.142765	-0.824437
H	-8.345658	3.645225	0.112930
H	-7.049259	4.788832	0.487784
H	-6.263515	5.427557	-2.465712
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H	-5.060256	4.139627	-2.670071
H	-1.542182	-5.743690	4.544716
H	-2.170386	-4.092675	4.637910
H	-2.390415	-5.213170	6.003137
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H	-3.482098	-4.535614	2.418054
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H	-9.296358	-4.896087	8.537547
H	-7.570203	-4.489454	8.581713
H	-8.713813	-3.415162	7.764577
H	-10.383603	-5.651836	6.370558
H	-9.832779	-4.181385	5.556698
H	-9.428356	-5.762837	4.879056
H	1.476009	0.580737	5.399371
H	-0.146885	0.577534	4.711947
H	0.296094	-3.632504	0.837185
H	-1.260099	-3.098418	1.518935

H	-0.179022	-1.913518	0.746341
H	2.621487	-2.311214	3.536740
H	3.095830	-0.996467	4.625552
H	2.474214	-2.507840	5.279295
H	1.959722	-0.802748	7.462485
H	0.616929	-1.319298	8.503947
H	1.019904	-2.242210	7.042904
H	0.840132	1.418261	7.550702
H	-0.706320	1.705839	6.723922
H	-1.271514	2.825213	8.712413
H	-2.811097	-3.407176	8.046435
H	-3.566128	-1.791443	7.915644
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H	-2.411341	2.576654	10.935721
H	-3.120882	1.509443	9.706017
H	-2.019403	0.845622	10.926892
H	0.097002	3.202392	10.762014
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134			
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C	-7.259991	-4.750905	5.694819
C	-7.278948	-3.392302	5.371551
O	-4.002429	-2.857345	3.885911
Y	-3.061228	-0.955117	3.876867
O	-2.077425	-0.759179	5.812186
C	-1.517454	-1.188012	6.924690
C	-0.754677	-0.464957	7.786237
C	1.209870	-0.817936	4.632732
C	1.408346	-1.498535	3.495395
C	2.761183	-1.816624	2.924021
C	-3.858837	-5.788184	4.162591
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C	-8.450841	-5.390533	6.421251
C	-8.226818	-6.881309	6.710297
C	-6.349784	-1.348716	4.263152
N	-5.366106	-0.363246	4.798552
C	-5.703857	0.958985	4.233737
C	-4.642060	2.014112	4.501628
N	-3.316508	1.659604	3.948706
C	-2.268253	2.261646	4.787906
O	-3.544628	-0.434284	1.818424
C	-4.225455	0.468527	1.123787
C	-4.135572	1.824929	1.524749
C	-4.891076	2.811859	0.897310
C	-5.750803	2.513978	-0.162606
C	-5.781288	1.180000	-0.584719

C	-5.040310	0.146132	0.002766	H	-8.036390	3.922815	-2.396711
C	-3.125835	2.198382	2.569233	H	-6.855218	2.663496	-2.770864
C	-5.078469	-1.277708	-0.574422	H	-8.168692	2.339991	-1.622711
C	-5.957071	-1.383085	-1.830172	H	-8.103165	5.070940	-0.214708
C	-6.582437	3.623939	-0.819554	H	-8.200110	3.523485	0.647927
C	-7.457334	3.098714	-1.966175	H	-6.940893	4.693615	1.064385
O	-0.955338	-1.678256	3.032635	H	-6.224454	5.513086	-1.854492
C	0.208083	-2.005315	2.787870	H	-5.016723	5.151298	-0.614444
O	0.506852	-2.871062	1.832747	H	-4.981294	4.282191	-2.153599
C	-0.589269	-3.438504	1.093735	H	-1.712039	-5.996551	4.455877
C	-3.647671	-1.689095	-0.974874	H	-2.306863	-4.339667	4.701782
C	-5.632514	-2.272506	0.462654	H	-2.594736	-5.578940	5.929836
C	-7.509165	4.265043	0.232721	H	-3.247700	-7.856840	4.051626
C	-5.644737	4.705276	-1.392165	H	-4.161510	-7.493316	5.516717
C	-3.720557	-5.627815	2.634596	H	-5.000359	-7.655231	3.958749
C	-2.539381	-5.394062	4.852186	H	-2.877999	-6.226765	2.265498
C	-5.427836	-0.333485	6.268629	H	-4.626721	-5.976623	2.127200
C	-8.677554	-4.674511	7.767493	H	-3.561736	-4.581971	2.364691
C	-9.719459	-5.255671	5.555958	H	-9.093205	-7.288480	7.242668
O	-1.677022	-2.532458	7.198922	H	-8.103676	-7.462497	5.790243
C	-3.003580	-2.928078	7.508655	H	-7.345034	-7.045020	7.339135
C	-0.431954	0.966517	7.521238	H	-9.531042	-5.112611	8.298623
O	-1.393241	1.830789	8.147076	H	-7.795027	-4.763376	8.409939
C	-0.958995	3.176331	8.304772	H	-8.883919	-3.608425	7.630113
C	-2.209791	4.033597	8.437807	H	-10.583583	-5.698652	6.065593
C	-0.229714	-1.032659	9.076284	H	-9.958006	-4.208102	5.346933
C	-0.044687	3.329871	9.520022	H	-9.592237	-5.765243	4.595059
H	-6.664524	1.311508	4.648432	H	2.052505	-0.443717	5.206604
H	-5.839122	0.844458	3.155215	H	0.213538	-0.649874	5.030218
H	-4.988333	2.974347	4.090101	H	-0.127971	-4.083087	0.347148
H	-4.527838	2.157151	5.580039	H	-1.232260	-4.017395	1.758770
H	-3.077161	3.298019	2.636709	H	-1.173135	-2.649448	0.618079
H	-2.133357	1.851694	2.249431	H	2.861738	-1.442058	1.900039
H	-7.365762	-0.997233	4.508117	H	3.546261	-1.366881	3.535903
H	-6.251200	-1.314157	3.171618	H	2.929044	-2.897457	2.884536
H	-6.104976	-6.534605	5.500238	H	0.870237	-1.027175	9.104549
H	-8.154429	-2.788601	5.605747	H	-0.567672	-0.431499	9.931110
H	-6.414670	0.927708	-1.425567	H	-0.559329	-2.061075	9.227134
H	-4.787375	3.838788	1.244708	H	0.569863	1.190126	7.920617
H	-6.390197	0.078909	6.612997	H	-0.410565	1.181234	6.443620
H	-5.334436	-1.350873	6.648609	H	-0.407065	3.488971	7.399799
H	-4.610124	0.259446	6.681781	H	-2.947930	-3.954655	7.876569
H	-2.349123	3.361115	4.796113	H	-3.426959	-2.289693	8.296353
H	-2.334716	1.885692	5.809268	H	-3.656162	-2.912852	6.629879
H	-1.284827	2.002236	4.384737	H	-1.949152	5.088300	8.572138
H	-3.636054	-2.721857	-1.344767	H	-2.840776	3.942163	7.549331
H	-3.266522	-1.039000	-1.770396	H	-2.794545	3.710152	9.305174
H	-2.980795	-1.611382	-0.114205	H	0.297634	4.365362	9.621593
H	-5.666328	-3.283109	0.037552	H	-0.584584	3.052306	10.431077
H	-5.013550	-2.302354	1.360663	H	0.841634	2.693259	9.444411
H	-6.655659	-2.000705	0.747506				
H	-5.915749	-2.408730	-2.212843				
H	-7.008299	-1.156169	-1.620497				
H	-5.614364	-0.719025	-2.631250				

scf done: -2511.198581				C	0.679014	-1.911782	4.799601
C	-5.013715	0.475982	0.252715	C	2.182289	-1.892607	4.689196
C	-4.456380	0.673849	1.546722	C	0.013039	-2.212960	5.970530
C	-4.486761	1.975086	2.108631	C	-0.076248	4.352230	6.207983
C	-5.110556	3.026725	1.440957	H	-7.549339	0.641666	4.474347
C	-5.712634	2.851938	0.193162	H	-6.362986	0.424407	3.179679
C	-5.628905	1.572276	-0.365844	H	-6.065664	2.580788	4.309178
O	-3.918738	-0.306474	2.262598	H	-5.896482	1.788496	5.869477
Y	-3.526513	-0.987194	4.265345	H	-3.788563	3.329781	3.587476
O	-1.367824	-1.442673	3.644089	H	-2.694636	1.978282	3.282154
C	-0.116946	-1.599113	3.655525	H	-7.828933	-1.693605	4.135202
O	0.580518	-1.456039	2.519762	H	-6.441599	-1.790871	3.045628
C	-0.159845	-1.184498	1.328785	H	-5.969268	-6.992986	5.460645
C	-3.755574	2.245247	3.393949	H	-8.569847	-3.647971	4.913485
N	-4.231306	1.539416	4.624148	H	-6.066169	1.416377	-1.343580
C	-3.561157	2.171557	5.775325	H	-5.110879	4.007373	1.914611
C	-6.409536	4.029146	-0.502137	H	-7.411263	-0.677313	6.458948
C	-5.401030	5.174334	-0.720286	H	-6.126344	-1.896238	6.621246
C	-4.922543	-0.880766	-0.466962	H	-5.736037	-0.180701	6.830453
C	-5.657013	-1.974350	0.331235	H	-3.872782	3.223406	5.880922
O	-4.164561	-3.005240	4.278961	H	-3.803299	1.631320	6.691495
C	-5.178059	-3.817770	4.572515	H	-2.476560	2.147673	5.662716
C	-6.493919	-3.294036	4.571810	H	-3.356169	-2.249148	-1.117875
C	-7.577373	-4.096289	4.922640	H	-2.901508	-0.537217	-1.221397
C	-7.421173	-5.440954	5.264405	H	-2.966998	-1.344374	0.362158
C	-6.118615	-5.948513	5.219377	H	-5.627805	-2.925557	-0.213664
C	-4.989841	-5.192838	4.878970	H	-5.188122	-2.128782	1.304145
C	-6.744505	-1.890449	4.094251	H	-6.709862	-1.707899	0.479869
N	-6.036857	-0.806918	4.833513	H	-5.421890	-1.824084	-2.343865
C	-6.346389	-0.888094	6.266176	H	-6.612713	-0.619072	-1.848418
C	-3.596106	-5.838687	4.829985	H	-5.050077	-0.106640	-2.520085
C	-2.685686	-5.186469	5.887419	H	-7.482477	4.507769	-2.321460
C	-8.640961	-6.287967	5.650525	H	-6.211826	3.303806	-2.561470
C	-9.635197	-6.328179	4.473158	H	-7.738563	2.844941	-1.782458
O	-2.794935	-0.716107	6.376302	H	-8.071184	5.386510	-0.088991
C	-1.896715	-0.747194	7.289616	H	-8.309202	3.745514	0.542037
O	-2.199402	-1.372478	8.452890	H	-7.210896	4.861339	1.364794
C	-3.475626	-1.987742	8.566986	H	-5.884791	6.026784	-1.211729
C	-0.575928	-0.292363	7.187237	H	-4.981231	5.531740	0.225282
C	0.325920	-0.321276	8.395622	H	-4.568320	4.845058	-1.350529
C	-0.214695	0.701179	6.133692	H	-1.676608	-5.613739	5.842499
O	-0.276563	2.033491	6.649997	H	-2.612852	-4.110981	5.720274
C	0.517125	2.977961	5.934301	H	-3.080681	-5.359089	6.895236
C	1.983067	2.903763	6.356812	H	-2.616602	-7.749997	5.057077
C	-3.632861	-7.346606	5.123462	H	-4.004889	-7.564897	6.130683
C	-2.983727	-5.658404	3.425757	H	-4.251027	-7.891750	4.401867
C	-8.262432	-7.733192	6.002250	H	-1.982219	-6.104403	3.391245
C	-9.332889	-5.664222	6.878645	H	-3.601434	-6.158519	2.671419
C	-6.476734	0.480756	4.264863	H	-2.905628	-4.602564	3.162615
C	-5.696077	1.669527	4.800482	H	-9.162466	-8.294170	6.276438
C	-5.540326	-0.842212	-1.873104	H	-7.797296	-8.249929	5.156035
C	-3.440807	-1.276387	-0.618223	H	-7.572954	-7.778572	6.852129
C	-6.990457	3.640280	-1.868584	H	-10.214785	-6.249686	7.165195
C	-7.566588	4.534661	0.382400	H	-8.651603	-5.633815	7.735761

H	-9.664579	-4.640142	6.680124
H	-10.519705	-6.921985	4.733493
H	-9.976964	-5.325805	4.196892
H	-9.171834	-6.776769	3.588191
H	-1.028093	-2.502959	5.919365
H	0.570997	-2.577445	6.827349
H	0.587192	-0.995717	0.557626
H	-0.772914	-2.046316	1.054056
H	-0.808980	-0.315418	1.455349
H	2.571006	-0.922625	4.358137
H	2.634788	-2.125070	5.657181
H	2.539275	-2.635108	3.966259
H	1.376608	-0.333013	8.081784
H	0.191348	0.565388	9.027461
H	0.145649	-1.202259	9.015552
H	0.803754	0.490144	5.776973
H	-0.878042	0.612943	5.261032
H	0.443092	2.765815	4.852909
H	-3.459677	-2.517084	9.520906
H	-4.274279	-1.239739	8.580269
H	-3.660844	-2.694703	7.754146
H	0.500229	5.132806	5.701653
H	-1.112102	4.407414	5.862300
H	-0.064384	4.557420	7.283292
H	2.587467	3.617572	5.787115
H	2.077908	3.140877	7.421348
H	2.403178	1.907394	6.191586

YT2S_NLFb.xyz
134

scf done: -2511.202236

C	-4.944195	0.556783	0.391332
C	-4.410526	0.724698	1.700586
C	-4.479680	2.008214	2.300432
C	-5.105799	3.068962	1.649648
C	-5.677458	2.922970	0.384061
C	-5.564388	1.660976	-0.208069
O	-3.863184	-0.266227	2.395191
Y	-3.555566	-0.990813	4.412478
O	-1.321730	-1.524114	3.646537
C	-0.134156	-1.855488	3.580095
O	0.579804	-1.669989	2.475473
C	-0.091900	-1.102262	1.341835
C	-3.795174	2.250395	3.616317
N	-4.300802	1.498333	4.805263
C	-3.662841	2.092156	5.997003
C	-6.371972	4.111425	-0.294005
C	-5.365488	5.265162	-0.473942
C	-4.827748	-0.777844	-0.365410
C	-5.562980	-1.900368	0.390177
O	-4.153733	-3.024748	4.372566
C	-5.165176	-3.857551	4.608736
C	-6.488005	-3.355658	4.550114

C	-7.574936	-4.183103	4.822360
C	-7.414191	-5.532798	5.141222
C	-6.101370	-6.014356	5.171256
C	-4.969132	-5.231330	4.915518
C	-6.736227	-1.943002	4.099806
N	-6.072519	-0.870956	4.896424
C	-6.429966	-1.004255	6.314766
C	-3.560528	-5.842532	4.969828
C	-2.757408	-5.175485	6.103137
C	-8.639164	-6.412710	5.423912
C	-9.550479	-6.440638	4.180830
O	-2.635877	-0.784277	6.354256
C	-1.875220	-0.550201	7.396316
O	-2.223427	-1.201707	8.556934
C	-3.550213	-1.669743	8.677899
C	-0.744449	0.209696	7.438502
C	0.027185	0.436418	8.708960
C	-0.186822	0.835553	6.208737
O	-0.292896	2.267070	6.270101
C	0.544351	2.956734	5.349729
C	1.971481	3.080893	5.882106
C	-3.581597	-7.353207	5.250295
C	-2.843723	-5.637787	3.619569
C	-8.254617	-7.858946	5.764099
C	-9.426258	-5.835587	6.617047
C	-6.520190	0.426622	4.354308
C	-5.770576	1.610647	4.942421
C	-5.420646	-0.707294	-1.780735
C	-3.340371	-1.155305	-0.499009
C	-6.933933	3.749640	-1.675743
C	-7.542581	4.593328	0.585701
C	0.661718	-2.473903	4.662130
C	2.098518	-2.821517	4.387225
C	0.050149	-2.684347	5.837438
C	-0.085588	4.321427	5.110569
H	-7.600205	0.562788	4.540467
H	-6.378445	0.402726	3.271124
H	-6.136485	2.529392	4.462523
H	-6.003297	1.701838	6.007553
H	-3.852691	3.327465	3.842785
H	-2.726641	2.004777	3.534279
H	-7.823392	-1.758634	4.104001
H	-6.394655	-1.809871	3.067064
H	-5.946337	-7.059410	5.406462
H	-8.573195	-3.751225	4.767798
H	-5.981719	1.526044	-1.197547
H	-5.133484	4.034542	2.152621
H	-7.511473	-0.857497	6.469248
H	-6.167343	-2.005892	6.659014
H	-5.885795	-0.275209	6.917815
H	-4.002299	3.130487	6.142360
H	-3.910114	1.507986	6.884714
H	-2.575533	2.101362	5.899487
H	-3.235324	-2.114306	-1.021213

H	-2.796009	-0.394901	-1.070605	H	-0.166169	4.867145	6.056295
H	-2.892063	-1.241967	0.491675	H	2.613669	3.595841	5.159434
H	-5.513931	-2.836920	-0.178299	H	1.972938	3.652074	6.816069
H	-5.107707	-2.073973	1.366439	H	2.414974	2.101455	6.083885
H	-6.620905	-1.649304	0.528202				
H	-5.283482	-1.674777	-2.275712	YT2S_NLff.xyz			
H	-6.495567	-0.495953	-1.769336	134			
H	-4.927209	0.050922	-2.398506	scf done: -2511.227885			
H	-7.425859	4.623976	-2.115422	C	-5.267087	0.179272	-0.167045
H	-6.145332	3.433114	-2.366734	C	-4.539793	0.478371	1.016352
H	-7.678094	2.948158	-1.615723	C	-4.420759	1.831528	1.423143
H	-8.045468	5.451687	0.124490	C	-5.083296	2.842334	0.730464
H	-8.282932	3.797439	0.720229	C	-5.864433	2.571762	-0.395588
H	-7.201341	4.902915	1.578618	C	-5.912963	1.238332	-0.818178
H	-5.847434	6.128016	-0.948750	O	-3.970736	-0.456711	1.766234
H	-4.955865	5.599744	0.484369	Y	-3.301073	-0.885520	3.748773
H	-4.525454	4.954506	-1.104041	O	-1.208177	-0.711761	3.386847
H	-1.733615	-5.568700	6.129797	C	0.093270	-0.569392	3.468569
H	-2.710775	-4.094699	5.963997	O	0.672572	0.228850	2.511291
H	-3.221491	-5.379157	7.074823	C	0.185817	0.048624	1.188434
H	-2.552983	-7.729757	5.264514	C	-3.465882	2.189282	2.528409
H	-4.027701	-7.588639	6.222790	N	-3.740643	1.645652	3.896024
H	-4.124686	-7.908867	4.477971	C	-2.762564	2.256033	4.811099
H	-1.833342	-6.063498	3.660371	C	-6.595871	3.710640	-1.118877
H	-3.389774	-6.144170	2.815676	C	-5.571883	4.747151	-1.622875
H	-2.769767	-4.578361	3.370426	C	-5.305434	-1.247733	-0.739348
H	-9.158796	-8.444926	5.961717	C	-5.958859	-2.223742	0.257956
H	-7.721840	-8.343613	4.939039	O	-4.026929	-2.890875	3.915795
H	-7.623852	-7.913253	6.657870	C	-5.017393	-3.577434	4.473623
H	-10.315046	-6.443484	6.824813	C	-6.263268	-2.933663	4.697259
H	-8.807360	-5.818109	7.520527	C	-7.300650	-3.604294	5.342554
H	-9.762491	-4.811983	6.423678	C	-7.174342	-4.926458	5.773877
H	-10.436737	-7.059792	4.364794	C	-5.958994	-5.560046	5.492669
H	-9.895258	-5.438043	3.908961	C	-4.880555	-4.944735	4.844674
H	-9.018342	-6.854477	3.317867	C	-6.511498	-1.560321	4.132394
H	-0.988924	-2.419658	5.988511	N	-5.681679	-0.457124	4.699335
H	0.583097	-3.129327	6.671940	C	-5.873157	-0.386349	6.151620
H	0.695583	-0.857939	0.630019	C	-3.609182	-5.738741	4.500347
H	-0.778174	-1.834645	0.913470	C	-2.384759	-5.133358	5.211970
H	-0.652301	-0.211071	1.628015	C	-8.339305	-5.622402	6.490434
H	2.678884	-1.937160	4.105362	C	-9.578685	-5.635772	5.573616
H	2.554936	-3.265103	5.275000	O	-2.635742	-1.002714	6.115673
H	2.185425	-3.534381	3.560858	C	-1.798876	-1.438593	6.914373
H	1.006539	-0.066413	8.689560	O	-2.145295	-2.217233	7.923854
H	0.224539	1.505956	8.850866	C	-3.530976	-2.563163	8.066393
H	-0.515063	0.068481	9.580942	C	-0.303927	-1.186620	6.820775
H	0.878417	0.566879	6.105562	C	0.442848	-1.708299	8.053600
H	-0.701360	0.474252	5.306552	C	-0.106479	0.328469	6.704510
H	0.565822	2.402929	4.393378	O	-0.703625	0.943099	7.832604
H	-3.593366	-2.198989	9.632393	C	-0.389325	2.324732	7.996730
H	-4.272504	-0.842216	8.702755	C	0.991331	2.511120	8.621725
H	-3.823465	-2.356817	7.871545	C	-3.702498	-7.212939	4.924316
H	0.520100	4.916277	4.419496	C	-3.387916	-5.710537	2.973852
H	-1.090090	4.217858	4.690933				

C	-8.011427	-7.074273	6.865913	H	-2.476577	-6.262279	2.713189
C	-8.677265	-4.858188	7.785861	H	-4.229113	-6.183972	2.455722
C	-6.087303	0.808424	4.059593	H	-3.291266	-4.686533	2.609378
C	-5.117910	1.946699	4.344706	H	-8.867574	-7.525811	7.378732
C	-6.101393	-1.328743	-2.051085	H	-7.797639	-7.684585	5.982068
C	-3.864772	-1.710286	-1.039744	H	-7.151251	-7.137705	7.541138
C	-7.403409	3.213346	-2.325797	H	-9.518592	-5.331001	8.306586
C	-7.571133	4.397030	-0.141928	H	-7.819462	-4.847500	8.467173
C	0.874924	-1.101905	4.443830	H	-8.954597	-3.819110	7.581313
C	2.368359	-0.937047	4.465647	H	-10.423356	-6.124323	6.073885
C	0.217309	-1.929390	5.511645	H	-9.894318	-4.623384	5.302697
C	-1.487401	2.922055	8.863647	H	-9.370858	-6.178693	4.645839
H	-7.096275	1.103668	4.397554	H	-0.620357	-2.475299	5.065898
H	-6.142313	0.643606	2.980811	H	0.924025	-2.692330	5.858809
H	-5.489699	2.859894	3.858472	H	0.693070	0.793815	0.572234
H	-5.088584	2.152209	5.419387	H	0.430000	-0.954381	0.813039
H	-3.416878	3.287933	2.604385	H	-0.896644	0.192603	1.126147
H	-2.458668	1.838491	2.269382	H	2.722321	-0.342349	5.322231
H	-7.576007	-1.307985	4.272049	H	2.876462	-1.909388	4.537480
H	-6.318600	-1.563466	3.053483	H	2.717996	-0.438828	3.559463
H	-5.844519	-6.596176	5.784117	H	1.512110	-1.512451	7.923801
H	-8.237416	-3.069676	5.493122	H	0.108206	-1.210797	8.966160
H	-6.483804	1.007025	-1.708212	H	0.308787	-2.786156	8.173028
H	-4.965259	3.867648	1.077984	H	0.971366	0.529453	6.656372
H	-6.903033	-0.081381	6.401650	H	-0.555192	0.698695	5.776367
H	-5.693505	-1.372040	6.579178	H	-0.405036	2.813223	7.007420
H	-5.175183	0.320353	6.604707	H	-3.565333	-3.276755	8.888552
H	-2.918827	3.342641	4.904869	H	-4.111191	-1.672540	8.315826
H	-2.830427	1.798418	5.801412	H	-3.913067	-3.017222	7.149779
H	-1.755344	2.088056	4.421901	H	-1.314588	3.989846	9.028587
H	-3.870227	-2.734491	-1.431824	H	-2.466648	2.796745	8.392834
H	-3.400595	-1.063067	-1.792323	H	-1.511063	2.422541	9.837586
H	-3.251620	-1.688927	-0.136888	H	1.221638	3.575572	8.733584
H	-6.026216	-3.225061	-0.184129	H	1.022192	2.044651	9.611577
H	-5.374017	-2.299088	1.175721	H	1.780353	2.066493	8.008537
H	-6.976587	-1.901401	0.507974				
H	-6.073394	-2.357865	-2.425030				
H	-7.154772	-1.059498	-1.913842	YT2S_TLB.xyz			
H	-5.679882	-0.685182	-2.830971	134			
H	-7.912960	4.057470	-2.803076	scf done: -2511.186017			
H	-6.762070	2.746230	-3.080714	C	-5.879380	-2.880016	4.701540
H	-8.169489	2.487681	-2.032220	C	-4.609693	-3.510351	4.732111
H	-8.101576	5.218957	-0.637552	C	-4.530855	-4.834352	5.250847
H	-8.316911	3.685663	0.228784	C	-5.712032	-5.445706	5.688851
H	-7.048225	4.814118	0.724782	C	-6.970522	-4.838917	5.663545
H	-6.078399	5.571104	-2.139592	C	-7.017100	-3.537113	5.165087
H	-4.992095	5.177809	-0.800394	O	-3.545289	-2.837080	4.287070
H	-4.865635	4.288692	-2.322847	Y	-2.832578	-0.877930	3.813476
H	-1.476218	-5.685285	4.942530	O	-0.718345	-0.433982	3.216406
H	-2.249293	-4.089822	4.925023	C	0.499281	-0.852296	3.170471
H	-2.498957	-5.189348	6.300774	C	0.932962	-2.147997	2.942001
H	-2.780075	-7.728188	4.635452	C	0.265612	-2.524298	5.325687
H	-3.814997	-7.328662	6.008333	C	0.339257	-1.542294	6.278684
H	-4.534281	-7.730732	4.434535	C	1.605039	-1.287647	7.058633

C	-3.191553	-5.575123	5.371315	H	-4.775953	3.623291	0.931637
C	-3.345773	-7.019076	5.875628	H	-6.388487	-0.237122	6.461533
C	-8.251625	-5.532876	6.143523	H	-5.022329	-1.373351	6.561971
C	-7.984698	-6.946396	6.678575	H	-4.715560	0.370504	6.587567
C	-6.041391	-1.513134	4.099801	H	-2.511980	3.481245	4.593881
N	-5.208673	-0.427284	4.695864	H	-2.357674	2.049304	5.649076
C	-5.664348	0.845110	4.107535	H	-1.337022	2.200013	4.211748
C	-4.679310	1.981118	4.322049	H	-3.481687	-3.022344	-1.280667
N	-3.327467	1.666650	3.814935	H	-3.116687	-1.343455	-1.718726
C	-2.330860	2.394510	4.613428	H	-2.879392	-1.892151	-0.048903
O	-3.600855	-0.613214	1.837435	H	-5.560881	-3.583233	0.050613
C	-4.228440	0.252206	1.050042	H	-4.927951	-2.571358	1.356473
C	-4.139341	1.631919	1.366682	H	-6.568051	-2.293822	0.724300
C	-4.872794	2.575514	0.651127	H	-5.729864	-2.805511	-2.214125
C	-5.697014	2.210218	-0.415686	H	-6.867099	-1.550094	-1.717429
C	-5.707892	0.854205	-0.760240	H	-5.443585	-1.130955	-2.694780
C	-4.989230	-0.140664	-0.084035	H	-7.903850	3.473343	-2.809975
C	-3.138353	2.091589	2.390174	H	-6.700297	2.206185	-3.068573
C	-4.974360	-1.590711	-0.597102	H	-8.054623	1.934260	-1.955351
C	-5.804707	-1.765662	-1.878327	H	-8.062058	4.739020	-0.695575
C	-6.509577	3.275119	-1.164532	H	-8.181234	3.238547	0.243615
C	-7.335969	2.679554	-2.312708	H	-6.946266	4.439810	0.644725
O	-1.940509	-0.757016	6.011922	H	-6.124292	5.101224	-2.298228
C	-0.845851	-0.797594	6.623569	H	-4.971192	4.833889	-0.984899
O	-0.710408	-0.118539	7.777953	H	-4.855808	3.871222	-2.463039
C	-1.874544	0.495171	8.322019	H	-1.305535	-5.264363	6.432547
C	-3.520495	-1.984896	-0.927595	H	-2.222789	-3.770413	6.137021
C	-5.540518	-2.563722	0.454150	H	-2.749672	-4.898252	7.393143
C	-7.479905	3.963174	-0.183951	H	-2.356436	-7.487281	5.924582
C	-5.558086	4.331575	-1.760431	H	-3.777532	-7.066526	6.881165
C	-2.499129	-5.652954	3.997906	H	-3.964002	-7.625934	5.205057
C	-2.310777	-4.827341	6.391247	H	-1.524259	-6.146884	4.092700
C	-5.343852	-0.412549	6.157625	H	-3.105689	-6.240103	3.299160
C	-8.896107	-4.708540	7.275586	H	-2.354763	-4.661857	3.568940
C	-9.245569	-5.644519	4.970362	H	-8.924862	-7.399447	7.011467
O	1.492244	0.036871	3.448824	H	-7.558751	-7.599220	5.909361
C	1.145770	1.377843	3.725915	H	-7.301321	-6.935347	7.534473
C	0.026275	-3.160722	2.325682	H	-9.817558	-5.188818	7.625855
O	0.405520	-3.354173	0.968793	H	-8.214643	-4.616581	8.128041
C	-0.246244	-4.436507	0.311694	H	-9.154983	-3.697623	6.945052
C	-0.123450	-4.166261	-1.180400	H	-10.172372	-6.133815	5.293679
C	2.398197	-2.487760	2.912051	H	-9.510246	-4.660674	4.570280
C	0.368098	-5.782835	0.694296	H	-8.817501	-6.231715	4.151290
H	-6.643857	1.133161	4.527090	H	1.082049	-3.229220	5.219766
H	-5.805527	0.689447	3.035807	H	-0.688328	-2.827150	4.910162
H	-5.070277	2.892002	3.844332	H	-1.575656	0.873241	9.299940
H	-4.592576	2.201156	5.391169	H	-2.217590	1.324681	7.697457
H	-3.104277	3.193197	2.369877	H	-2.684243	-0.231236	8.427783
H	-2.142263	1.727595	2.106771	H	1.470523	-1.489504	8.126820
H	-7.101533	-1.222673	4.181098	H	2.407160	-1.930378	6.687957
H	-5.792979	-1.529386	3.032855	H	1.943413	-0.249522	6.970364
H	-5.640745	-6.453950	6.075292	H	2.554035	-3.524273	3.241259
H	-7.967065	-3.007584	5.116592	H	2.809295	-2.420510	1.897408
H	-6.305139	0.550969	-1.610275	H	2.983681	-1.831237	3.558629

H	0.101668	-4.116633	2.872676
H	-1.030355	-2.847307	2.372246
H	-1.314262	-4.434976	0.589695
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H	0.539413	1.810936	2.923458
H	0.612973	1.472387	4.677597
H	-0.615806	-4.952775	-1.761208
H	-0.578499	-3.205560	-1.433601
H	0.932255	-4.132697	-1.469505
H	-0.140907	-6.600260	0.172604
H	1.427689	-5.803202	0.418457
H	0.289362	-5.979676	1.767424

YT2S_TLBb.xyz
134

scf done: -2511.198619

C	-6.034223	-2.786522	4.765738
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C	-5.928528	-5.444690	5.511122
C	-7.031629	-4.689843	5.925193
C	-7.061562	-3.354465	5.517026
O	-3.902725	-2.974244	3.746379
Y	-2.995608	-1.066742	3.448252
O	-0.966718	-1.221946	2.818081
C	0.126642	-0.958713	2.128555
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C	0.672765	-0.449359	5.576902
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C	0.869983	-1.061041	8.005956
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C	-3.940624	-7.317823	4.686064
C	-8.185719	-5.273058	6.751773
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C	-6.192373	-1.382414	4.242341
N	-5.183380	-0.390319	4.715402
C	-5.507240	0.928543	4.140287
C	-4.377102	1.935232	4.310542
N	-3.114704	1.490202	3.680350
C	-1.961286	1.978065	4.455947
O	-3.894973	-0.531925	1.590452
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C	-4.090821	1.802612	1.319257
C	-4.706671	2.901631	0.724726
C	-5.664564	2.754822	-0.281313
C	-5.945635	1.446982	-0.691996
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C	-2.960154	2.022159	2.287609
C	-5.663773	-1.097072	-0.701492
C	-6.645019	-1.047470	-1.883129
C	-6.330660	3.991670	-0.898687
C	-7.376592	3.623326	-1.960142
O	-2.077964	-1.191603	5.743222

C	-1.260367	-1.447860	6.630918
O	-1.553042	-2.221843	7.668024
C	-2.863749	-2.804383	7.742786
C	-4.355826	-1.738027	-1.208458
C	-6.287037	-2.003038	0.377741
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C	-5.259003	4.875299	-1.567914
C	-3.669728	-5.820538	2.725996
C	-2.377644	-5.401645	4.848765
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C	-9.496503	-5.177103	5.945817
O	0.058174	0.206335	1.374725
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C	1.389118	-2.916411	2.967422
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C	3.228747	-5.427995	3.193600
H	-6.422414	1.336923	4.604453
H	-5.716163	0.797430	3.075982
H	-4.695908	2.901260	3.893144
H	-4.184977	2.101810	5.375391
H	-2.775290	3.106450	2.361222
H	-2.040628	1.564685	1.900747
H	-7.199173	-1.018601	4.508110
H	-6.128556	-1.384349	3.148495
H	-5.895662	-6.491621	5.783802
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H	-6.662018	1.307371	-1.491208
H	-4.410410	3.896735	1.052934
H	-6.149321	0.093439	6.549428
H	-5.100759	-1.340859	6.574454
H	-4.374006	0.275527	6.557458
H	-1.978425	3.074911	4.557504
H	-1.959267	1.529684	5.452468
H	-1.037238	1.697493	3.944871
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H	-3.915327	-1.136465	-2.011316
H	-3.627360	-1.828511	-0.400567
H	-6.552597	-2.975363	-0.054233
H	-5.586006	-2.178007	1.194978
H	-7.203638	-1.556843	0.781224
H	-6.808814	-2.064213	-2.255823
H	-7.621692	-0.643592	-1.593580
H	-6.258881	-0.451288	-2.717094
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H	-4.504462	5.211380	-0.849463	O	-3.771753	-2.838948	4.103400
H	-4.740578	4.326369	-2.360981	Y	-2.926968	-0.907399	3.840952
H	-1.570763	-6.039723	4.469358	O	-0.733120	-1.079088	2.954407
H	-2.156343	-4.370254	4.570015	C	0.487748	-1.231240	3.040559
H	-2.379033	-5.484131	5.942217	C	1.144947	-2.332037	3.851205
H	-3.115928	-7.924051	4.295962	C	0.506632	-2.354838	5.270442
H	-3.950391	-7.442492	5.774916	C	0.516596	-1.093130	6.095688
H	-4.871129	-7.732486	4.283697	C	1.756442	-0.743276	6.875456
H	-2.863241	-6.470635	2.366275	C	-3.566278	-5.699932	4.758145
H	-4.610850	-6.181709	2.296842	C	-3.784491	-7.170758	5.145367
H	-3.489522	-4.808832	2.359510	C	-8.526903	-5.377204	6.019849
H	-8.798616	-7.114941	7.712820	C	-8.341769	-6.863766	6.353705
H	-7.882617	-7.380463	6.226529	C	-6.162714	-1.332689	4.189168
H	-7.046240	-6.882622	7.709602	N	-5.207907	-0.364751	4.807984
H	-9.166165	-4.873767	8.662670	C	-5.581524	0.990256	4.354853
H	-7.424854	-4.536528	8.663882	C	-4.476884	2.015561	4.563982
H	-8.545284	-3.418728	7.872245	N	-3.230128	1.681636	3.845092
H	-10.336098	-5.584457	6.521794	C	-2.092889	2.323961	4.529358
H	-9.739711	-4.140937	5.690345	O	-3.545548	-0.509004	1.804860
H	-9.420182	-5.740005	5.009750	C	-4.304330	0.334535	1.120248
H	1.697287	-0.088879	5.567440	C	-4.289196	1.704881	1.487835
H	0.124049	-0.443862	4.640326	C	-5.138530	2.619734	0.869710
H	-2.777860	-3.620091	8.459337	C	-6.017175	2.234909	-0.146237
H	-3.571800	-2.059081	8.111572	C	-5.964615	0.893538	-0.543308
H	-3.184907	-3.177780	6.769929	C	-5.128158	-0.070447	0.034131
H	0.989912	-2.109284	8.297077	C	-3.234119	2.191317	2.441837
H	1.861390	-0.610160	7.922475	C	-5.067657	-1.504045	-0.519863
H	0.331430	-0.565439	8.820496	C	-5.956919	-1.688481	-1.759384
H	3.376004	-1.182335	2.004882	C	-6.951723	3.266287	-0.792924
H	2.736573	-2.052098	0.616445	C	-7.825785	2.653377	-1.895645
H	2.349217	-0.330010	0.840148	O	-1.798097	-0.647946	5.682715
H	2.256894	-2.847079	3.649224	C	-0.641867	-0.396415	6.248840
H	0.490123	-3.062534	3.582004	O	-0.627160	0.720928	7.075601
H	1.119353	-5.324002	3.630971	C	-1.526554	0.632617	8.169180
H	-0.521812	0.975679	-0.415314	C	-3.617645	-1.823470	-0.939649
H	0.057077	-0.711399	-0.496503	C	-5.533011	-2.523313	0.537470
H	-1.561819	-0.348665	0.173720	C	-7.884653	3.861093	0.280761
H	1.495817	-7.349722	2.197860	C	-6.117850	4.400269	-1.421701
H	0.318038	-6.230973	1.471598	C	-3.075660	-5.681634	3.296511
H	1.977858	-6.291428	0.855515	C	-2.480639	-5.134513	5.694213
H	3.376164	-6.387697	3.700845	C	-5.253004	-0.462667	6.273895
H	3.895478	-5.389434	2.325846	C	-8.992350	-4.654381	7.299244
H	3.528135	-4.636690	3.887609	C	-9.625720	-5.262875	4.944517
				O	1.323265	-0.452749	2.380849
YT2S_TLbf.xyz				C	0.754691	0.545238	1.519979
134				C	0.767589	-3.653258	3.150123
scf done: -2511.230967				O	1.228767	-3.613292	1.819810
C	-6.069792	-2.757526	4.663263	C	0.883509	-4.750726	1.027133
C	-4.855984	-3.478074	4.539127	C	1.019806	-4.320059	-0.424497
C	-4.843477	-4.856061	4.888596	C	2.669664	-2.191130	3.887077
C	-6.032739	-5.427228	5.356695	C	1.769024	-5.949560	1.357304
C	-7.235204	-4.729062	5.504282	H	-6.491244	1.329438	4.879214
C	-7.218826	-3.380279	5.145641	H	-5.822668	0.936078	3.290449
				H	-4.847271	3.006650	4.255978

H	-4.233821	2.089077	5.628650	H	-2.560896	0.498448	7.833232
H	-3.275171	3.292949	2.480953	H	-1.261837	-0.204319	8.829695
H	-2.250518	1.921369	2.035750	H	1.539520	0.008269	7.636381
H	-7.188464	-0.972936	4.370664	H	2.168486	-1.630990	7.376145
H	-5.990203	-1.279019	3.107047	H	2.564449	-0.340323	6.249720
H	-6.016905	-6.476647	5.621162	H	3.083417	-2.965574	4.540931
H	-8.127466	-2.785695	5.226592	H	3.092731	-2.319485	2.889244
H	-6.606409	0.579439	-1.356535	H	2.979688	-1.219554	4.274192
H	-5.091191	3.660896	1.186349	H	1.224055	-4.476980	3.721207
H	-6.265050	-0.251541	6.654341	H	-0.324161	-3.790415	3.176237
H	-4.968497	-1.469850	6.582394	H	-0.168897	-5.011250	1.228006
H	-4.551084	0.243783	6.720349	H	1.587696	0.929977	0.933307
H	-2.212183	3.419209	4.559633	H	-0.008660	0.104519	0.876554
H	-1.978724	1.934169	5.540855	H	0.313182	1.347273	2.116065
H	-1.168797	2.100268	3.989440	H	0.757207	-5.142398	-1.096670
H	-3.553569	-2.847805	-1.326638	H	0.361693	-3.473537	-0.637822
H	-3.287052	-1.142138	-1.732054	H	2.051120	-4.018218	-0.634637
H	-2.937801	-1.727401	-0.090916	H	1.498930	-6.807355	0.733211
H	-5.494631	-3.538831	0.124777	H	2.820186	-5.705245	1.172618
H	-4.901097	-2.496636	1.426367	H	1.666697	-6.259280	2.401634
H	-6.569628	-2.327755	0.835526				
H	-5.847832	-2.713098	-2.131007				
H	-7.018324	-1.535224	-1.534521	YT2S_TLF.xyz			
H	-5.675909	-1.011124	-2.573313	134			
H	-8.480038	3.423158	-2.319059	scf done: -2511.193386			
H	-7.222498	2.246913	-2.714357	C	-5.401804	-5.178724	4.917571
H	-8.464529	1.851248	-1.510907	C	-5.457248	-3.788194	4.628173
H	-8.551147	4.613045	-0.158394	C	-6.721487	-3.148350	4.591631
H	-8.504964	3.080407	0.734105	C	-7.882373	-3.857155	4.893568
H	-7.319204	4.345558	1.083183	C	-7.856783	-5.213890	5.222055
H	-6.770939	5.148726	-1.886586	C	-6.603528	-5.834839	5.211806
H	-5.503924	4.914388	-0.675502	O	-4.363639	-3.068883	4.385036
H	-5.445959	4.008499	-2.192518	Y	-3.572023	-1.107279	4.404739
H	-1.544348	-5.694743	5.578284	O	-1.406836	-1.329987	4.061344
H	-2.289682	-4.082061	5.480898	C	-0.197519	-0.921965	4.210326
H	-2.794186	-5.218369	6.740841	C	0.725772	-1.417700	5.122781
H	-2.842778	-7.717077	5.022527	C	0.497517	-2.770885	5.716927
H	-4.092819	-7.282630	6.190483	O	1.140939	-3.742870	4.897249
H	-4.532381	-7.658444	4.510604	C	1.194925	-5.047009	5.462261
H	-2.147853	-6.259786	3.201466	C	1.291692	-6.023614	4.299445
H	-3.822672	-6.135866	2.636037	C	-6.830699	-1.719315	4.133931
H	-2.895183	-4.661472	2.954208	N	-6.094956	-0.713169	4.953108
H	-9.286544	-7.281665	6.717879	C	-6.402919	0.624267	4.416474
H	-8.041713	-7.443825	5.474452	C	-5.491752	1.706967	4.971799
H	-7.590582	-7.015352	7.136253	N	-4.062248	1.478677	4.666096
H	-9.922937	-5.094988	7.676956	C	-3.243006	2.085330	5.729470
H	-8.235280	-4.730562	8.086994	C	-9.160456	-5.955076	5.548314
H	-9.178188	-3.590977	7.117869	C	-9.855184	-5.277675	6.746039
H	-10.558894	-5.720216	5.294762	C	-4.071762	-5.949493	4.884292
H	-9.840861	-4.219196	4.694368	C	-3.426336	-5.812899	3.490168
H	-9.322278	-5.769737	4.022530	O	-3.916111	-0.466589	2.393423
H	1.035017	-3.147125	5.821499	C	-4.419878	0.492303	1.626220
H	-0.529241	-2.693051	5.167107	C	-4.945369	0.247741	0.329151
H	-1.442374	1.569111	8.725477	C	-5.543947	1.322947	-0.340757

C	-5.632551	2.622478	0.170725	H	-4.875914	-0.422945	-2.418353
C	-5.042728	2.844703	1.417494	H	-7.356494	4.187270	-2.432349
C	-4.434574	1.816076	2.133718	H	-6.087766	2.970526	-2.607001
C	-4.823853	-1.132841	-0.338694	H	-7.627596	2.547038	-1.834020
C	-3.334821	-1.527401	-0.426016	H	-7.974418	5.154509	-0.243095
C	-3.663746	2.139186	3.384711	H	-8.229440	3.538984	0.444227
C	-6.313017	3.774979	-0.580154	H	-7.138099	4.679727	1.241870
C	-7.480718	4.318566	0.266864	H	-5.766157	5.738419	-1.365095
O	-3.109333	-1.010397	6.702667	H	-4.892864	5.303315	0.109346
C	-2.349371	-1.319612	7.659345	H	-4.452658	4.547064	-1.426939
C	-0.972765	-0.945891	7.831743	H	-2.162333	-5.942154	5.931537
C	-0.371474	-0.153849	6.883915	H	-2.911774	-4.340800	5.797771
O	-2.819205	-2.056301	8.675364	H	-3.543104	-5.530015	6.960950
C	-4.172410	-2.503580	8.614735	H	-3.281207	-7.946892	5.103328
C	-5.295783	4.906372	-0.827778	H	-4.665249	-7.644131	6.156512
C	-6.875192	3.335957	-1.939187	H	-4.909040	-7.926225	4.419529
C	-5.587272	-2.203268	0.464335	H	-2.473746	-6.355215	3.460844
C	-5.388148	-1.140386	-1.767990	H	-4.080559	-6.239996	2.722068
C	-6.506222	-0.815017	6.357197	H	-3.238164	-4.767721	3.241087
C	-3.115139	-5.400521	5.959866	H	-9.874861	-7.909935	6.147787
C	-4.255875	-7.450115	5.158734	H	-8.468901	-7.982634	5.081235
C	-10.098072	-5.908929	4.325407	H	-8.270951	-7.530348	6.785729
C	-8.920758	-7.427346	5.909959	H	-10.795637	-5.787802	6.986354
O	0.187499	0.180436	3.501889	H	-9.216227	-5.306986	7.635273
C	-0.366553	0.330515	2.196021	H	-10.090599	-4.229006	6.538646
C	2.149000	-0.926767	5.126361	H	-11.039877	-6.427958	4.539909
C	2.374991	-5.184912	6.423855	H	-10.342035	-4.880620	4.040582
C	-0.231436	-1.451728	9.044224	H	-9.632128	-6.391339	3.459879
H	-7.450827	0.894191	4.637625	H	-0.970921	0.347494	6.137206
H	-6.301010	0.587124	3.329718	H	0.614384	0.259961	7.066608
H	-5.815575	2.682446	4.578062	H	-4.291890	-3.181020	9.460305
H	-5.598988	1.759722	6.059763	H	-4.861053	-1.660808	8.715487
H	-3.700683	3.230175	3.540570	H	-4.371082	-3.030558	7.679025
H	-2.608860	1.876939	3.235067	H	-0.212107	-2.545459	9.095183
H	-7.897136	-1.439187	4.106324	H	0.802011	-1.095470	9.028513
H	-6.445732	-1.620080	3.112522	H	-0.694813	-1.101786	9.973619
H	-6.557038	-6.891586	5.441090	H	2.569680	-0.974355	6.139339
H	-8.831181	-3.324372	4.854998	H	2.784825	-1.558828	4.493807
H	-5.960464	1.133248	-1.321634	H	2.230995	0.101201	4.768699
H	-5.035395	3.845219	1.847708	H	0.917421	-2.801945	6.734960
H	-7.568672	-0.547285	6.481582	H	-0.575821	-2.992935	5.790568
H	-6.370975	-1.843092	6.693603	H	0.258675	-5.240379	6.013170
H	-5.899435	-0.160228	6.985284	H	-0.105109	1.338819	1.870257
H	-3.489528	3.150128	5.868948	H	0.084026	-0.397351	1.510853
H	-3.392147	1.552111	6.670330	H	-1.450745	0.198757	2.187388
H	-2.185966	2.021640	5.459593	H	1.337202	-7.057318	4.657419
H	-3.232113	-2.513203	-0.895249	H	0.427430	-5.917324	3.638555
H	-2.778670	-0.805208	-1.034337	H	2.194886	-5.821035	3.714386
H	-2.882515	-1.570441	0.566359	H	2.398186	-6.183696	6.872916
H	-5.524797	-3.172113	-0.045404	H	3.316224	-5.024853	5.887855
H	-5.166636	-2.322699	1.463704	H	2.319198	-4.455920	7.238017
H	-6.648410	-1.942273	0.552411				
H	-5.248302	-2.135527	-2.203241				
H	-6.461708	-0.921931	-1.791423				

YT2S_TLFb.xyz

134				O	-0.209914	0.521977	3.452700
scf done: -2511.198715				C	-0.356084	0.341849	2.045828
C	-5.427930	-5.215839	4.943955	C	2.241315	-0.733577	4.192710
C	-5.480733	-3.823527	4.654307	C	2.805732	-4.863673	6.096401
C	-6.739850	-3.167077	4.682504	C	-1.332043	-1.162277	9.940815
C	-7.887147	-3.858831	5.066644	H	-7.445431	0.914914	4.564855
C	-7.857138	-5.211241	5.414344	H	-6.270066	0.527548	3.301167
C	-6.616224	-5.851476	5.325071	H	-5.742704	2.652252	4.465905
O	-4.393241	-3.125855	4.350336	H	-5.608705	1.798523	5.999087
Y	-3.619397	-1.138832	4.413883	H	-3.515100	3.103954	3.558536
O	-1.490703	-1.072681	4.447132	H	-2.512596	1.671148	3.292006
C	-0.267073	-0.672863	4.159374	H	-7.933772	-1.481260	4.152627
C	0.883799	-1.271663	4.544395	H	-6.478339	-1.675677	3.166028
C	0.855344	-2.552482	5.315622	H	-6.570359	-6.908107	5.555785
O	1.445652	-3.583607	4.527224	H	-8.831333	-3.316179	5.076336
C	1.574562	-4.832027	5.189849	H	-5.839781	1.172334	-1.345764
C	1.644804	-5.896148	4.103760	H	-4.761815	3.810409	1.836711
C	-6.864270	-1.748821	4.189054	H	-7.644972	-0.424109	6.455963
N	-6.138451	-0.713206	4.980751	H	-6.520852	-1.769732	6.742353
C	-6.399888	0.609344	4.382859	H	-5.976061	-0.103943	7.003420
C	-5.468844	1.688339	4.918939	H	-3.359109	2.999743	5.893707
N	-4.042862	1.385735	4.668411	H	-3.448402	1.407058	6.698463
C	-3.209887	1.916215	5.761405	H	-2.156966	1.742158	5.527042
C	-9.145293	-5.929676	5.838757	H	-3.390098	-2.656845	-0.903448
C	-9.732258	-5.242390	7.087660	H	-2.820416	-0.984044	-1.044214
C	-4.118774	-6.010716	4.793937	H	-2.977686	-1.737851	0.557165
C	-3.598602	-5.874181	3.347784	H	-5.734051	-3.151987	-0.056026
O	-3.953300	-0.572672	2.386573	H	-5.293895	-2.338594	1.452074
C	-4.380888	0.423715	1.619326	H	-6.754119	-1.843065	0.560320
C	-4.909696	0.217430	0.316969	H	-5.380960	-2.145517	-2.209130
C	-5.421420	1.332158	-0.360400	H	-6.504624	-0.847366	-1.798544
C	-5.421018	2.634548	0.150967	H	-4.888729	-0.464586	-2.430315
C	-4.836209	2.812549	1.407091	H	-7.007183	4.321336	-2.463762
C	-4.312676	1.744181	2.131986	H	-5.854586	2.993555	-2.631175
C	-4.883379	-1.169819	-0.348284	H	-7.420736	2.718905	-1.843373
C	-3.425311	-1.665534	-0.435717	H	-7.511317	5.374491	-0.297422
C	-3.549288	2.013325	3.400861	H	-7.916738	3.805040	0.423921
C	-5.992418	3.837035	-0.612443	H	-6.718078	4.853355	1.194699
C	-7.097846	4.505740	0.228600	H	-5.261627	5.730360	-1.419709
O	-3.439253	-1.313591	6.879181	H	-4.421503	5.221826	0.051602
C	-2.907697	-1.580927	7.960092	H	-4.072227	4.414918	-1.481924
C	-1.658414	-0.974728	8.485320	H	-2.111587	-6.041411	5.637941
C	-0.867344	-0.332290	7.614999	H	-2.853574	-4.432454	5.621114
O	-3.420411	-2.461229	8.809794	H	-3.373095	-5.648479	6.814851
C	-4.628759	-3.147441	8.446245	H	-3.352256	-8.024903	4.933309
C	-4.870435	4.860274	-0.879014	H	-4.636268	-7.704158	6.100992
C	-6.601251	3.435665	-1.963110	H	-5.031266	-7.967930	4.389391
C	-5.717025	-2.183745	0.458564	H	-2.664551	-6.436082	3.228082
C	-5.449316	-1.141657	-1.776608	H	-4.328707	-6.278565	2.638123
C	-6.593684	-0.747096	6.373503	H	-3.411054	-4.830209	3.092620
C	-3.051212	-5.493992	5.778063	H	-9.847590	-7.873697	6.486300
C	-4.308680	-7.509820	5.073303	H	-8.527684	-7.966887	5.316249
C	-10.175689	-5.864187	4.693986	H	-8.193495	-7.525820	7.002132
C	-8.905624	-7.407210	6.178309	H	-10.664007	-5.731222	7.396231

H	-9.029436	-5.291669	7.926594
H	-9.956600	-4.187321	6.901020
H	-11.106420	-6.367354	4.982334
H	-10.424446	-4.831467	4.430162
H	-9.788422	-6.352649	3.793832
H	-1.114292	-0.279751	6.559678
H	0.070103	0.108999	7.940412
H	-4.667358	-4.027114	9.087216
H	-5.486136	-2.502079	8.650025
H	-4.617205	-3.436814	7.395010
H	-1.200269	-2.221645	10.182240
H	-0.409951	-0.633381	10.192278
H	-2.133632	-0.787433	10.585851
H	2.847756	-0.575721	5.096859
H	2.796168	-1.443838	3.568222
H	2.171180	0.219327	3.665407
H	1.424831	-2.436896	6.256515
H	-0.175782	-2.825119	5.579434
H	0.673770	-5.009688	5.804174
H	-0.298714	1.333784	1.590669
H	0.452490	-0.285093	1.649635
H	-1.322349	-0.112660	1.799794
H	1.741550	-6.896152	4.539008
H	0.745725	-5.867430	3.482386
H	2.510513	-5.715060	3.458196
H	2.888417	-5.828442	6.608660
H	3.712196	-4.708807	5.501985
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YT2S_Tlff.xyz

134

scf done: -2511.229028

C	-5.433470	-5.332454	4.768563
C	-5.524803	-3.938417	4.509815
C	-6.804382	-3.331952	4.491159
C	-7.948791	-4.078774	4.760988
C	-7.889759	-5.445370	5.040702
C	-6.619309	-6.030316	5.027718
O	-4.454611	-3.181181	4.280791
Y	-3.709733	-1.200896	4.414926
O	-1.476989	-1.712960	3.683975
C	-0.249742	-1.670616	3.808933
C	0.461858	-1.355016	5.114164
C	0.294450	-2.616415	5.985738
O	0.891089	-3.702326	5.308574
C	0.953461	-4.912921	6.062000
C	1.117875	-6.039604	5.054476
C	-6.943318	-1.891450	4.085573
N	-6.201362	-0.898242	4.916062
C	-6.560352	0.445203	4.422728
C	-5.723353	1.555853	5.036387
N	-4.268529	1.354509	4.856338
C	-3.562409	1.867798	6.043354

C	-9.175335	-6.232930	5.326922
C	-9.895605	-5.621936	6.545020
C	-4.078428	-6.056506	4.759937
C	-3.398434	-5.876015	3.387483
O	-3.947177	-0.395727	2.426646
C	-4.431297	0.630506	1.740021
C	-4.941259	0.505363	0.417819
C	-5.506912	1.642247	-0.173787
C	-5.580024	2.897750	0.439390
C	-5.019534	3.002288	1.714465
C	-4.448103	1.906753	2.357660
C	-4.845028	-0.820290	-0.356666
C	-3.364801	-1.239115	-0.458228
C	-3.745958	2.100505	3.672424
C	-6.214746	4.124696	-0.228931
C	-7.374802	4.643246	0.643954
O	-2.865853	-1.085411	6.398450
C	-2.057222	-0.706256	7.357286
C	-0.778434	-0.275340	7.189017
C	-0.239899	-0.112850	5.793533
O	-2.591321	-0.692588	8.626688
C	-3.412184	-1.799395	8.963850
C	-5.158067	5.236992	-0.379818
C	-6.774515	3.807465	-1.622445
C	-5.637360	-1.931815	0.357248
C	-5.395139	-0.706043	-1.786388
C	-6.549780	-1.057189	6.334395
C	-3.178861	-5.485825	5.873395
C	-4.215613	-7.566497	5.007923
C	-10.105491	-6.163073	4.099438
C	-8.899364	-7.711744	5.631775
O	0.548888	-1.917328	2.789365
C	-0.073751	-2.285173	1.546934
C	1.954355	-1.078723	4.897084
C	2.097283	-4.880239	7.073511
C	0.102561	0.116678	8.342292
H	-7.626036	0.651463	4.626369
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H	-6.040011	2.514092	4.599959
H	-5.925686	1.620171	6.109691
H	-3.752011	3.176389	3.913709
H	-2.690949	1.806902	3.571791
H	-8.013201	-1.624879	4.094052
H	-6.585605	-1.753059	3.058371
H	-6.545063	-7.091130	5.229594
H	-8.910385	-3.568145	4.736432
H	-5.910292	1.540837	-1.173084
H	-5.009610	3.962529	2.228156
H	-7.614624	-0.834774	6.512468
H	-6.359591	-2.088902	6.635813
H	-5.941163	-0.397174	6.955562
H	-3.771934	2.938667	6.198270
H	-3.860847	1.308644	6.930994
H	-2.484285	1.741860	5.927232

H	-3.275008	-2.191316	-0.995494	H	0.278383	-6.053968	4.354497
H	-2.785744	-0.485273	-1.003643	H	2.041264	-5.901597	4.482424
H	-2.939158	-1.357590	0.539775	H	2.131459	-5.814978	7.642559
H	-5.597535	-2.860053	-0.225553	H	3.054546	-4.755635	6.556935
H	-5.222526	-2.135835	1.345582	H	1.986992	-4.062988	7.792556
H	-6.691599	-1.651325	0.464155				
H	-5.273966	-1.668192	-2.295704				
H	-6.463004	-0.461415	-1.800396	YT2R_NRBb.xyz			
H	-4.861419	0.047609	-2.375603	134			
H	-7.223181	4.708401	-2.054759	scf done: -2511.198053			
H	-5.991636	3.467531	-2.308785	C	-5.518176	-5.257800	4.777194
H	-7.552562	3.037540	-1.582993	C	-5.450201	-3.875285	4.452206
H	-7.838459	5.526196	0.187877	C	-6.573446	-3.055149	4.722517
H	-8.147642	3.876047	0.761407	C	-7.714046	-3.588869	5.317198
H	-7.032490	4.927705	1.644042	C	-7.809409	-4.940526	5.652942
H	-5.596340	6.125321	-0.849974	C	-6.696195	-5.736087	5.363825
H	-4.748480	5.541903	0.588375	O	-4.369289	-3.320873	3.908210
H	-4.322988	4.898859	-1.002228	Y	-3.323164	-1.489364	3.718089
H	-2.206355	-5.993004	5.870384	O	-2.096288	-1.440764	5.481471
H	-3.015194	-4.415821	5.736548	C	-0.993296	-1.369812	6.182418
H	-3.636852	-5.643149	6.856602	C	-0.889032	-1.629832	7.513036
H	-3.222790	-8.028530	4.974344	C	0.416222	-1.721512	8.258808
H	-4.645744	-7.788249	5.990865	C	-6.578935	-1.614116	4.291408
H	-4.830895	-8.054942	4.244470	N	-5.481355	-0.757745	4.833453
H	-2.423307	-6.378861	3.379543	C	-5.751238	0.629799	4.411562
H	-4.011180	-6.319956	2.594864	C	-4.574316	1.563868	4.640932
H	-3.251522	-4.819363	3.158815	N	-3.340915	1.125820	3.952719
H	-9.842422	-8.228956	5.839205	C	-2.168854	1.567350	4.727630
H	-8.423781	-8.220447	4.786487	C	-9.087478	-5.487231	6.302117
H	-8.256234	-7.832767	6.510120	C	-8.992286	-6.988219	6.607081
H	-10.824997	-6.163968	6.757419	C	-4.332617	-6.197963	4.503325
H	-9.262044	-5.670688	7.437126	C	-4.633607	-7.657544	4.877580
H	-10.155006	-4.571849	6.377588	O	-3.897739	-0.838076	1.715474
H	-11.034634	-6.714837	4.285860	C	-4.564125	0.155994	1.143720
H	-10.374744	-5.131021	3.853646	C	-5.497425	-0.039244	0.086960
H	-9.621080	-6.598284	3.219051	C	-6.195871	1.082315	-0.379976
H	-1.045785	0.219996	5.128717	C	-6.018791	2.383695	0.103590
H	0.500464	0.697092	5.793071	C	-5.053956	2.552532	1.099383
H	-3.791380	-1.604246	9.969252	C	-4.332966	1.476337	1.610661
H	-4.250302	-1.912549	8.270840	C	-5.718642	-1.425723	-0.545957
H	-2.835676	-2.734237	8.973934	C	-6.702428	-1.379860	-1.725910
H	1.059245	-0.426335	8.337388	C	-3.218163	1.720072	2.589273
H	0.359322	1.186686	8.316561	C	-6.800617	3.591523	-0.429735
H	-0.388271	-0.083121	9.296283	C	-7.841444	3.193164	-1.485231
H	2.412958	-0.842029	5.862407	O	-1.379455	-2.280753	2.614650
H	2.463166	-1.945517	4.473931	C	-0.342192	-2.684306	2.086220
H	2.106587	-0.222595	4.232778	C	0.480588	-3.810835	2.582161
H	0.777475	-2.421248	6.952562	C	1.574274	-4.342317	1.700544
H	-0.770321	-2.806504	6.173797	O	0.154189	-2.139907	0.980747
H	-0.000452	-5.045501	6.598002	C	-0.535527	-1.010848	0.412431
H	0.748893	-2.485726	0.862128	C	-7.542622	4.282327	0.731769
H	-0.689846	-3.175679	1.683978	C	-5.824300	4.595020	-1.074683
H	-0.694983	-1.467679	1.177656	C	-4.378277	-1.965549	-1.083608
H	1.167630	-7.008304	5.560915	C	-6.286981	-2.416170	0.488316

C	-5.411833	-0.865222	6.298892	H	-5.477728	-8.061710	4.307832
C	-3.975639	-6.176783	3.003261	H	-3.115387	-6.830155	2.811232
C	-3.122765	-5.746947	5.345336	H	-4.816718	-6.543713	2.404331
C	-9.352073	-4.749264	7.629732	H	-3.731826	-5.167167	2.670387
C	-10.282057	-5.265217	5.353453	H	-9.922567	-7.330219	7.073611
O	0.100171	-1.049970	5.389818	H	-8.842607	-7.580902	5.698444
C	0.963800	-0.014791	5.830599	H	-8.173560	-7.211066	7.299922
C	-2.135619	-1.853995	8.306139	H	-10.270013	-5.120852	8.100646
O	-2.453242	-0.675803	9.064536	H	-8.524371	-4.899404	8.331046
C	-3.498858	-0.856477	10.008891	H	-9.469664	-3.671871	7.478892
C	-4.111374	0.515310	10.261709	H	-11.209266	-5.638235	5.805046
C	-2.982574	-1.489612	11.300813	H	-10.426115	-4.204173	5.125565
C	0.215880	-4.263480	3.814316	H	-10.129103	-5.790472	4.404852
H	-6.630103	1.025856	4.949713	H	0.798424	-5.070384	4.248124
H	-6.002806	0.616107	3.347923	H	-0.565762	-3.823418	4.420117
H	-4.859912	2.577210	4.318818	H	-0.264824	-1.003132	-0.642794
H	-4.355562	1.626549	5.711114	H	-0.177346	-0.096925	0.894284
H	-3.077494	2.808623	2.699447	H	-1.614588	-1.097012	0.547204
H	-2.283121	1.317026	2.177341	H	1.176467	-4.702073	0.745881
H	-7.544991	-1.167498	4.578323	H	2.090391	-5.169892	2.192592
H	-6.504159	-1.543147	3.199119	H	2.309184	-3.565681	1.466017
H	-6.744483	-6.789050	5.610391	H	1.244665	-2.008895	7.604772
H	-8.551391	-2.919871	5.509086	H	0.341137	-2.493346	9.034717
H	-6.918925	0.929187	-1.170525	H	0.698003	-0.793603	8.774856
H	-4.839398	3.546966	1.488310	H	-1.991843	-2.699629	8.999017
H	-6.325438	-0.467988	6.769738	H	-2.975582	-2.103694	7.645992
H	-5.311197	-1.915980	6.575154	H	1.871088	-0.410249	6.300922
H	-4.543244	-0.329051	6.685837	H	0.459008	0.643744	6.545070
H	-2.135513	2.666156	4.810199	H	1.258699	0.565415	4.948672
H	-2.192953	1.127790	5.725902	H	-4.270713	-1.516874	9.573886
H	-1.254127	1.229141	4.235127	H	-3.796220	-1.636139	12.019719
H	-4.524341	-2.947636	-1.549112	H	-2.227623	-0.842117	11.759024
H	-3.963391	-1.290077	-1.840429	H	-2.525160	-2.466078	11.115047
H	-3.657264	-2.071716	-0.271712	H	-4.930997	0.456216	10.985232
H	-6.453259	-3.395035	0.022337	H	-4.499495	0.942490	9.332556
H	-5.603115	-2.556392	1.326752	H	-3.350926	1.197414	10.657132
H	-7.251907	-2.064601	0.871531				
H	-6.804321	-2.385748	-2.147392				
H	-7.701761	-1.052630	-1.418672	YT3RR_NRB.xyz			
H	-6.355507	-0.720562	-2.529046	149			
H	-8.385398	4.082120	-1.822865	scf done: -2856.871806			
H	-7.376626	2.738390	-2.366413	C	-5.242472	0.376477	0.656202
H	-8.577406	2.487691	-1.084636	C	-4.292529	0.405370	1.712515
H	-8.098868	5.155126	0.369649	C	-4.067812	1.624684	2.398732
H	-8.255244	3.596250	1.201930	C	-4.837912	2.751122	2.117956
H	-6.850958	4.628788	1.506366	C	-5.839444	2.730848	1.143770
H	-6.365262	5.468367	-1.458158	C	-5.992560	1.538108	0.427881
H	-5.079097	4.953755	-0.357416	O	-3.593092	-0.660602	2.084491
H	-5.286773	4.133039	-1.909421	Y	-2.923086	-1.712236	3.817574
H	-2.252865	-6.381725	5.134594	O	-1.277999	-2.675331	2.572262
H	-2.860248	-4.710121	5.131549	C	-0.247311	-3.402236	2.452426
H	-3.347726	-5.829158	6.414611	O	0.536120	-3.227834	1.372175
H	-3.757242	-8.274776	4.650419	C	0.090605	-2.291782	0.392076
H	-4.848421	-7.778032	5.944764	C	-2.877618	1.742422	3.310520

N	-2.793170	0.893439	4.537799	H	-3.544688	0.853338	6.480534
C	-1.535697	1.264367	5.206125	H	-2.778284	2.797268	3.618465
C	-6.686614	3.983512	0.880599	H	-1.979477	1.493423	2.729453
C	-7.434508	4.376829	2.169885	H	-7.111266	-1.061561	4.711345
C	-5.409759	-0.863272	-0.239593	H	-6.045851	-1.190553	3.310997
C	-4.045600	-1.229947	-0.859757	H	-7.281627	-6.743410	3.894880
O	-4.134009	-3.464330	3.897211	H	-8.486003	-2.750130	4.792203
C	-5.378828	-3.935825	4.015512	H	-6.733301	1.510184	-0.360682
C	-6.421248	-3.031986	4.337591	H	-4.631543	3.667403	2.669196
C	-7.724115	-3.484272	4.535311	H	-5.935979	-1.299143	7.034442
C	-8.071905	-4.827137	4.391121	H	-4.977329	-2.665174	6.418951
C	-7.040144	-5.697588	4.030828	H	-4.152400	-1.222480	7.033589
C	-5.708367	-5.309320	3.836790	H	-1.574574	2.301447	5.578178
C	-6.193390	-1.545571	4.339370	H	-1.337782	0.581367	6.032898
N	-5.038028	-1.020193	5.119682	H	-0.710925	1.194864	4.495640
C	-5.025414	-1.576408	6.479453	H	-4.148526	-2.117022	-1.496418
C	-4.648845	-6.364401	3.479431	H	-3.671179	-0.408918	-1.481897
C	-3.832879	-5.935734	2.243905	H	-3.310378	-1.441711	-0.081398
C	-9.519119	-5.283282	4.618141	H	-6.076232	-2.928510	-0.092131
C	-9.941374	-4.951016	6.062974	H	-5.263554	-2.349247	1.366105
O	-1.336097	-1.830788	5.444490	H	-6.923596	-1.831205	1.005335
C	-0.298087	-2.528009	5.738420	H	-6.434476	-1.512131	-2.026317
O	0.914079	-2.148165	5.273325	H	-7.406042	-0.412628	-1.047773
C	1.049707	-0.960176	4.517009	H	-6.070726	0.216789	-2.036486
C	-0.277453	-3.760611	6.407598	H	-8.313238	4.678411	-0.368589
C	1.050479	-4.375618	6.777025	H	-7.260092	3.517940	-1.183563
C	-1.521063	-4.206052	7.137794	H	-8.428415	2.960526	0.030271
C	-1.564797	-4.077333	8.697722	H	-8.040735	5.275972	2.007342
C	-3.040128	-4.209407	9.113638	H	-8.101756	3.570965	2.493945
O	-3.138809	-4.082647	10.513108	H	-6.741982	4.587543	2.991119
C	-4.394046	-4.453749	11.071374	H	-6.361658	6.054158	0.267772
C	-4.163396	-4.627985	12.564447	H	-5.028575	5.385083	1.217715
C	-0.751739	-5.168992	9.402997	H	-5.233071	4.900667	-0.470219
C	-1.023482	-2.712477	9.117713	H	-2.900352	-7.231737	4.465428
O	0.067672	-2.513017	9.602999	H	-3.315966	-5.597983	5.024465
C	-3.729627	-6.553126	4.700228	H	-4.292326	-6.980874	5.537951
C	-5.262512	-7.735155	3.148909	H	-4.460932	-8.427081	2.868185
C	-10.454399	-4.550709	3.635749	H	-5.786440	-8.178844	4.002280
C	-9.695812	-6.792904	4.405828	H	-5.960669	-7.678678	2.306563
C	-5.179587	0.447099	5.147418	H	-3.083085	-6.700305	2.007901
C	-3.889000	1.164578	5.488427	H	-4.489479	-5.829436	1.373025
C	-5.946466	-2.060993	0.566006	H	-3.323796	-4.986191	2.404022
C	-6.388092	-0.615644	-1.398783	H	-10.740442	-7.071428	4.582278
C	-5.772101	5.147798	0.450330	H	-9.443011	-7.092531	3.383202
C	-7.728618	3.763464	-0.224659	H	-9.077789	-7.376777	5.096297
C	0.190703	-4.421772	3.339025	H	-10.978380	-5.258598	6.243183
C	-0.623303	-4.754039	4.414360	H	-9.301850	-5.469888	6.784968
C	1.495412	-5.126596	3.064166	H	-9.872302	-3.877905	6.267681
O	-1.896024	-1.709559	8.871006	H	-11.495010	-4.860520	3.790167
C	-1.439795	-0.417461	9.272578	H	-10.408968	-3.464790	3.764913
C	-5.479755	-3.421176	10.775020	H	-10.182595	-4.773875	2.598759
H	-5.956927	0.740243	5.873803	H	-0.423026	-5.681552	4.942740
H	-5.520543	0.772391	4.162500	H	-1.662466	-4.443010	4.407511
H	-4.084860	2.248522	5.549150	H	0.842334	-2.317972	-0.397353

H	0.019208	-1.283578	0.809183
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H	1.516154	-5.557559	2.057042
H	1.643645	-5.939503	3.780501
H	2.359048	-4.455750	3.139220
H	0.934883	-5.449461	6.963041
H	1.471709	-3.927569	7.684867
H	1.781266	-4.248445	5.976266
H	-2.373451	-3.654582	6.727983
H	-1.704915	-5.269626	6.924512
H	-0.945666	-5.136391	10.477024
H	0.318912	-5.046236	9.248968
H	-1.054147	-6.153052	9.028467
H	2.041626	-1.009621	4.064795
H	0.995416	-0.079620	5.164142
H	0.295225	-0.886938	3.728741
H	-3.407501	-5.198368	8.787865
H	-3.636998	-3.443887	8.600991
H	-2.262223	0.268422	9.065827
H	-0.547875	-0.127708	8.710619
H	-1.197660	-0.408073	10.338291
H	-4.697806	-5.423228	10.638092
H	-6.427096	-3.717607	11.236959
H	-5.656899	-3.313649	9.700773
H	-5.189747	-2.444510	11.176425
H	-5.081430	-4.953100	13.063208
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H	-3.383608	-5.372182	12.746955

YT3RR_NRBb.xyz

149

scf done: -2856.882956

C	-5.072287	0.579493	0.568153
C	-4.177649	0.380723	1.657110
C	-3.820932	1.498707	2.455358
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C	-5.310972	2.963610	1.201859
C	-5.611711	1.860771	0.393921
O	-3.659441	-0.800075	1.963663
Y	-3.091135	-2.021827	3.689402
O	-1.308196	-2.588420	2.205237
C	-0.418849	-2.885707	1.406510
O	0.079196	-2.010311	0.542965
C	-0.439564	-0.669254	0.574782
C	-2.733062	1.350088	3.482186
N	-2.971484	0.427736	4.632190
C	-1.828545	0.567949	5.550925
C	-5.922718	4.354507	0.986836
C	-6.659457	4.798512	2.265805
C	-5.418519	-0.559255	-0.407890
C	-4.125660	-1.102726	-1.049378
O	-4.247860	-3.765865	3.396905
C	-5.360628	-4.388301	3.780408

C	-6.449373	-3.609539	4.242108
C	-7.622233	-4.219601	4.680824
C	-7.781370	-5.606783	4.669766
C	-6.701203	-6.355725	4.191016
C	-5.496491	-5.801786	3.741603
C	-6.375408	-2.109056	4.180332
N	-5.252363	-1.477564	4.933980
C	-5.258900	-1.932134	6.331378
C	-4.361497	-6.698106	3.222020
C	-4.006665	-6.306791	1.772949
C	-9.091893	-6.239776	5.155806
C	-9.346082	-5.841117	6.623107
O	-1.758961	-2.509260	5.306831
C	-0.796785	-3.230195	5.851886
O	0.377190	-3.284937	5.106610
C	0.994458	-2.039651	4.865691
C	-0.850686	-3.962466	6.992086
C	0.330983	-4.775164	7.451370
C	-2.156156	-4.072294	7.738265
C	-2.163591	-3.764639	9.271393
C	-3.622581	-3.483185	9.667588
O	-3.686742	-3.191144	11.045134
C	-4.998650	-3.123756	11.589904
C	-4.846561	-3.260323	13.097066
C	-1.640892	-4.935813	10.111272
C	-1.309684	-2.531847	9.552836
O	-0.234329	-2.533888	10.108209
C	-3.128080	-6.550202	4.133822
C	-4.744281	-8.186455	3.209303
C	-10.261221	-5.739472	4.284717
C	-9.063266	-7.772355	5.078414
C	-5.426083	-0.014558	4.852492
C	-4.218798	0.761624	5.354846
C	-6.136728	-1.709127	0.323409
C	-6.337546	-0.091760	-1.547406
C	-4.804737	5.367677	0.669523
C	-6.929150	4.376940	-0.172051
C	0.212600	-4.220813	1.287591
C	0.060260	-5.064876	2.316573
C	1.017495	-4.524160	0.055381
O	-1.882180	-1.390329	9.099650
C	-1.130593	-0.208471	9.376850
C	-5.709120	-1.828113	11.201181
H	-6.313944	0.295680	5.430783
H	-5.612443	0.243127	3.806976
H	-4.434305	1.837811	5.276474
H	-4.058116	0.551772	6.416443
H	-2.495381	2.348062	3.886904
H	-1.821123	0.980271	2.993158
H	-7.324995	-1.693052	4.555324
H	-6.265677	-1.778511	3.141010
H	-6.799753	-7.433221	4.162606
H	-8.433612	-3.580896	5.026706
H	-6.304416	2.005690	-0.425034

H	-4.078975	3.578513	2.864969	H	-2.871627	-3.405442	7.250660
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H	-5.195741	-3.021075	6.356339	H	-1.782136	-4.726719	11.173518
H	-4.402153	-1.525044	6.871557	H	-0.582375	-5.122527	9.938556
H	-1.782232	1.583851	5.976022	H	-2.202176	-5.842452	9.859992
H	-1.898956	-0.170935	6.349831	H	1.939318	-2.247104	4.356737
H	-0.898226	0.382346	5.009292	H	1.206562	-1.509896	5.805241
H	-4.364458	-1.898296	-1.765346	H	0.382470	-1.393290	4.223058
H	-3.596308	-0.309408	-1.589383	H	-4.227448	-4.377174	9.433985
H	-3.464001	-1.514178	-0.285168	H	-4.009722	-2.648963	9.067823
H	-6.404690	-2.500104	-0.387330	H	-1.737410	0.624565	9.019739
H	-5.497387	-2.149338	1.090153	H	-0.167765	-0.230136	8.858975
H	-7.062986	-1.355263	0.790601	H	-0.946147	-0.111417	10.449815
H	-6.533318	-0.933948	-2.219633	H	-5.583614	-3.978999	11.207617
H	-7.306000	0.263154	-1.178168	H	-6.708761	-1.788371	11.646306
H	-5.882747	0.706641	-2.144162	H	-5.826704	-1.738628	10.117053
H	-7.347739	5.383487	-0.278996	H	-5.137061	-0.964870	11.556558
H	-6.459402	4.113230	-1.125622	H	-5.823714	-3.245681	13.589640
H	-7.763207	3.688257	0.000213	H	-4.246780	-2.434143	13.492261
H	-7.096986	5.795173	2.133581	H	-4.342929	-4.197780	13.347393
H	-7.468512	4.102317	2.511453				
H	-5.985170	4.844111	3.126888				
H	-5.222769	6.370310	0.519868	YT3RR_NRBf.xyz			
H	-4.073093	5.430484	1.481336	149			
H	-4.267833	5.083128	-0.241507	scf done: -2856.899327			
H	-2.298794	-7.160954	3.755337	C	-5.527615	0.075136	0.320365
H	-2.797854	-5.512370	4.192865	C	-4.405375	0.153472	1.188056
H	-3.358476	-6.892133	5.148995	C	-3.920858	1.434381	1.558070
H	-3.904621	-8.768815	2.814166	C	-4.592106	2.592300	1.173878
H	-4.960811	-8.568297	4.213093	C	-5.750067	2.542541	0.393076
H	-5.611254	-8.384238	2.569451	C	-6.166228	1.273973	-0.025646
H	-3.183044	-6.930862	1.404556	O	-3.778438	-0.913875	1.668718
H	-4.867781	-6.463719	1.113587	Y	-2.851615	-1.594683	3.473681
H	-3.710099	-5.259288	1.707495	O	-0.913396	-2.046699	2.702594
H	-10.014610	-8.179257	5.437801	C	0.361631	-2.246329	2.932753
H	-8.921195	-8.124990	4.051305	O	1.222302	-1.453503	2.207554
H	-8.266528	-8.196361	5.698909	C	0.834995	-1.200034	0.863532
H	-10.283270	-6.279556	6.986605	C	-2.580239	1.533512	2.228486
H	-8.533755	-6.192073	7.268538	N	-2.397957	0.930215	3.583663
H	-9.420366	-4.755388	6.741396	C	-0.986278	1.139750	3.945361
H	-11.209191	-6.174881	4.623260	C	-6.476598	3.836596	0.002750
H	-10.361021	-4.650349	4.327495	C	-6.916465	4.586050	1.275957
H	-10.113033	-6.018730	3.236315	C	-5.997675	-1.267085	-0.263077
H	0.522468	-6.047482	2.301129	C	-4.828356	-1.921790	-1.028253
H	-0.491791	-4.781846	3.204294	O	-4.133004	-3.260922	3.835856
H	-0.177628	-0.231880	-0.387746	C	-5.338766	-3.590193	4.291687
H	0.051687	-0.114556	1.379464	C	-6.205124	-2.569450	4.768670
H	-1.519858	-0.672568	0.729510	C	-7.430440	-2.898885	5.346531
H	0.408666	-4.432098	-0.850368	C	-7.875002	-4.218179	5.447371
H	1.412255	-5.541534	0.102341	C	-7.044895	-5.197242	4.892321
H	1.857139	-3.830628	-0.053312	C	-5.804213	-4.935069	4.298206
H	0.042508	-5.819847	7.633675	C	-5.936262	-1.111919	4.481247
H	0.756593	-4.392237	8.386862	N	-4.651041	-0.524746	4.954348
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C	-5.017468	-6.064339	3.605862	H	-4.506275	-1.284282	-1.859470
C	-4.835359	-5.717344	2.114064	H	-3.973221	-2.090668	-0.370977
C	-9.245109	-4.530981	6.064103	H	-6.822017	-3.160425	0.420439
C	-9.338394	-3.934377	7.481326	H	-5.684171	-2.435059	1.562893
O	-1.495639	-1.703216	5.598245	H	-7.326019	-1.773599	1.395124
C	-0.619649	-2.254145	6.267783	H	-7.429714	-2.076595	-1.660521
O	0.074818	-1.606305	7.194596	H	-8.055181	-0.684191	-0.775652
C	-0.154101	-0.217876	7.424466	H	-6.892548	-0.452665	-2.099418
C	-0.222144	-3.721759	6.162101	H	-8.220111	4.519178	-1.086544
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C	-1.411772	-4.595568	6.667559	H	-8.454154	2.946372	-0.314959
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C	-3.090157	-5.412557	8.299883	H	-7.607711	3.976828	1.868354
O	-3.349821	-5.685697	9.656865	H	-6.062894	4.838332	1.913628
C	-4.629422	-6.251171	9.928591	H	-6.032689	5.666669	-1.103701
C	-4.519680	-6.929344	11.285446	H	-4.634697	5.009700	-0.242523
C	-0.711221	-6.065810	8.661399	H	-5.198494	4.228977	-1.725196
C	-1.472194	-3.737874	9.109644	H	-3.084762	-7.054105	3.746063
O	-0.654890	-3.634696	9.994967	H	-3.052675	-5.335449	4.190494
C	-3.636380	-6.253512	4.254168	H	-3.739154	-6.533509	5.308397
C	-5.747206	-7.415271	3.675995	H	-5.151507	-8.170702	3.152304
C	-10.349609	-3.911862	5.183569	H	-5.882488	-7.762130	4.706664
C	-9.505041	-6.040373	6.170379	H	-6.729486	-7.379734	3.192588
C	-4.665445	0.918075	4.635564	H	-4.273408	-6.511478	1.607137
C	-3.277235	1.541949	4.600071	H	-5.807050	-5.621468	1.618373
C	-6.480723	-2.212065	0.852131	H	-4.291319	-4.779409	1.991665
C	-7.159422	-1.096271	-1.253951	H	-10.475557	-6.217528	6.646451
C	-5.528197	4.737332	-0.813251	H	-9.532161	-6.522146	5.187330
C	-7.727642	3.570806	-0.845972	H	-8.740442	-6.540506	6.774730
C	0.899130	-3.129380	3.818457	H	-10.320408	-4.144227	7.921275
C	-0.019869	-4.013156	4.617020	H	-8.573388	-4.362155	8.137477
C	2.390165	-3.354562	3.863760	H	-9.205107	-2.848079	7.478350
O	-2.397087	-2.780333	8.859837	H	-11.341958	-4.112686	5.605579
C	-2.430058	-1.723339	9.819202	H	-10.233711	-2.826523	5.100156
C	-5.729097	-5.193066	9.897912	H	-10.318735	-4.327722	4.171134
H	-5.290527	1.464180	5.362440	H	0.332176	-5.054745	4.560035
H	-5.129205	1.042133	3.654209	H	-1.014961	-4.010984	4.157756
H	-3.378164	2.625644	4.426884	H	1.609196	-0.555214	0.442524
H	-2.790006	1.424981	5.574230	H	-0.136943	-0.701551	0.803678
H	-2.291832	2.595836	2.292219	H	0.784494	-2.130202	0.283189
H	-1.837785	1.034098	1.593498	H	2.854123	-3.071888	2.915520
H	-6.763281	-0.520715	4.908462	H	2.618003	-4.411599	4.053141
H	-5.960436	-0.950306	3.396194	H	2.908622	-2.778809	4.644444
H	-7.385212	-6.224340	4.912006	H	1.365002	-5.050878	6.749259
H	-8.062752	-2.086120	5.700539	H	1.021828	-3.813576	7.973117
H	-7.035808	1.209976	-0.667064	H	1.897713	-3.386555	6.503323
H	-4.181497	3.552758	1.482078	H	-2.330690	-4.152752	6.267881
H	-5.322210	-0.273619	6.957743	H	-1.307981	-5.561655	6.160080
H	-4.503476	-1.816159	6.606823	H	-1.020581	-6.386372	9.657644
H	-3.549164	-0.336633	6.747501	H	0.332989	-5.763356	8.716208
H	-0.733769	2.211882	3.988092	H	-0.794618	-6.920275	7.980930
H	-0.791966	0.686820	4.915274	H	0.164826	-0.028701	8.449389
H	-0.339571	0.653514	3.211402	H	-1.207918	0.037027	7.297252
H	-5.142982	-2.886267	-1.444812	H	0.461475	0.371171	6.739516

H	-3.218391	-6.323325	7.691520
H	-3.769652	-4.646891	7.902720
H	-3.130104	-0.982932	9.431051
H	-1.437301	-1.290625	9.959770
H	-2.782431	-2.101022	10.783307
H	-4.845773	-7.014836	9.161881
H	-6.699778	-5.643949	10.128797
H	-5.810298	-4.717662	8.916133
H	-5.525474	-4.416696	10.642670
H	-5.463472	-7.413335	11.554299
H	-4.276192	-6.193248	12.058544
H	-3.729971	-7.685285	11.273368

YT3RR_NRF.xyz
149

scf done: -2856.869214

C	-5.518541	-0.784540	-0.278691
C	-4.300984	-0.633184	0.438935
C	-3.634630	0.616517	0.393049
C	-4.207899	1.709395	-0.252079
C	-5.446110	1.614809	-0.892529
C	-6.051821	0.353098	-0.899484
O	-3.748954	-1.607799	1.151317
Y	-2.780176	-1.925785	3.041237
O	-1.259373	-3.366841	2.214080
C	-0.305754	-4.200721	2.270013
O	-0.435194	-5.375806	1.630281
C	-1.651415	-5.597474	0.915302
C	-2.228936	0.705425	0.915951
N	-1.973715	0.479566	2.371252
C	-0.521962	0.647627	2.561939
C	-6.057756	2.845097	-1.576404
C	-6.239944	3.973301	-0.541816
C	-6.204446	-2.154106	-0.412400
C	-5.210288	-3.157070	-1.033554
O	-4.282502	-3.161309	3.880122
C	-5.380742	-3.155353	4.632840
C	-6.036134	-1.923852	4.882807
C	-7.138608	-1.871689	5.732536
C	-7.661925	-3.014378	6.340578
C	-7.042012	-4.227317	6.025014
C	-5.930756	-4.345245	5.181270
C	-5.645913	-0.681326	4.127000
N	-4.236404	-0.216060	4.263115
C	-3.888537	-0.052408	5.682268
C	-5.352085	-5.725769	4.830514
C	-5.399535	-5.933452	3.303433
C	-8.873447	-2.906651	7.276213
C	-8.537079	-1.968043	8.451578
O	-1.344811	-1.720848	4.811613
C	-0.237269	-1.594502	5.408409
O	0.106303	-0.291742	5.657542
C	0.499159	0.088252	6.980197

C	0.683013	-2.654834	5.628324
C	0.064582	-4.010404	5.907820
C	0.268739	-4.635137	7.325188
C	-0.897169	-5.625207	7.530757
O	-0.760608	-6.238881	8.791488
C	-1.854811	-7.061848	9.185968
C	-1.723953	-7.252756	10.689067
C	2.053393	-2.355000	6.192615
C	-3.899954	-5.833418	5.328743
C	-6.142258	-6.877033	5.472116
C	-10.076977	-2.335859	6.499976
C	-9.285286	-4.266041	7.857861
C	-4.117274	1.064676	3.538091
C	-2.679887	1.455851	3.228649
C	-6.668704	-2.671215	0.961779
C	-7.438204	-2.103094	-1.327258
C	-5.118855	3.334000	-2.697334
C	-7.429006	2.547878	-2.198697
C	0.938460	-4.018264	2.924013
C	1.204244	-2.778182	3.509559
C	1.953172	-5.136000	2.910068
C	1.591197	-5.402713	7.451363
C	0.083758	-3.579576	8.411352
O	-0.819278	-2.765502	8.424179
O	1.008106	-3.649144	9.385117
C	0.814172	-2.753366	10.480802
C	-1.861488	-8.392115	8.436391
H	-4.588057	1.875257	4.120884
H	-4.673079	0.977401	2.601621
H	-2.678276	2.451733	2.755916
H	-2.110928	1.545903	4.159229
H	-1.817803	1.693866	0.650870
H	-1.619815	-0.046531	0.396830
H	-6.315213	0.137683	4.438659
H	-5.811748	-0.837415	3.053854
H	-7.447759	-5.134578	6.453792
H	-7.605920	-0.903214	5.903223
H	-6.991558	0.243424	-1.425214
H	-3.658202	2.649502	-0.261739
H	-4.540058	0.696577	6.161260
H	-4.014220	-1.005076	6.199398
H	-2.846086	0.250491	5.784417
H	-0.197058	1.657765	2.262007
H	-0.255655	0.486820	3.606983
H	0.015238	-0.072461	1.937533
H	-5.674401	-4.147567	-1.115601
H	-4.916998	-2.836832	-2.039754
H	-4.311415	-3.241420	-0.419995
H	-7.165191	-3.642839	0.851054
H	-5.829612	-2.796708	1.647314
H	-7.391303	-1.981094	1.412418
H	-7.858279	-3.110509	-1.418437
H	-8.226591	-1.457198	-0.924849
H	-7.189461	-1.756823	-2.336446

H	-7.831100	3.456910	-2.659176
H	-7.366141	1.783972	-2.980921
H	-8.151144	2.209437	-1.447867
H	-6.664215	4.867034	-1.014674
H	-6.915873	3.659971	0.261035
H	-5.288125	4.260925	-0.083909
H	-5.537280	4.217851	-3.193696
H	-4.132227	3.606524	-2.309257
H	-4.974837	2.554687	-3.452952
H	-3.475248	-6.808218	5.057111
H	-3.277542	-5.047778	4.897985
H	-3.866781	-5.741246	6.419435
H	-5.696081	-7.831211	5.170741
H	-6.118742	-6.836286	6.566777
H	-7.189167	-6.887686	5.150147
H	-4.963173	-6.905381	3.040335
H	-6.434684	-5.921276	2.945594
H	-4.849870	-5.147208	2.783352
H	-10.145896	-4.138060	8.523496
H	-9.578279	-4.972963	7.074327
H	-8.478378	-4.719297	8.443739
H	-9.395518	-1.872944	9.127327
H	-7.689851	-2.353840	9.028378
H	-8.273973	-0.963658	8.105204
H	-10.950945	-2.241693	7.155865
H	-9.861398	-1.344317	6.089552
H	-10.347015	-2.989866	5.664183
H	2.240689	-2.536674	3.729111
H	0.598418	-1.938002	3.192776
H	-2.509615	-5.600779	1.592078
H	-1.802224	-4.831078	0.150971
H	-1.538972	-6.577241	0.450261
H	2.260200	-5.388494	1.887875
H	2.849943	-4.840205	3.462300
H	1.575620	-6.062215	3.358085
H	2.088789	-2.291405	7.287321
H	2.755146	-3.143529	5.902096
H	2.446698	-1.415574	5.792488
H	-1.008696	-3.921539	5.717472
H	0.435501	-4.749660	5.183937
H	1.624430	-5.948654	8.395032
H	1.665639	-6.125973	6.632227
H	2.461568	-4.746492	7.406118
H	0.030760	1.056592	7.175019
H	0.141749	-0.639261	7.712544
H	1.584817	0.198244	7.056659
H	-1.847734	-5.075854	7.471295
H	-0.874922	-6.360029	6.710287
H	-2.794766	-6.524566	8.972333
H	1.576727	-3.014549	11.214696
H	0.937820	-1.714115	10.162992
H	-0.185745	-2.873612	10.904282
H	-2.692800	-9.018609	8.775488
H	-1.975117	-8.252598	7.357470

H	-0.925851	-8.931424	8.617676
H	-2.552201	-7.853453	11.076834
H	-0.785138	-7.764021	10.925621
H	-1.725057	-6.285556	11.198782

YT3RR_NRFb.xyz

149

scf done: -2856.883756

C	-5.137611	-1.021090	-0.337941
C	-4.048626	-0.841057	0.558944
C	-3.293302	0.355377	0.475673
C	-3.657995	1.372934	-0.402482
C	-4.764677	1.252598	-1.246552
C	-5.461777	0.040110	-1.192705
O	-3.700092	-1.739279	1.470941
Y	-3.058686	-1.863079	3.543317
O	-1.634433	-3.599187	2.751738
C	-0.905278	-4.346017	2.100749
O	-1.318307	-5.515127	1.642083
C	-2.678435	-5.887405	1.939026
C	-2.014675	0.457813	1.255480
N	-2.089211	0.454908	2.746475
C	-0.714105	0.651839	3.239428
C	-5.143501	2.398221	-2.194775
C	-5.419566	3.676297	-1.378311
C	-5.906458	-2.350339	-0.400762
C	-4.914447	-3.484300	-0.732391
O	-4.705489	-2.988746	4.266284
C	-5.745835	-2.862301	5.087750
C	-6.381298	-1.599857	5.189466
C	-7.433628	-1.407154	6.081389
C	-7.916498	-2.440205	6.887046
C	-7.310777	-3.691653	6.729598
C	-6.253091	-3.948681	5.849075
C	-5.985455	-0.487970	4.256571
N	-4.575009	-0.011358	4.367698
C	-4.275468	0.381238	5.753130
C	-5.696189	-5.371158	5.675165
C	-5.906363	-5.811508	4.211413
C	-9.066507	-2.180178	7.868577
C	-8.645548	-1.091730	8.875767
O	-1.684775	-1.749771	5.205988
C	-0.728910	-1.374406	6.017361
O	-0.852142	-0.037096	6.416387
C	-1.226129	0.135653	7.775652
C	0.344852	-2.097619	6.432547
C	0.434611	-3.561434	6.088777
C	0.550164	-4.579438	7.272060
C	0.101313	-5.944630	6.730261
O	0.268830	-6.920155	7.734903
C	-0.400776	-8.152330	7.501731
C	-0.445195	-8.874717	8.839330
C	1.488302	-1.443095	7.163688

C	-4.197734	-5.421275	6.027531	H	-3.770607	1.774996	-3.776872
C	-6.409810	-6.395647	6.570357	H	-3.819702	-6.443971	5.895772
C	-10.310843	-1.701310	7.095056	H	-3.619294	-4.749473	5.392564
C	-9.454325	-3.435713	8.661873	H	-4.016997	-5.129091	7.065367
C	-4.403260	1.126691	3.443479	H	-5.983934	-7.388926	6.389991
C	-2.949936	1.542523	3.260662	H	-6.279108	-6.172594	7.634802
C	-6.601783	-2.644985	0.941694	H	-7.482850	-6.455533	6.357827
C	-6.988445	-2.354802	-1.491633	H	-5.490885	-6.815451	4.052917
C	-3.982930	2.664232	-3.174107	H	-6.973924	-5.848710	3.967735
C	-6.398667	2.083241	-3.020005	H	-5.423424	-5.113844	3.524020
C	0.510985	-4.055203	1.761888	H	-10.270144	-3.198147	9.353322
C	1.117543	-3.079985	2.451989	H	-9.801994	-4.241011	8.006005
C	1.180955	-4.893798	0.711748	H	-8.616971	-3.816141	9.256508
C	1.983879	-4.697017	7.803485	H	-9.457352	-0.883162	9.583155
C	-0.455420	-4.183088	8.352619	H	-7.767676	-1.409866	9.448136
O	-1.656136	-4.313552	8.254302	H	-8.392927	-0.152391	8.373566
O	0.127597	-3.652007	9.445909	H	-11.143260	-1.508630	7.782628
C	-0.776518	-3.269409	10.483300	H	-10.115090	-0.776204	6.543720
C	0.296695	-8.980430	6.423562	H	-10.634233	-2.456997	6.371509
H	-4.975646	1.997957	3.807548	H	2.158935	-2.833543	2.267174
H	-4.825279	0.844011	2.475692	H	0.599882	-2.532614	3.233692
H	-2.916584	2.413215	2.587887	H	-2.827887	-5.942427	3.018467
H	-2.536767	1.868703	4.219373	H	-3.369761	-5.160454	1.510477
H	-1.485215	1.373549	0.942907	H	-2.813184	-6.865044	1.479698
H	-1.368936	-0.391187	0.991555	H	0.648317	-4.834553	-0.242992
H	-6.658273	0.369881	4.421412	H	2.209322	-4.560903	0.555547
H	-6.118816	-0.809643	3.216431	H	1.196790	-5.949287	1.000996
H	-7.684120	-4.516977	7.322005	H	1.514522	-1.674081	8.236940
H	-7.888194	-0.418926	6.130989	H	2.447921	-1.781877	6.749442
H	-6.304079	-0.093101	-1.859359	H	1.451945	-0.355934	7.055225
H	-3.044860	2.272585	-0.430917	H	-0.456476	-3.818813	5.507886
H	-4.883883	1.249132	6.056194	H	1.308627	-3.757913	5.446598
H	-4.507827	-0.453869	6.416287	H	2.044096	-5.471921	8.570054
H	-3.215882	0.615755	5.860029	H	2.650519	-4.981827	6.981215
H	-0.294721	1.603552	2.873374	H	2.347037	-3.762326	8.229725
H	-0.699944	0.645213	4.329283	H	-1.399137	1.205600	7.923773
H	-0.075023	-0.156543	2.873017	H	-2.147968	-0.413497	8.003654
H	-5.430632	-4.452388	-0.738910	H	-0.437840	-0.192796	8.462253
H	-4.469457	-3.331381	-1.722158	H	-0.954672	-5.880765	6.432017
H	-4.109827	-3.515345	0.005156	H	0.704228	-6.179428	5.836695
H	-7.150883	-3.592836	0.883620	H	-1.432961	-7.936364	7.176655
H	-5.883252	-2.717393	1.759612	H	-0.154091	-2.889494	11.294045
H	-7.327432	-1.858479	1.179764	H	-1.464122	-2.495379	10.132765
H	-7.477323	-3.334998	-1.508633	H	-1.362267	-4.128507	10.820038
H	-7.766919	-1.606374	-1.306200	H	-0.217304	-9.936205	6.277668
H	-6.570923	-2.178019	-2.488962	H	0.311441	-8.462368	5.459544
H	-6.636415	2.931793	-3.670558	H	1.331531	-9.185797	6.717202
H	-6.255442	1.207048	-3.661201	H	-0.984038	-9.823162	8.751577
H	-7.269954	1.901129	-2.381727	H	0.570211	-9.084781	9.191147
H	-5.682483	4.509125	-2.041469	H	-0.946212	-8.254911	9.587432
H	-6.250043	3.521518	-0.681239				
H	-4.545370	3.981195	-0.794309				
H	-4.232609	3.486702	-3.855152				
H	-3.062523	2.936330	-2.647966				

scf done: -2856.881291				C	-5.087719	3.499120	-2.587698
C	-5.586861	-0.687739	-0.308514	C	-7.414511	2.766922	-2.087508
C	-4.351064	-0.602178	0.388955	C	0.857863	-4.187866	3.033908
C	-3.647849	0.628420	0.378678	C	1.193349	-2.942496	3.780422
C	-4.197386	1.761937	-0.215430	C	1.828640	-5.345061	3.018263
C	-5.446663	1.728746	-0.839476	C	1.346885	-5.342379	7.777625
C	-6.093118	0.487676	-0.878848	C	-0.049739	-3.273055	8.257137
O	-3.813612	-1.621384	1.046931	O	-0.753133	-2.319705	7.970158
Y	-2.762571	-2.040330	2.869482	O	0.622264	-3.349170	9.413764
O	-1.179584	-3.306180	2.156922	C	0.361030	-2.308391	10.358106
C	-0.267195	-4.231704	2.262361	C	-2.330905	-7.883219	8.825984
O	-0.447984	-5.365741	1.517505	H	-4.576166	1.696932	4.163757
C	-1.518799	-5.370602	0.587692	H	-4.676389	0.811020	2.638637
C	-2.232950	0.657112	0.882086	H	-2.719286	2.338506	2.756558
N	-1.972575	0.389665	2.330737	H	-2.091576	1.435036	4.134970
C	-0.519995	0.538494	2.521085	H	-1.794240	1.638987	0.637563
C	-6.027960	3.000492	-1.472163	H	-1.652930	-0.100797	0.338913
C	-6.163004	4.097145	-0.397251	H	-6.239332	-0.092637	4.565081
C	-6.322186	-2.028062	-0.472962	H	-5.782899	-1.012451	3.125473
C	-5.378533	-3.042768	-1.151421	H	-7.158762	-5.465697	6.418264
O	-4.218409	-3.329935	3.717389	H	-7.357326	-1.208127	6.138801
C	-5.254426	-3.374346	4.548562	H	-7.045018	0.425878	-1.390259
C	-5.886538	-2.161643	4.923494	H	-3.618859	2.684473	-0.199939
C	-6.906978	-2.162899	5.871744	H	-4.424577	0.487941	6.196351
C	-7.370744	-3.341999	6.459373	H	-3.845400	-1.196103	6.187537
C	-6.788764	-4.532951	6.012362	H	-2.732899	0.102125	5.755647
C	-5.760969	-4.598178	5.063687	H	-0.182290	1.551340	2.245491
C	-5.566392	-0.883692	4.193199	H	-0.258086	0.353821	3.563298
N	-4.163223	-0.386555	4.274952	H	0.008481	-0.178509	1.886394
C	-3.767757	-0.232623	5.681432	H	-5.880141	-4.012349	-1.257489
C	-5.233283	-5.953412	4.562302	H	-5.095944	-2.697252	-2.152300
C	-5.462529	-6.060468	3.040833	H	-4.469679	-3.183051	-0.563670
C	-8.484076	-3.295596	7.514541	H	-7.309172	-3.524067	0.761337
C	-8.023531	-2.439502	8.710975	H	-5.923339	-2.758373	1.552356
O	-1.279153	-1.871042	4.767552	H	-7.458283	-1.875806	1.386074
C	-0.211697	-1.702583	5.361212	H	-8.034110	-2.890483	-1.466141
O	-0.001152	-0.429844	5.732529	H	-8.327515	-1.239781	-0.915142
C	0.900245	0.052573	6.732493	H	-7.335931	-1.535870	-2.359854
C	0.825514	-2.818197	5.366873	H	-7.793781	3.703396	-2.510865
C	0.149242	-4.125485	5.852760	H	-7.382997	2.029502	-2.896506
C	0.134788	-4.493105	7.368022	H	-8.138417	2.423732	-1.340583
C	-1.150661	-5.327431	7.583162	H	-6.567766	5.018351	-0.833214
O	-1.241212	-5.699747	8.936271	H	-6.836410	3.775823	0.404543
C	-2.418103	-6.429096	9.282021	H	-5.196839	4.341464	0.055784
C	-2.566140	-6.309705	10.790716	H	-5.485946	4.410015	-3.050834
C	2.150418	-2.563379	6.093664	H	-4.089563	3.731237	-2.202808
C	-3.732228	-6.098313	4.870788	H	-4.974362	2.740802	-3.369411
C	-5.952902	-7.142326	5.218108	H	-3.354684	-7.053253	4.484525
C	-9.753505	-2.669922	6.903191	H	-3.158073	-5.289346	4.417080
C	-8.847858	-4.690514	8.041018	H	-3.564770	-6.082040	5.952996
C	-4.099134	0.903795	3.561665	H	-5.552767	-8.075792	4.807439
C	-2.680847	1.338471	3.217653	H	-5.802203	-7.171053	6.303269
C	-6.773575	-2.576328	0.893750	H	-7.030286	-7.132053	5.021024
C	-7.574072	-1.902657	-1.355355	H	-5.079101	-7.017600	2.666136

H	-6.531762	-6.011050	2.807638
H	-4.958224	-5.251215	2.510545
H	-9.630864	-4.606901	8.802606
H	-9.230389	-5.338812	7.245497
H	-7.987885	-5.187445	8.502826
H	-8.808698	-2.386792	9.474926
H	-7.126575	-2.865876	9.172863
H	-7.785706	-1.415185	8.407117
H	-10.558656	-2.622755	7.646471
H	-9.571221	-1.651735	6.545399
H	-10.107863	-3.262197	6.053113
H	2.280041	-2.789689	3.740053
H	0.755511	-2.084914	3.260339
H	-2.492590	-5.297803	1.082338
H	-1.431786	-4.554883	-0.137912
H	-1.450240	-6.329119	0.068956
H	2.075357	-5.656400	1.995716
H	2.768720	-5.069410	3.511264
H	1.452859	-6.246076	3.524785
H	2.063970	-2.430138	7.174226
H	2.793770	-3.431344	5.923833
H	2.679902	-1.701270	5.679938
H	-0.874223	-4.120142	5.470431
H	0.644866	-4.950229	5.335667
H	1.227061	-5.709825	8.797154
H	1.423959	-6.203699	7.106258
H	2.283854	-4.784313	7.721184
H	0.531936	1.050124	6.977434
H	0.858676	-0.572191	7.622453
H	1.919620	0.132451	6.351461
H	-2.024063	-4.725731	7.288939
H	-1.101764	-6.201262	6.914354
H	-3.284890	-5.949124	8.796750
H	0.874906	-2.605128	11.272182
H	0.751366	-1.349717	10.004636
H	-0.712428	-2.209430	10.533529
H	-3.229968	-8.432233	9.123659
H	-2.241920	-7.967170	7.739056
H	-1.462166	-8.369006	9.282207
H	-3.467841	-6.826387	11.132650
H	-1.700905	-6.755040	11.292587
H	-2.632361	-5.259471	11.087563

YT3RS_NLB.xyz

149

scf done: -2856.876327

C	-5.776064	-0.499509	-0.264435
C	-4.614516	-0.256361	0.516523
C	-4.094857	1.059233	0.574059
C	-4.755647	2.117330	-0.044059
C	-5.938562	1.922141	-0.761680
C	-6.399894	0.604658	-0.860769
O	-3.983481	-1.202470	1.202345

Y	-2.935209	-1.587629	3.030675
O	-1.361109	-2.841712	1.999167
C	-2.743898	1.272585	1.191819
N	-2.567163	0.978730	2.646790
C	-1.191706	1.381253	2.984622
C	-6.652628	3.113916	-1.413537
C	-7.061385	4.124685	-0.323565
C	-6.312343	-1.923286	-0.480080
C	-5.202209	-2.794793	-1.102927
O	-4.248913	-3.156051	3.651389
C	-5.201158	-3.430581	4.542555
C	-5.964069	-2.360783	5.075146
C	-6.870819	-2.584459	6.108516
C	-7.090442	-3.859094	6.635506
C	-6.407905	-4.913010	6.019550
C	-5.492470	-4.755289	4.970173
C	-5.913805	-1.008193	4.416363
N	-4.615496	-0.277540	4.460972
C	-4.206532	-0.064878	5.856452
C	-4.912151	-5.984309	4.245338
C	-5.338315	-5.916154	2.764423
C	-8.067298	-4.057183	7.802217
C	-7.591228	-3.230257	9.013152
O	-1.410348	-1.370700	4.773839
C	-0.484516	-2.081921	5.310971
O	-0.812899	-3.285375	5.853305
C	-2.131512	-3.435298	6.367610
C	0.890044	-1.807132	5.352908
C	1.370041	-0.394397	5.144667
C	1.582079	0.500555	6.416901
C	0.359744	0.400002	7.336934
O	0.521297	1.328305	8.388083
C	-0.608601	1.482147	9.238020
C	-0.420379	2.803603	9.967227
C	1.794433	-2.796559	6.049376
C	-3.376701	-6.040727	4.337124
C	-5.447165	-7.308034	4.814534
C	-9.474938	-3.584719	7.387890
C	-8.166198	-5.525085	8.239120
C	-4.808810	1.010208	3.761571
C	-3.510416	1.750514	3.486601
C	-6.763853	-2.539408	0.857221
C	-7.515492	-1.957966	-1.435051
C	-5.704302	3.804100	-2.413986
C	-7.919227	2.694273	-2.172067
C	2.856704	0.144596	7.189188
C	1.608919	1.945429	5.908599
O	0.664722	2.493124	5.373651
O	2.793092	2.553032	6.077629
C	2.857513	3.903901	5.614036
C	-0.753034	0.308042	10.204427
H	-5.472099	1.664561	4.353657
H	-5.315749	0.806901	2.814920
H	-3.748094	2.714637	3.012172

H	-3.007124	1.983041	4.429501
H	-2.440419	2.318433	1.020569
H	-2.012784	0.637964	0.672154
H	-6.690556	-0.368754	4.868038
H	-6.163446	-1.117284	3.354498
H	-6.605129	-5.918864	6.367021
H	-7.427306	-1.731643	6.494062
H	-7.295492	0.421662	-1.440476
H	-4.317466	3.111563	0.028558
H	-4.901527	0.618960	6.370825
H	-4.216836	-1.023032	6.378110
H	-3.195033	0.340431	5.906589
H	-1.022160	2.447541	2.771254
H	-0.991100	1.210333	4.040323
H	-0.481120	0.800768	2.388087
H	-5.560708	-3.822398	-1.240219
H	-4.910915	-2.404669	-2.084654
H	-4.319298	-2.813794	-0.461228
H	-7.164374	-3.547103	0.693556
H	-5.933303	-2.615254	1.560801
H	-7.559522	-1.936865	1.311100
H	-7.832267	-2.996931	-1.575851
H	-8.375280	-1.406215	-1.038824
H	-7.270072	-1.551470	-2.422309
H	-8.395597	3.577141	-2.611925
H	-7.693678	2.000283	-2.988772
H	-8.651675	2.218454	-1.511267
H	-7.566504	4.991270	-0.766966
H	-7.745830	3.664586	0.397275
H	-6.192785	4.494252	0.230814
H	-6.198120	4.662597	-2.884746
H	-4.795897	4.171059	-1.925910
H	-5.399990	3.110265	-3.204540
H	-2.999287	-6.902932	3.773913
H	-2.918532	-5.137715	3.932333
H	-3.051588	-6.158458	5.376059
H	-5.026056	-8.140973	4.241017
H	-5.160720	-7.455499	5.861829
H	-6.537615	-7.377737	4.741583
H	-4.924876	-6.767078	2.208742
H	-6.429416	-5.954009	2.676078
H	-4.993233	-4.990166	2.300169
H	-8.854998	-5.612709	9.086275
H	-8.548974	-6.164861	7.436920
H	-7.196113	-5.920416	8.559080
H	-8.282101	-3.345766	9.856924
H	-6.597734	-3.554930	9.340817
H	-7.531910	-2.163364	8.775530
H	-10.185132	-3.715461	8.213085
H	-9.481995	-2.526431	7.108717
H	-9.840695	-4.157483	6.529302
H	1.582822	-3.819586	5.727644
H	2.843674	-2.579192	5.819732
H	1.692800	-2.785028	7.143112

H	0.652832	0.121796	4.505226
H	2.330349	-0.400388	4.606105
H	3.002711	0.834378	8.022242
H	2.784433	-0.866426	7.595105
H	3.738331	0.194541	6.544662
H	-2.145323	-4.407335	6.860837
H	-2.346577	-2.654233	7.105643
H	-2.891128	-3.420434	5.586425
H	-0.552164	0.621840	6.763099
H	0.285328	-0.630648	7.712319
H	-1.515545	1.544637	8.610796
H	3.873466	4.239679	5.822101
H	2.648198	3.956383	4.542386
H	2.132284	4.526320	6.144171
H	-1.617418	0.452918	10.860716
H	-0.894085	-0.640021	9.676765
H	0.143224	0.222116	10.827347
H	-1.271469	3.010685	10.623122
H	0.487138	2.771173	10.578831
H	-0.321777	3.623300	9.250594
C	-0.484355	-3.752674	2.031955
C	0.796109	-3.665423	2.656963
C	1.200462	-2.435189	3.132274
O	-0.710909	-4.906171	1.394066
C	-1.936881	-5.025369	0.667262
C	1.676853	-4.887384	2.705916
H	2.247300	-2.291923	3.380298
H	0.641862	-1.547010	2.859129
H	-1.901011	-6.010397	0.202070
H	-2.796234	-4.957288	1.336925
H	-2.010824	-4.247170	-0.096127
H	1.879008	-5.279617	1.702866
H	2.634512	-4.643530	3.173599
H	1.222431	-5.702985	3.279156

YT3RS_NLBb.xyz

149

scf done: -2856.907163

C	-5.966427	-0.525476	-0.451692
C	-4.736472	-0.335904	0.233365
C	-4.105113	0.930205	0.169874
C	-4.714512	1.998684	-0.483704
C	-5.955130	1.862246	-1.111230
C	-6.533841	0.588016	-1.084877
O	-4.145294	-1.291441	0.940170
Y	-2.960880	-1.609897	2.684586
O	-1.253126	-2.632156	1.901927
C	-2.709173	1.074262	0.705167
N	-2.496085	0.904276	2.177952
C	-1.091995	1.260066	2.443623
C	-6.601550	3.064156	-1.813437
C	-6.798998	4.209485	-0.800753
C	-6.633512	-1.907967	-0.527339

C	-5.653486	-2.910940	-1.170195	H	-4.190155	2.952874	-0.512043
O	-4.225635	-3.101120	3.547867	H	-4.588496	0.925930	6.056043
C	-5.062787	-3.279902	4.563726	H	-3.843850	-0.686787	6.148486
C	-5.726463	-2.150771	5.110256	H	-2.920615	0.667137	5.476504
C	-6.506486	-2.279013	6.257554	H	-0.871266	2.288934	2.116591
C	-6.691630	-3.510495	6.891134	H	-0.882182	1.191815	3.511568
C	-6.112447	-4.624431	6.272875	H	-0.429885	0.580788	1.899451
C	-5.329645	-4.565088	5.112217	H	-6.107354	-3.908455	-1.212872
C	-5.728982	-0.850314	4.349713	H	-5.407959	-2.607401	-2.194094
N	-4.429636	-0.130771	4.216300	H	-4.727226	-2.974249	-0.596365
C	-3.913630	0.219057	5.545085	H	-7.529559	-3.370793	0.813568
C	-4.860429	-5.852593	4.407303	H	-6.151742	-2.514842	1.520405
C	-5.428739	-5.862363	2.972722	H	-7.723957	-1.696265	1.352491
C	-7.535376	-3.605505	8.169739	H	-8.321241	-2.909051	-1.427875
C	-6.916421	-2.713325	9.263973	H	-8.684841	-1.245502	-0.963888
O	-1.431995	-1.563814	4.615094	H	-7.711195	-1.576207	-2.413221
C	-0.498860	-2.138635	5.183887	H	-8.397464	3.611914	-2.893074
O	-0.704003	-3.049759	6.118116	H	-7.898842	1.942459	-3.180364
C	-2.063867	-3.335428	6.490043	H	-8.679616	2.386527	-1.650333
C	0.968780	-1.846013	4.909930	H	-7.249180	5.082783	-1.287547
C	1.230109	-0.333094	5.160579	H	-7.458509	3.897882	0.016330
C	1.278888	0.308642	6.580013	H	-5.849400	4.529225	-0.359835
C	0.159485	-0.205817	7.500032	H	-6.126114	4.415205	-3.462507
O	0.165575	0.586619	8.666353	H	-4.699799	3.849034	-2.581860
C	-0.909837	0.345428	9.569894	H	-5.532985	2.758839	-3.695801
C	-0.992850	1.566734	10.471915	H	-3.031950	-6.864695	3.809484
C	1.901580	-2.774718	5.688527	H	-2.887254	-5.103243	3.820925
C	-3.325075	-5.953942	4.344812	H	-2.894478	-6.013825	5.350584
C	-5.370576	-7.120208	5.111131	H	-5.040835	-7.999610	4.547603
C	-8.972063	-3.126669	7.880246	H	-4.975407	-7.218979	6.128630
C	-7.611720	-5.038524	8.714129	H	-6.464252	-7.152934	5.161459
C	-4.667334	1.083779	3.409114	H	-5.107085	-6.768332	2.444781
C	-3.386055	1.780464	2.974944	H	-6.523956	-5.852742	2.992283
C	-7.026959	-2.398382	0.879373	H	-5.086599	-4.992224	2.409796
C	-7.908989	-1.895356	-1.384048	H	-8.203569	-5.053374	9.635739
C	-5.684764	3.549715	-2.953886	H	-8.092037	-5.719817	8.003883
C	-7.971605	2.722833	-2.415448	H	-6.619144	-5.436493	8.951269
C	2.642366	0.139884	7.260433	H	-7.517589	-2.751626	10.180281
C	0.931829	1.791827	6.352998	H	-5.901758	-3.045048	9.510115
O	-0.099058	2.165026	5.825851	H	-6.858409	-1.666877	8.948073
O	1.876610	2.637069	6.777590	H	-9.589109	-3.185951	8.784829
C	1.578758	4.026420	6.607351	H	-8.991289	-2.089058	7.532487
C	-0.701409	-0.942403	10.363462	H	-9.439833	-3.744904	7.107086
H	-5.287477	1.801155	3.974756	H	1.726952	-3.814860	5.409971
H	-5.236420	0.795044	2.521506	H	2.940403	-2.528702	5.446868
H	-3.654437	2.679741	2.401808	H	1.773092	-2.697374	6.770036
H	-2.828583	2.121667	3.852276	H	0.464399	0.197290	4.593290
H	-2.329814	2.070223	0.424348	H	2.188629	-0.106454	4.676191
H	-2.057879	0.332750	0.222495	H	2.651744	0.645326	8.227131
H	-6.458721	-0.169340	4.819369	H	2.859545	-0.917659	7.424717
H	-6.076702	-1.039521	3.327102	H	3.442765	0.560060	6.645567
H	-6.291516	-5.598974	6.708713	H	-2.010090	-4.214193	7.129978
H	-6.995411	-1.387015	6.646664	H	-2.476420	-2.489321	7.044930
H	-7.479789	0.449261	-1.592405	H	-2.675769	-3.534648	5.612513

H	-0.809473	-0.113741	6.985542
H	0.331942	-1.265329	7.732992
H	-1.845283	0.264090	8.989036
H	2.443125	4.562985	6.997933
H	1.425794	4.261521	5.551077
H	0.677187	4.294529	7.163351
H	-1.532234	-1.103964	11.057777
H	-0.640713	-1.820144	9.712969
H	0.225491	-0.881879	10.942876
H	-1.818760	1.468259	11.182699
H	-0.062550	1.682624	11.037179
H	-1.148524	2.471047	9.877688
C	-0.323060	-3.541876	2.073496
C	0.843004	-3.391243	2.765172
C	1.173059	-2.054138	3.364066
O	-0.556030	-4.763373	1.495257
C	-1.544734	-4.820032	0.480927
C	1.870818	-4.494656	2.776823
H	2.234039	-1.822041	3.183798
H	0.587998	-1.281217	2.855372
H	-1.496700	-5.835282	0.081205
H	-2.550582	-4.638871	0.873169
H	-1.346237	-4.102047	-0.322901
H	1.776427	-5.123865	1.887506
H	2.886823	-4.077904	2.788378
H	1.798844	-5.170215	3.641977

YT3RS_NLBf.xyz

149

scf done: -2856.884501

C	-5.729636	-0.530215	-0.280783
C	-4.548099	-0.309199	0.478401
C	-4.034486	1.007790	0.567131
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Y	-3.133824	-1.670145	3.791340	O	2.565961	1.304412	6.033832
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C	-3.222471	-5.888347	5.553548	H	-5.613686	0.545524	3.207051
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C	-4.164086	1.541118	4.436204	H	-6.314286	-1.554956	3.319855
N	-2.952692	0.936906	3.841133	H	-6.905451	-6.515296	6.171119
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O	-1.380167	-2.730217	2.596195	H	-5.626614	-2.628411	1.474655
C	-0.665736	-3.338049	1.797398	H	-7.190242	-1.933589	0.980477
C	-0.181708	-4.726327	1.991191	H	-6.779621	-2.593878	-2.011942
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				H	-7.364826	4.041068	-2.392036
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H	-7.045294	5.247441	-0.269220
H	-7.449215	3.799266	0.672599
H	-5.932944	4.659266	0.973289
H	-5.199435	5.170555	-2.015921
H	-4.051672	4.588685	-0.801826
H	-4.291640	3.671167	-2.293644
H	-2.458508	-6.637531	5.311445
H	-2.855371	-4.908025	5.248135
H	-3.350353	-5.883716	6.641547
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H	-5.097870	-7.674956	6.418463
H	-5.898710	-7.968081	4.859445
H	-3.564952	-7.063604	3.092052
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H	-4.026484	-5.355545	2.916969
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H	-9.024039	-7.122213	6.470761
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H	0.639558	-6.485614	1.084441
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149			
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Y	-3.073603	-1.771448	2.826128
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C	-3.524811	1.558179	3.419253
N	-2.596940	0.738728	2.608976
C	-1.204543	0.996732	3.015957
O	-4.255844	-1.267250	1.127739
C	-4.740150	-0.242547	0.437134
C	-4.056145	0.997193	0.506648
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C	-5.755460	2.081506	-0.863968
C	-6.382062	0.834334	-0.966518
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C	-2.698386	1.057239	1.150929
C	-6.622311	-1.684614	-0.576436
C	-7.130378	-2.259084	0.759852
C	-6.296133	3.350495	-1.536890
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O	-1.334558	-2.439088	1.802985
C	-0.106655	-2.718713	1.442879
C	0.782193	-3.435137	2.180205
C	2.150494	-3.787344	1.664589
O	0.298360	-2.199689	0.235886
C	-0.656070	-2.279407	-0.814352
C	-7.832747	-1.561518	-1.515211
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C	-7.608323	3.097751	-2.291987
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C	-5.123650	-6.223863	2.942244
C	-4.197596	-0.215208	5.799250

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O	-1.076077	-3.456997	6.509816	H	-4.611355	-8.287577	4.577698
C	-2.377177	-3.262013	7.084320	H	-4.780894	-7.497121	6.147103
C	1.347903	-1.830464	4.498609	H	-6.176771	-7.625449	5.055867
C	1.958354	-0.906677	5.602668	H	-4.647995	-7.086985	2.460877
C	3.268876	-1.447212	6.197726	H	-6.209149	-6.350778	2.866112
C	0.346163	-3.989349	3.503006	H	-4.842739	-5.322160	2.395834
C	2.216064	0.415822	4.863309	H	-8.495342	-5.717878	9.370443
O	3.464783	0.504170	4.381801	H	-8.233685	-6.323640	7.731990
C	3.746320	1.682202	3.619934	H	-6.848186	-5.984313	8.787084
C	0.960111	-0.584818	6.719497	H	-7.976585	-3.400175	10.027690
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C	0.682529	1.062627	8.435264	H	-7.314813	-2.237510	8.870432
C	0.072927	0.192888	9.532857	H	-9.930575	-3.907012	8.486814
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C	1.489274	2.220040	9.002162	H	-9.641875	-4.403050	6.807654
H	-5.485452	1.501450	4.305018	H	0.863267	-4.942848	3.662184
H	-5.347583	0.629207	2.771531	H	-0.720183	-4.232080	3.453077
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H	-3.021850	1.818944	4.355518	H	-0.210005	-1.770862	-1.671490
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H	-6.332106	-6.050123	6.587121	H	0.873635	-5.019550	5.913605
H	-7.315611	-1.892603	6.578618	H	2.377413	-4.231962	5.415981
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H	-4.873258	0.485167	6.317880	H	2.168364	-2.099524	3.828630
H	-4.211548	-1.164704	6.333521	H	3.749316	-0.679067	6.806489
H	-3.182439	0.185330	5.828701	H	3.084517	-2.309372	6.840376
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H	-1.047876	0.721578	4.059586	H	-2.414615	-3.931019	7.942945
H	-0.526686	0.402299	2.398507	H	-2.486154	-2.225206	7.409246
H	-6.117996	-3.653473	-1.363644	H	-3.161572	-3.516949	6.369775
H	-5.305618	-2.317869	-2.200479	H	0.053117	-0.141278	6.283520
H	-4.755491	-2.820071	-0.587902	H	0.679090	-1.513840	7.237930
H	-7.673964	-3.195419	0.585457	H	-0.128459	1.466023	7.803858
H	-6.302183	-2.470955	1.437487	H	4.790458	1.596555	3.319691
H	-7.820591	-1.559435	1.246042	H	3.098952	1.735237	2.740923
H	-8.279257	-2.551692	-1.656453	H	3.593172	2.577877	4.226877
H	-8.610535	-0.907423	-1.105276	H	-0.593592	0.784692	10.168668
H	-7.551514	-1.184761	-2.504657	H	-0.513052	-0.633494	9.118370
H	-7.960691	4.031257	-2.743920	H	0.862696	-0.231157	10.161553
H	-7.480098	2.369287	-3.099646	H	0.859263	2.865174	9.622036
H	-8.397839	2.734420	-1.625446	H	2.310808	1.842959	9.619792
H	-6.937533	5.348358	-0.929567	H	1.914043	2.818479	8.192127
H	-7.308930	4.082044	0.256317				
H	-5.653054	4.681678	0.087268				
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C	-0.237224	-3.673366	6.110031	H	-6.756431	0.494474	5.254233
C	-1.283255	-4.176226	7.070485	H	-5.904460	0.424487	3.705711
C	-1.128356	-3.769335	8.567397	H	-4.859101	2.059196	5.189939
C	-0.013639	-4.605729	9.198658	H	-4.668614	0.858296	6.458162
O	0.924989	-3.870647	9.819447	H	-2.629612	2.434724	4.106456
C	1.961326	-4.625445	10.451314	H	-1.992321	0.985021	3.324738
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N	-5.626153	-1.266269	4.889961	H	-6.460305	-1.627997	3.023488
C	-5.812539	0.189255	4.768357	H	-7.432654	-7.184508	4.141145
C	-4.674421	0.990308	5.371820	H	-8.946453	-3.206728	4.470299
N	-3.345999	0.591868	4.859796	H	-6.041161	2.332966	-0.517315
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C	-9.806179	-5.809631	4.522345	H	-6.673531	-1.397850	6.746419
C	-9.872316	-7.342707	4.490016	H	-5.655589	-2.795065	6.326621
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C	-3.882784	1.656404	2.582622	H	-5.653596	-1.898339	1.027167
C	-5.361024	-0.288030	-0.418755	H	-7.139286	-1.001191	0.634099
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O	-1.854078	-2.978985	2.424976	H	-5.938872	4.437677	-1.242460
C	-0.816654	-3.669571	2.202483	H	-7.380412	4.143210	-0.250265
C	-0.185849	-4.586065	3.086857	H	-6.745245	6.205356	1.938418
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C	-6.204508	-1.402970	0.226739	H	-3.575646	-5.569696	5.275293
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C	-3.987696	-6.347053	2.568244	H	-4.426202	-8.770284	3.568549
C	-3.912330	-6.590820	5.092418	H	-5.821811	-8.460137	4.600631
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C	-10.702876	-5.268058	3.391426	H	-3.155113	-7.053909	2.470204
O	0.571359	-2.027340	4.700812	H	-4.619516	-6.446399	1.678010
C	0.415685	-0.923799	3.825518	H	-3.584730	-5.334875	2.590513

H	-10.909256	-7.670460	4.621393	C	-0.595417	-3.319340	5.588348
H	-9.517370	-7.745869	3.535626	C	-0.583907	-4.046363	6.732041
H	-9.279309	-7.793142	5.293201	C	-1.824343	-4.171857	7.572668
H	-11.387467	-5.694761	6.025089	C	-1.762838	-3.592738	9.021421
H	-9.748488	-5.715085	6.704896	C	-0.917478	-4.519075	9.896542
H	-10.377768	-4.243915	5.951697	O	0.120205	-3.901594	10.492548
H	-11.731798	-5.628977	3.507869	C	0.918007	-4.741369	11.328429
H	-10.732920	-4.173904	3.387211	C	-6.254577	-1.908636	4.237649
H	-10.335721	-5.594187	2.412729	N	-5.060056	-1.386303	4.966155
H	-0.470088	-5.731031	4.861062	C	-5.144526	0.086821	4.959674
H	-1.849165	-4.602695	4.426135	C	-3.848954	0.760767	5.379894
H	-0.191759	-2.768130	-0.846023	N	-2.700210	0.398490	4.522251
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H	-1.832035	-3.141967	-0.236280	C	-9.300760	-5.815059	5.136342
H	0.999488	-5.772647	1.715390	C	-9.420398	-7.338210	4.987108
H	1.414574	-5.975039	3.424170	C	-4.632233	-6.630647	3.169542
H	1.923122	-4.527258	2.545989	C	-5.134727	-8.082454	3.138580
H	1.210102	-5.190848	6.574091	O	-3.563085	-0.798238	1.877270
H	1.674754	-3.588535	7.145428	C	-4.118258	0.381069	1.630475
H	1.790463	-3.968484	5.425794	C	-5.089800	0.587297	0.612018
H	-2.267365	-3.824576	6.742276	C	-5.655959	1.864842	0.502884
H	-1.306549	-5.273599	7.042898	C	-5.310225	2.955978	1.307907
H	-0.916706	-1.993459	9.796064	C	-4.311087	2.737526	2.259601
H	-1.754816	-1.735020	8.250054	C	-3.717495	1.488471	2.423003
H	0.003570	-1.928036	8.281782	C	-5.485886	-0.536123	-0.363250
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H	-2.573335	-5.292017	9.102198	C	-7.042886	4.374761	0.086722
H	-3.267997	-3.670736	8.831614	O	-1.350658	-2.767984	2.026042
H	2.621629	-3.892012	10.914548	C	-0.493258	-3.135063	1.223113
H	2.507585	-5.223145	9.716919	C	0.048404	-4.509601	1.118410
H	1.542545	-5.295776	11.206065	C	0.939903	-4.843773	-0.044240
H	-3.343743	-5.647804	11.185262	O	0.048326	-2.306173	0.337475
H	-5.372925	-4.423389	12.000128	C	-0.389545	-0.936558	0.351937
H	-5.034057	-4.026495	10.313960	C	-6.579267	4.770712	2.499684
H	-4.596570	-2.878228	11.595463	C	-4.862751	5.368250	0.765304
H	-3.423533	-5.008022	13.598512	C	-4.232396	-1.044546	-1.102522
H	-2.656258	-3.453726	13.212289	C	-6.139843	-1.711346	0.388515
H	-1.760470	-4.965603	12.973891	C	-5.033369	-1.906934	6.339525
				C	-4.245786	-6.249155	1.726097
				C	-3.390012	-6.593634	4.081653
YT3SR_NRBb.xyz				C	-9.490301	-5.464202	6.625296
149				C	-10.432252	-5.165406	4.315175
scf done: -2856.885374				O	0.528425	-3.381755	4.772817
C	-5.688719	-5.651882	3.704547	C	1.117127	-2.137980	4.464715
C	-5.435418	-4.255534	3.768403	C	0.625230	-4.838813	7.152050
C	-6.448956	-3.399420	4.262778	C	-3.184038	-3.685502	9.599495
C	-7.665646	-3.918441	4.699605	O	-3.170792	-3.240655	10.938836
C	-7.944199	-5.285327	4.652819	C	-4.309682	-3.608052	11.708054
C	-6.934478	-6.111617	4.148205	C	-5.548050	-2.806799	11.310292
O	-4.279093	-3.718519	3.383733	C	-1.276802	-2.144339	9.028680
Y	-3.007953	-2.043838	3.587253	C	-3.931072	-3.390198	13.164770
O	-1.589940	-2.592685	5.110254	O	-1.155704	-5.698287	10.052780

H	-10.327841	-5.402762	3.251305
H	0.116531	-6.384907	2.088840
H	-0.891964	-5.072668	2.929224
H	-0.136862	-0.538202	-0.629979
H	0.162389	-0.392401	1.124191
H	-1.461673	-0.869737	0.546283
H	0.428506	-4.682386	-0.998878
H	1.253156	-5.888902	0.006845
H	1.835192	-4.213953	-0.053359
H	0.359888	-5.887367	7.342982
H	1.065543	-4.455884	8.082943
H	1.401002	-4.815013	6.385813
H	-2.650729	-3.671677	7.058323
H	-2.096057	-5.233018	7.671093
H	-1.282633	-1.731530	10.039082
H	-1.941222	-1.538737	8.401307
H	-0.267668	-2.068948	8.618097
H	2.039372	-2.350130	3.917242
H	1.367177	-1.574809	5.375101
H	0.467454	-1.518158	3.832414
H	-3.523463	-4.730863	9.545883
H	-3.857493	-3.071934	8.980190
H	1.698595	-4.098640	11.736516
H	1.357584	-5.557514	10.748808
H	0.314775	-5.169917	12.132966
H	-4.512332	-4.680823	11.545409
H	-6.405258	-3.089868	11.929880
H	-5.825232	-2.980657	10.266024
H	-5.363790	-1.735521	11.444935
H	-4.748868	-3.689480	13.827406
H	-3.708213	-2.333443	13.345014
H	-3.043103	-3.975394	13.417901

149

scf done: -2856.898654

C	-5.780116	-5.146555	3.990082
C	-5.407875	-3.781042	4.143221
C	-6.405636	-2.853368	4.533464
C	-7.683461	-3.286965	4.881965
C	-8.054421	-4.630562	4.818933
C	-7.083256	-5.517321	4.347027
O	-4.165569	-3.342648	3.930878
Y	-2.903317	-1.633353	3.746217
O	-1.163064	-1.790303	5.504120
C	-0.194627	-2.496316	5.817120
C	-0.238262	-4.005973	5.943401
C	-1.462512	-4.466544	6.765082
C	-1.462434	-4.289312	8.304715
C	-0.572697	-5.361388	8.943549
O	0.315572	-4.866136	9.821539
C	1.128896	-5.845011	10.474930
C	-6.182446	-1.369350	4.414658

N	-4.993298	-0.789171	5.092318	H	-6.088112	-1.096973	3.356944
C	-5.097951	0.675620	4.973232	H	-7.353101	-6.560422	4.246742
C	-3.779901	1.391722	5.203474	H	-8.410446	-2.536730	5.188888
N	-2.714451	0.976842	4.268585	H	-6.811365	1.485221	-0.518489
C	-1.425432	1.348025	4.867899	H	-4.390119	3.716803	2.204439
C	-9.468086	-5.065536	5.225122	H	-5.862562	-0.879647	7.040617
C	-9.675184	-6.580367	5.087220	H	-4.908408	-2.296304	6.549468
C	-4.803129	-6.202144	3.445065	H	-4.084489	-0.787732	7.002964
C	-5.475414	-7.561980	3.195470	H	-1.386256	2.424776	5.101344
O	-3.798872	-0.726655	2.041158	H	-1.266825	0.775862	5.782313
C	-4.403766	0.357180	1.579179	H	-0.617442	1.123357	4.167597
C	-5.391877	0.317607	0.558640	H	-4.560832	-2.420246	-1.400859
C	-6.040573	1.518094	0.240733	H	-3.954451	-0.759402	-1.536140
C	-5.750381	2.754416	0.829435	H	-3.630451	-1.706515	-0.068037
C	-4.706560	2.774685	1.758622	H	-6.522281	-2.954476	0.103958
C	-4.031066	1.611624	2.122427	H	-5.594933	-2.348683	1.481385
C	-5.686590	-0.975029	-0.221749	H	-7.221149	-1.711806	1.150633
C	-6.678142	-0.742839	-1.373009	H	-6.820862	-1.682018	-1.918322
C	-2.785987	1.701335	2.959223	H	-7.662910	-0.422112	-1.014459
C	-6.492130	4.049266	0.470263	H	-6.312976	0.000608	-2.090158
C	-7.589556	3.823678	-0.579135	H	-8.096108	4.771042	-0.792639
O	-1.202468	-2.320357	2.650741	H	-7.180307	3.448933	-1.523321
C	-0.023302	-2.893553	2.606324	H	-8.347380	3.114802	-0.228647
C	0.433252	-3.904589	3.396497	H	-7.677369	5.564982	1.506371
C	1.780422	-4.531323	3.140877	H	-7.886150	3.924980	2.149814
O	0.843310	-2.380089	1.668048	H	-6.417956	4.841842	2.516428
C	0.245643	-1.865101	0.487638	H	-6.008139	6.013847	-0.353610
C	-7.155369	4.628253	1.735910	H	-4.708026	5.322736	0.625475
C	-5.494768	5.079807	-0.095696	H	-5.010422	4.696266	-0.999836
C	-4.372428	-1.496327	-0.840780	H	-2.930174	-7.127130	4.078179
C	-6.288256	-2.058580	0.691494	H	-3.178066	-5.481244	4.691189
C	-4.960074	-1.206717	6.498531	H	-4.076391	-6.835176	5.401274
C	-4.212322	-5.739695	2.098109	H	-4.736331	-8.250471	2.771581
C	-3.676196	-6.423457	4.467542	H	-5.851755	-8.020322	4.116803
C	-9.721465	-4.681531	6.696518	H	-6.304426	-7.486988	2.483051
C	-10.505875	-4.358012	4.331242	H	-3.510659	-6.491710	1.717504
O	1.005637	-1.994238	6.048788	H	-5.006948	-5.613904	1.354154
C	1.266401	-0.625473	5.728500	H	-3.683512	-4.791536	2.196614
C	1.064768	-4.583556	6.503880	H	-10.693050	-6.844442	5.394121
C	-2.889193	-4.645063	8.772593	H	-9.545699	-6.917168	4.053153
O	-2.921552	-4.608881	10.179870	H	-8.981671	-7.145017	5.719751
C	-4.046406	-5.247540	10.778858	H	-10.732341	-4.974364	7.005068
C	-5.328338	-4.441975	10.581287	H	-9.005773	-5.181210	7.358210
C	-1.122421	-2.869359	8.764157	H	-9.625470	-3.602699	6.855447
C	-3.700643	-5.425994	12.248600	H	-11.523818	-4.655200	4.610988
O	-0.668971	-6.544436	8.695405	H	-10.441991	-3.268869	4.419254
C	-0.474380	-4.500229	4.445971	H	-10.352821	-4.615781	3.278135
H	-5.845227	1.066993	5.685347	H	-0.378242	-5.594774	4.444224
H	-5.457695	0.906563	3.968919	H	-1.516632	-4.293631	4.176979
H	-3.943635	2.480231	5.140136	H	1.066987	-1.474513	-0.117318
H	-3.420847	1.189613	6.219252	H	-0.469334	-1.066350	0.703724
H	-2.576959	2.767067	3.152821	H	-0.272686	-2.653386	-0.073542
H	-1.945480	1.309896	2.370476	H	2.118381	-4.321025	2.123565
H	-7.082362	-0.859095	4.797438	H	1.731019	-5.621614	3.265440

H	2.575878	-4.175625	3.813151
H	0.976022	-5.672913	6.548661
H	1.281314	-4.216746	7.510172
H	1.914294	-4.333828	5.869214
H	-2.352338	-3.963765	6.367658
H	-1.592866	-5.534277	6.560791
H	-1.251037	-2.782080	9.844145
H	-1.795964	-2.155591	8.278249
H	-0.091869	-2.592075	8.527637
H	2.338517	-0.496271	5.872598
H	0.716524	0.039305	6.397120
H	0.998033	-0.432550	4.688638
H	-3.149024	-5.648647	8.403815
H	-3.594691	-3.923437	8.331233
H	1.771938	-5.288024	11.156593
H	1.728559	-6.397408	9.746684
H	0.506195	-6.553630	11.026305
H	-4.172104	-6.240579	10.314416
H	-6.170087	-4.933767	11.079343
H	-5.588183	-4.340141	9.523287
H	-5.213541	-3.439575	11.007828
H	-4.503533	-5.952653	12.773167
H	-3.556429	-4.451380	12.726330
H	-2.777090	-6.001191	12.355754

YT3SR_NRF.xyz
149

scf done: -2856.865237

C	-5.781275	-2.973878	4.792746
C	-4.914341	-3.892544	4.147846
C	-5.172870	-5.284471	4.278538
C	-6.202240	-5.678166	5.143732
C	-7.015069	-4.790269	5.856500
C	-6.790472	-3.429740	5.638352
O	-3.904004	-3.419557	3.421789
Y	-2.741822	-1.690879	3.050770
O	-1.314263	-1.893744	4.903270
C	-0.262416	-1.594306	5.522481
C	0.984172	-2.289319	5.421577
C	2.194147	-1.734450	6.151179
C	-4.401059	-6.325034	3.448750
C	-2.903928	-6.308466	3.796504
C	-8.131538	-5.247305	6.805148
C	-9.488438	-4.714695	6.303316
C	-5.730802	-1.508654	4.448333
N	-4.457129	-0.784360	4.726353
C	-4.667983	0.638785	4.394611
C	-3.373486	1.426129	4.251779
N	-2.495590	0.922745	3.174143
C	-1.111488	1.344855	3.452515
O	-3.886472	-1.028700	1.366538
C	-4.634305	-0.016004	0.946073
C	-4.219346	1.297306	1.278612

C	-5.008003	2.398989	0.956444
C	-6.221961	2.257103	0.279431
C	-6.576479	0.958565	-0.103870
C	-5.820442	-0.186123	0.182610
C	-2.839829	1.499559	1.837776
C	-6.238803	-1.566083	-0.350594
C	-6.547245	-2.530402	0.809524
C	-7.077847	3.490534	-0.038256
C	-6.276756	4.461941	-0.927811
O	-0.917133	-2.224586	1.896297
C	0.204199	-2.813824	1.743272
C	1.371579	-2.615821	2.503963
C	2.596941	-3.440818	2.194476
O	0.330172	-3.696166	0.734241
C	-0.812860	-3.918859	-0.089203
C	-7.491215	-1.494874	-1.238531
C	-5.095686	-2.142911	-1.211204
C	-8.374714	3.129118	-0.775742
C	-7.459202	4.204102	1.273965
C	-4.909610	-7.756224	3.684979
C	-4.589507	-6.014851	1.949402
C	-4.081656	-0.946924	6.136294
C	-8.227694	-6.776184	6.901482
C	-7.863819	-4.695931	8.219516
O	-0.289866	-0.364379	6.149966
C	-0.226408	-0.345161	7.574529
C	0.949242	-3.791686	5.209438
C	0.582710	-4.739213	6.395812
C	1.436726	-4.537509	7.651178
C	1.379957	-1.627389	3.511215
C	0.753861	-6.149309	5.812598
O	1.628712	-6.908058	6.495288
C	1.813260	-8.227875	5.977091
C	-0.903138	-4.601314	6.757935
O	-1.216658	-5.599717	7.705035
C	-2.583747	-5.635681	8.109692
C	-2.875624	-4.566773	9.160870
O	0.188830	-6.539266	4.813734
C	-2.840458	-7.039171	8.636131
H	-5.293133	1.120218	5.166490
H	-5.221841	0.688401	3.454403
H	-3.620471	2.486803	4.083110
H	-2.805510	1.378218	5.186205
H	-2.635058	2.582494	1.877440
H	-2.114945	1.059675	1.140138
H	-6.546397	-0.997312	4.986448
H	-5.923597	-1.379799	3.376471
H	-6.384410	-6.738966	5.257078
H	-7.428139	-2.689151	6.118545
H	-7.492391	0.826163	-0.664930
H	-4.647987	3.389642	1.230531
H	-4.848905	-0.516074	6.800457
H	-3.985180	-2.010490	6.360056
H	-3.121171	-0.467831	6.329612

H	-1.028787	2.444071	3.477391
H	-0.779269	0.946040	4.411617
H	-0.452489	0.978825	2.660338
H	-5.371873	-3.134138	-1.590795
H	-4.896243	-1.494567	-2.071894
H	-4.178248	-2.236439	-0.627369
H	-6.855099	-3.506502	0.416196
H	-5.673648	-2.683780	1.444627
H	-7.369672	-2.147777	1.425156
H	-7.721678	-2.497717	-1.613964
H	-8.371281	-1.143670	-0.688233
H	-7.344779	-0.843732	-2.107372
H	-8.955973	4.037636	-0.967237
H	-8.175748	2.656015	-1.743157
H	-9.002825	2.452314	-0.186730
H	-8.066351	5.093904	1.068422
H	-8.038698	3.540379	1.924639
H	-6.573853	4.528047	1.830529
H	-6.871474	5.353421	-1.160501
H	-5.356803	4.795097	-0.437043
H	-5.995526	3.983808	-1.871916
H	-2.357645	-7.031445	3.180456
H	-2.465920	-5.324042	3.630758
H	-2.738927	-6.585891	4.842238
H	-4.340564	-8.446305	3.052715
H	-4.771855	-8.078327	4.723212
H	-5.968042	-7.868840	3.425155
H	-4.038625	-6.743716	1.342134
H	-5.647450	-6.074102	1.670960
H	-4.227698	-5.014006	1.707435
H	-9.023992	-7.053615	7.600748
H	-8.465797	-7.231120	5.934180
H	-7.295926	-7.220447	7.267576
H	-8.660142	-4.997681	8.910590
H	-6.913228	-5.073504	8.611465
H	-7.814988	-3.602369	8.224879
H	-10.299127	-5.030203	6.971076
H	-9.502912	-3.621270	6.257226
H	-9.706505	-5.092926	5.299219
H	2.355546	-1.235024	3.790588
H	0.616181	-0.860966	3.432559
H	-1.633279	-4.357182	0.485688
H	-0.484234	-4.621144	-0.855957
H	-1.155164	-2.989171	-0.551022
H	3.437993	-3.121395	2.818061
H	2.901296	-3.331991	1.146913
H	2.441330	-4.512498	2.364921
H	2.245474	-0.644677	6.064086
H	3.104487	-2.147063	5.702546
H	2.239309	-1.990667	7.213777
H	0.268489	-4.024903	4.386421
H	1.947282	-4.084308	4.862338
H	1.218800	-5.314990	8.384070
H	1.202691	-3.573137	8.111303

H	2.506213	-4.566417	7.425535
H	-0.194113	0.706281	7.865707
H	0.662649	-0.849010	7.960561
H	-1.121446	-0.809513	8.004302
H	-1.521538	-4.712442	5.857776
H	-1.076841	-3.593618	7.166358
H	-3.221200	-5.460504	7.228111
H	2.537637	-8.706066	6.636738
H	2.191795	-8.191780	4.952174
H	0.868687	-8.777405	5.981688
H	-3.927759	-4.598024	9.461489
H	-2.671922	-3.560607	8.781105
H	-2.255769	-4.729994	10.048850
H	-3.880871	-7.149030	8.956762
H	-2.190216	-7.247877	9.492208
H	-2.633725	-7.780905	7.860138

YT3SR_NRFb.xyz

149

scf done: -2856.890108

C	-6.753664	-2.809163	5.029315
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C	-7.258808	-5.340099	6.002950
C	-8.188793	-4.333514	6.282106
C	-7.906653	-3.066963	5.767122
O	-4.694806	-3.536459	4.115412
Y	-3.329175	-1.920504	3.840526
O	-2.109744	-2.039919	5.609290
C	-1.348510	-1.707473	6.624354
C	-0.013877	-1.914936	6.764564
C	0.724336	-1.388712	7.967828
C	-5.138662	-6.317543	4.969080
C	-3.745330	-6.046701	5.568816
C	-9.469004	-4.570600	7.094338
C	-10.699647	-4.257049	6.220212
C	-6.556132	-1.447616	4.422939
N	-5.328332	-0.719118	4.855154
C	-5.359072	0.621390	4.240210
C	-4.056471	1.386677	4.412142
N	-2.886250	0.656551	3.876994
C	-1.702595	0.955716	4.701432
O	-3.909005	-1.310931	1.841823
C	-4.226727	-0.256662	1.106039
C	-3.667627	1.000969	1.451265
C	-4.041601	2.157718	0.771049
C	-4.955445	2.128100	-0.284974
C	-5.445162	0.869593	-0.651999
C	-5.105817	-0.328114	-0.010312
C	-2.568675	1.063484	2.475477
C	-5.635549	-1.677843	-0.523218
C	-6.480014	-2.382365	0.555614
C	-5.356594	3.426672	-0.997682

C	-4.107490	4.086409	-1.615414	H	-7.333198	-1.759501	0.848743
O	-1.453187	-2.766342	2.649256	H	-6.844816	-2.516935	-2.105001
C	-0.782163	-3.155637	1.691667	H	-7.420235	-0.935914	-1.572015
C	0.292014	-2.360196	1.039862	H	-5.980223	-1.059792	-2.604449
C	0.819503	-2.830320	-0.284931	H	-6.635689	4.140737	-2.592800
O	-0.951208	-4.335427	1.129073	H	-5.967650	2.535341	-2.904931
C	-1.903275	-5.221355	1.743304	H	-7.297654	2.736699	-1.747937
C	-6.518643	-1.525614	-1.771807	H	-6.272072	5.338546	-0.468086
C	-4.441788	-2.575616	-0.907676	H	-6.891425	3.961578	0.464014
C	-6.372356	3.186851	-2.123161	H	-5.299222	4.637709	0.832686
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C	-5.636742	-7.646969	5.556494	H	-3.357944	4.327213	-0.854962
C	-5.034394	-6.500863	3.441755	H	-3.637654	3.420737	-2.347058
C	-5.273047	-0.628215	6.321873	H	-3.060531	-6.867350	5.320337
C	-9.589927	-6.019737	7.585090	H	-3.324451	-5.113219	5.193564
C	-9.476208	-3.647147	8.328529	H	-3.805609	-5.977919	6.660885
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C	-2.718282	-1.854344	8.525333	H	-5.707057	-7.615485	6.649346
C	0.752693	-2.582681	5.650905	H	-6.614796	-7.934762	5.156066
C	1.388222	-3.985180	5.939524	H	-4.322520	-7.300340	3.199690
C	2.651249	-3.895559	6.802427	H	-6.007442	-6.778316	3.021670
C	0.750116	-1.283405	1.689973	H	-4.709509	-5.575583	2.963416
C	1.677011	-4.615774	4.574331	H	-10.512174	-6.138327	8.164212
O	2.978714	-4.873737	4.366276	H	-9.630559	-6.730092	6.752515
C	3.290395	-5.479137	3.111403	H	-8.753521	-6.300731	8.234138
C	0.346268	-4.886546	6.612109	H	-10.387813	-3.798626	8.918851
O	0.905200	-6.177110	6.755651	H	-8.614727	-3.852278	8.972909
C	0.038940	-7.145293	7.336315	H	-9.436379	-2.590896	8.044343
C	-0.037856	-6.989224	8.853960	H	-11.626173	-4.410385	6.786656
O	0.828459	-4.850383	3.734660	H	-10.692568	-3.220443	5.868633
C	0.579278	-8.507766	6.928980	H	-10.727500	-4.906186	5.338737
H	-6.180597	1.218735	4.673561	H	1.544980	-0.672002	1.273788
H	-5.572274	0.499235	3.175299	H	0.355650	-1.008803	2.661699
H	-4.157201	2.367507	3.924855	H	-1.627602	-5.383208	2.785988
H	-3.878455	1.579114	5.474104	H	-1.838536	-6.148558	1.176326
H	-2.175442	2.093538	2.499868	H	-2.908241	-4.802151	1.671234
H	-1.741645	0.414514	2.155739	H	1.592887	-2.151501	-0.651457
H	-7.435309	-0.825192	4.658427	H	0.021161	-2.882936	-1.032304
H	-6.495942	-1.524248	3.331053	H	1.243774	-3.835686	-0.203002
H	-7.458055	-6.336743	6.375216	H	0.128157	-0.638809	8.492170
H	-8.602979	-2.245853	5.929762	H	1.674020	-0.923573	7.670757
H	-6.128300	0.814629	-1.489576	H	0.979862	-2.168082	8.699721
H	-3.589272	3.101357	1.073254	H	0.079070	-2.705555	4.799515
H	-6.085594	0.007703	6.710221	H	1.578887	-1.928390	5.327220
H	-5.389388	-1.628270	6.742275	H	3.090645	-4.883810	6.947575
H	-4.309569	-0.234316	6.649467	H	2.406150	-3.484836	7.783938
H	-1.451312	2.028301	4.664899	H	3.401619	-3.248518	6.339753
H	-1.880896	0.662880	5.736411	H	-3.315460	-1.214811	9.180748
H	-0.841517	0.390078	4.336917	H	-2.016527	-2.435870	9.137776
H	-4.797337	-3.554380	-1.252354	H	-3.382398	-2.544458	7.991148
H	-3.862804	-2.120646	-1.719213	H	-0.563264	-4.924071	5.995222
H	-3.781798	-2.724555	-0.050973	H	0.079625	-4.444781	7.582400
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H	2.761266	-6.428935	2.999702
H	-0.706646	-7.740955	9.286007
H	-0.418521	-6.004553	9.140957
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H	1.594389	-8.643004	7.316844
H	0.615287	-8.594328	5.839570

YT3SR_NRFf.xyz
149

C	-5.799608	-3.166244	4.572898
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C	-5.025802	-5.431654	4.072728
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O	-3.947267	-3.491204	3.137794
Y	-2.858282	-1.715784	2.790347
O	-1.357965	-2.058780	4.697617
C	-0.397781	-1.793586	5.417935
C	0.944737	-2.475624	5.199027
C	2.139643	-1.876968	5.954192
C	-4.154989	-6.413986	3.272030
C	-2.662322	-6.213213	3.594496
C	-7.982964	-5.594322	6.593063
C	-9.370890	-5.215168	6.038569
C	-5.809183	-1.691881	4.266037
N	-4.557676	-0.939142	4.575953
C	-4.798012	0.488825	4.293704
C	-3.516649	1.308361	4.201709
N	-2.600058	0.839793	3.139412
C	-1.211426	1.178167	3.494002
O	-4.028446	-0.952893	1.171006
C	-4.725694	0.120462	0.820581
C	-4.250799	1.389967	1.235243
C	-4.989642	2.544356	0.987695
C	-6.208544	2.501998	0.306136
C	-6.622915	1.247601	-0.157029
C	-5.920111	0.054022	0.053935
C	-2.871500	1.494414	1.820952
C	-6.398573	-1.270067	-0.564968
C	-6.739576	-2.299643	0.529140
C	-7.007427	3.790968	0.069872
C	-6.162075	4.780865	-0.756012
O	-0.991751	-2.121504	1.781062
C	-0.071101	-3.047914	1.727277
C	0.992105	-3.200046	2.573269
C	2.007617	-4.287246	2.315798
O	-0.175997	-3.955810	0.707419
C	-1.089963	-3.660311	-0.335457
C	-7.653586	-1.088109	-1.433128

C	-5.285426	-1.832759	-1.472566
C	-8.317231	3.536359	-0.688357
C	-7.358647	4.434655	1.425891
C	-4.493732	-7.880935	3.578565
C	-4.399088	-6.189008	1.765229
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C	-7.930280	-7.121268	6.741637
C	-7.811674	-4.974853	7.993716
O	-0.620293	-0.763118	6.262617
C	0.062023	-0.471589	7.486743
C	0.822953	-4.011327	5.375572
C	0.533838	-4.688691	6.750108
C	1.608336	-4.444840	7.824900
C	1.270592	-2.184234	3.627805
C	0.500688	-6.191354	6.424324
O	1.742069	-6.685026	6.251995
C	1.800289	-8.068567	5.890347
C	-0.849362	-4.322620	7.295451
O	-1.021990	-4.949029	8.543925
C	-2.372107	-5.231673	8.904020
C	-3.113029	-3.965038	9.323944
O	-0.496685	-6.864660	6.296978
C	-2.308796	-6.262359	10.019527
H	-5.444853	0.929653	5.072428
H	-5.339321	0.563074	3.347375
H	-3.781735	2.365316	4.044093
H	-2.977702	1.255656	5.152905
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H	-7.448520	-2.992595	5.916582
H	-7.543393	1.193265	-0.723880
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H	-3.224720	-0.665803	6.194855
H	-1.070240	2.268850	3.569874
H	-0.948675	0.725865	4.451075
H	-0.535989	0.798532	2.722374
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H	-5.069069	-1.138566	-2.292309
H	-4.367184	-1.996657	-0.905955
H	-7.096401	-3.230095	0.071359
H	-5.868132	-2.539487	1.140427
H	-7.537613	-1.925348	1.181156
H	-7.929547	-2.053285	-1.871322
H	-8.513430	-0.736567	-0.851811
H	-7.486516	-0.388291	-2.259439
H	-8.856148	4.480555	-0.822661
H	-8.136248	3.115745	-1.683071
H	-8.977278	2.853246	-0.143126
H	-7.922484	5.363655	1.278770

H	-7.970660	3.757971	2.031877
H	-6.460276	4.678709	2.001792
H	-6.716171	5.711078	-0.930018
H	-5.229202	5.040985	-0.245946
H	-5.900711	4.352527	-1.729233
H	-2.054546	-6.898765	2.991391
H	-2.344456	-5.193695	3.372940
H	-2.453721	-6.426046	4.647200
H	-3.853001	-8.529918	2.971910
H	-4.314002	-8.134576	4.629129
H	-5.533482	-8.126408	3.335276
H	-3.771399	-6.868035	1.175320
H	-5.445915	-6.387369	1.509034
H	-4.164012	-5.162527	1.478476
H	-8.712567	-7.453092	7.433024
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H	-6.968194	-7.457250	7.143229
H	-8.591807	-5.336564	8.674260
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H	-7.876660	-3.882595	7.965696
H	-10.166221	-5.584018	6.697678
H	-9.488110	-4.130469	5.949474
H	-9.523889	-5.647771	5.044356
H	2.350803	-1.987900	3.628517
H	0.786596	-1.236482	3.369410
H	-2.129871	-3.683765	0.006389
H	-0.944981	-4.444092	-1.081787
H	-0.891212	-2.682146	-0.786382
H	2.996510	-3.991579	2.690970
H	2.105991	-4.489206	1.245089
H	1.762613	-5.248328	2.790936
H	2.298554	-0.831127	5.667729
H	3.035032	-2.427661	5.651399
H	2.087698	-1.937496	7.038508
H	0.064235	-4.345111	4.658994
H	1.772701	-4.422484	5.019925
H	1.483181	-5.153212	8.645989
H	1.512295	-3.445155	8.256931
H	2.614997	-4.557658	7.417398
H	-0.630750	0.157486	8.047942
H	0.987968	0.077098	7.310845
H	0.258357	-1.379049	8.060208
H	-1.621461	-4.640421	6.582286
H	-0.921587	-3.227403	7.402289
H	-2.877790	-5.675742	8.032098
H	2.859887	-8.303527	5.789723
H	1.277436	-8.241436	4.946429
H	1.341642	-8.688088	6.665049
H	-4.146213	-4.194844	9.602756
H	-3.147126	-3.233547	8.510449
H	-2.617457	-3.502536	10.184717
H	-3.315483	-6.558217	10.329751
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H	-1.771847	-7.151827	9.680251

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149			
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C	-5.869451	1.516270	-0.362782
O	-3.760328	-0.630094	1.710134
Y	-2.978050	-1.379956	3.557053
O	-1.229689	-2.358515	2.504454
C	-0.402989	-3.317336	2.534633
O	-0.543802	-4.332943	1.675070
C	-1.606395	-4.241497	0.722787
C	-2.674071	1.818163	2.418972
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C	-5.718892	-1.035245	-0.471879
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O	-4.241598	-3.102819	3.669557
C	-5.278086	-3.597391	4.348399
C	-6.209239	-2.694316	4.919436
C	-7.232445	-3.157149	5.743682
C	-7.401328	-4.515848	6.018101
C	-6.533008	-5.395248	5.363324
C	-5.495041	-4.993428	4.511875
C	-6.182678	-1.245375	4.517105
N	-4.971848	-0.464768	4.899058
C	-4.785106	-0.505537	6.355589
C	-4.699325	-6.034263	3.703645
C	-4.949570	-5.763214	2.205559
C	-8.521808	-4.983932	6.956161
C	-8.352648	-4.316017	8.334977
O	-1.684728	-1.406930	5.474024
C	-0.811016	-2.147810	6.059294
O	-1.172852	-3.397224	6.447683
C	-2.553653	-3.655776	6.658026
C	0.544460	-1.862622	6.283870
C	1.382142	-2.891831	7.005263
C	1.026733	-0.435201	6.244307
C	1.301948	0.303427	7.597381
C	0.157768	0.045508	8.574709
O	0.217167	-0.667990	9.550109
C	2.617810	-0.130698	8.253019
C	-3.190619	-5.970211	4.000751
C	-5.153392	-7.474623	3.989599
C	-9.889321	-4.586940	6.365111
C	-8.513743	-6.504917	7.162399
C	-5.172978	0.919578	4.427322

C	-3.927430	1.782434	4.542493	H	-4.574011	-8.163278	3.365032
C	-6.340420	-1.927469	0.619066	H	-4.985905	-7.761463	5.033821
C	-6.752240	-0.898591	-1.600403	H	-6.211384	-7.630228	3.753765
C	-5.078361	4.955313	-1.144052	H	-4.369770	-6.459910	1.587619
C	-7.260174	3.802033	-1.476153	H	-6.009261	-5.898843	1.963485
C	0.741876	-3.412124	3.379645	H	-4.671358	-4.741168	1.940151
C	1.121877	-2.281824	4.074548	H	-9.311614	-6.787664	7.857471
C	1.542654	-4.688408	3.402065	H	-8.687500	-7.045886	6.226187
O	-0.972103	0.705191	8.230457	H	-7.565667	-6.851724	7.587359
C	-2.056421	0.537708	9.145709	H	-9.151409	-4.630877	9.016959
C	1.380723	1.806143	7.274390	H	-7.392970	-4.590334	8.785839
O	1.607379	2.525059	8.463636	H	-8.388837	-3.224350	8.264212
C	1.915731	3.903692	8.291741	H	-10.704018	-4.908772	7.024835
C	2.551237	4.366435	9.593738	H	-9.975414	-3.503438	6.235354
C	0.677261	4.723256	7.934395	H	-10.040677	-5.051527	5.385154
H	-5.987356	1.398347	4.999338	H	2.122810	-2.241838	4.491995
H	-5.492731	0.877976	3.383148	H	0.656999	-1.332937	3.830668
H	-4.169365	2.797973	4.195711	H	-1.539235	-5.151955	0.127450
H	-3.636778	1.871229	5.593640	H	-2.575552	-4.188701	1.221529
H	-2.401196	2.882317	2.513235	H	-1.478437	-3.362094	0.086763
H	-1.824356	1.309269	1.942705	H	1.906809	-4.955200	2.403552
H	-7.069993	-0.745869	4.940834	H	2.407691	-4.578127	4.061333
H	-6.259747	-1.170870	3.426276	H	0.953921	-5.538604	3.763421
H	-6.676456	-6.457379	5.513960	H	2.448089	-2.703557	6.832497
H	-7.920169	-2.425726	6.165257	H	1.218262	-2.878627	8.089725
H	-6.641859	1.438763	-1.117160	H	1.158125	-3.901361	6.653923
H	-4.104253	3.827696	1.355531	H	0.295988	0.151009	5.684254
H	-5.587460	0.044663	6.874354	H	1.973961	-0.372796	5.683812
H	-4.813550	-1.545265	6.684770	H	2.849847	0.532059	9.089084
H	-3.816862	-0.086182	6.632758	H	2.566308	-1.149071	8.633913
H	-1.438010	2.710649	4.585843	H	3.433054	-0.064675	7.524059
H	-1.522313	1.168111	5.492501	H	-2.608708	-4.681694	7.022432
H	-0.669762	1.246487	3.939305	H	-2.958337	-2.981686	7.421173
H	-4.748264	-2.717081	-1.461182	H	-3.138942	-3.569442	5.742142
H	-4.056365	-1.139786	-1.883729	H	2.209169	1.967625	6.561768
H	-3.705583	-1.862342	-0.300709	H	0.450768	2.128377	6.787195
H	-6.653924	-2.886742	0.189725	H	-2.855379	1.186436	8.785153
H	-5.626866	-2.131532	1.418815	H	-2.389265	-0.503258	9.168768
H	-7.229817	-1.451325	1.048668	H	-1.755835	0.830110	10.154812
H	-6.989625	-1.893362	-1.992453	H	2.654555	3.999603	7.476412
H	-7.690588	-0.453548	-1.250978	H	0.935950	5.781165	7.822379
H	-6.375068	-0.297631	-2.435005	H	0.227733	4.391544	6.993647
H	-7.697620	4.747757	-1.813857	H	-0.074852	4.632818	8.724761
H	-6.880823	3.280397	-2.361216	H	2.842199	5.419465	9.531602
H	-8.066818	3.200300	-1.043913	H	1.843543	4.250978	10.420931
H	-7.223939	5.795935	0.363987	H	3.439701	3.770728	9.819381
H	-7.534246	4.274038	1.221520				
H	-6.007865	5.134176	1.464823				
H	-5.522014	5.885651	-1.518352	YT3SS_NLBb.xyz			
H	-4.271722	5.226014	-0.455345	149			
H	-4.628800	4.426926	-1.991205	scf done: -2856.904111			
H	-2.654461	-6.697796	3.379889	C	-5.609192	0.201725	-0.203524
H	-2.785614	-4.979406	3.795511	C	-4.511604	0.309441	0.692033
H	-2.989233	-6.217886	5.048125	C	-3.949175	1.587111	0.933099

C	-4.511856	2.731604	0.372511	O	-1.016878	-0.363204	8.481683
C	-5.632871	2.665853	-0.458094	C	-1.948521	-0.894072	9.429686
C	-6.135362	1.388084	-0.730954	C	1.003527	1.493376	7.935915
O	-3.985620	-0.734062	1.321098	O	1.183127	1.819646	9.291291
Y	-2.992566	-1.322924	3.115066	C	1.252375	3.213174	9.580278
O	-1.170391	-2.118219	2.349872	C	1.837624	3.330146	10.978635
C	-0.178942	-2.972266	2.454287	C	-0.113846	3.886597	9.470760
O	-0.252727	-4.084965	1.656468	H	-5.731264	1.682481	4.598301
C	-1.129661	-4.026055	0.544287	H	-5.398618	0.949977	3.023410
C	-2.656633	1.683368	1.691285	H	-3.961271	2.906006	3.468408
N	-2.650905	1.260021	3.128115	H	-3.315830	2.135837	4.913206
C	-1.332491	1.620136	3.671167	H	-2.301818	2.725989	1.645404
C	-6.232847	3.948253	-1.050252	H	-1.898190	1.061752	1.195831
C	-6.641992	4.902132	0.089256	H	-6.858272	-0.464087	4.911901
C	-6.173102	-1.168353	-0.612810	H	-6.197645	-1.050578	3.379420
C	-5.048934	-2.006674	-1.256052	H	-6.504354	-6.108702	5.962519
O	-4.215321	-3.010948	3.583766	H	-7.564520	-1.995913	6.408370
C	-5.178390	-3.402226	4.411865	H	-6.983705	1.307487	-1.398640
C	-6.015907	-2.420815	5.002880	H	-4.042903	3.691996	0.582282
C	-6.945324	-2.780984	5.976689	H	-5.227874	0.533555	6.584266
C	-7.113411	-4.106824	6.383215	H	-4.477214	-1.077443	6.524549
C	-6.350613	-5.067569	5.709667	H	-3.483774	0.355963	6.231271
C	-5.409590	-4.772618	4.714374	H	-1.164691	2.708893	3.638060
C	-6.016644	-1.015878	4.460266	H	-1.250884	1.279648	4.704346
N	-4.771318	-0.215501	4.644207	H	-0.547184	1.135737	3.085053
C	-4.470120	-0.084272	6.073723	H	-5.429401	-2.995768	-1.538491
C	-4.722734	-5.897702	3.916516	H	-4.673896	-1.517687	-2.162077
C	-5.056126	-5.716212	2.420862	H	-4.215327	-2.139316	-0.563971
C	-8.125283	-4.457334	7.482599	H	-7.165094	-2.875670	0.303424
C	-7.753409	-3.712459	8.780149	H	-5.956930	-2.115018	1.348359
O	-1.637345	-1.423795	5.168280	H	-7.535124	-1.332624	1.087111
C	-0.751598	-2.053752	5.758073	H	-7.649959	-2.053015	-1.916113
O	-1.028801	-3.077622	6.540796	H	-8.172994	-0.506667	-1.244836
C	-2.406871	-3.463481	6.678683	H	-6.980360	-0.551785	-2.561151
C	0.735551	-1.729312	5.661490	H	-7.877200	4.613350	-2.292935
C	1.590639	-2.813503	6.320962	H	-7.247942	3.032527	-2.764772
C	0.973570	-0.300553	6.239962	H	-8.270521	3.188770	-1.323135
C	1.234352	-0.023947	7.748565	H	-7.068166	5.827715	-0.315541
C	0.265016	-0.749536	8.681601	H	-7.393220	4.436453	0.736160
O	0.575599	-1.558772	9.524250	H	-5.787031	5.177925	0.714928
C	2.670294	-0.352325	8.174267	H	-5.592769	5.568420	-2.368504
C	-3.193663	-5.887212	4.100936	H	-4.283738	4.906281	-1.379911
C	-5.220822	-7.291443	4.331185	H	-4.882925	3.992190	-2.768837
C	-9.539797	-4.030780	7.042649	H	-2.739109	-6.687176	3.504837
C	-8.154990	-5.960548	7.791241	H	-2.756496	-4.941509	3.777212
C	-4.984899	1.106641	4.023050	H	-2.923721	-6.064836	5.147915
C	-3.711449	1.932134	3.913219	H	-4.730852	-8.046899	3.707751
C	-6.736476	-1.914630	0.611817	H	-4.981009	-7.525387	5.374644
C	-7.307786	-1.049501	-1.641767	H	-6.301717	-7.401860	4.192753
C	-5.185345	4.643748	-1.942381	H	-4.578468	-6.506550	1.829321
C	-7.477175	3.670543	-1.904718	H	-6.137544	-5.777227	2.256902
C	0.905574	-2.860329	3.272259	H	-4.706658	-4.749029	2.055296
C	1.069167	-1.637025	4.127853	H	-8.874723	-6.159819	8.592494
C	2.027731	-3.864833	3.187373	H	-8.460946	-6.549882	6.920420

H	-7.177968	-6.326172	8.125119	C	-1.519725	-4.553812	0.645448
H	-8.471228	-3.941264	9.576886	C	-2.729589	1.824948	2.107387
H	-6.756828	-4.006759	9.126997	N	-2.770677	1.345547	3.518780
H	-7.751064	-2.627100	8.637008	C	-1.528271	1.819784	4.151889
H	-10.274903	-4.270226	7.820295	C	-6.373978	3.735474	-0.811802
H	-9.597917	-2.954708	6.851063	C	-7.021610	4.536967	0.334604
H	-9.834356	-4.548273	6.123838	C	-5.653464	-1.341748	-0.576070
H	2.120802	-1.313424	4.090809	C	-4.379040	-2.017214	-1.121389
H	0.470344	-0.818518	3.714419	O	-4.357490	-3.037809	3.595935
H	-0.967028	-4.954909	-0.006682	C	-5.310127	-3.483903	4.406051
H	-2.179867	-3.970588	0.847945	C	-6.196500	-2.542968	4.990173
H	-0.905843	-3.172939	-0.106552	C	-7.154675	-2.945512	5.917338
H	2.056943	-4.331637	2.199177	C	-7.303903	-4.283585	6.288851
H	2.997094	-3.377908	3.359101	C	-6.476519	-5.206547	5.639150
H	1.956166	-4.684384	3.916674	C	-5.500769	-4.865083	4.693672
H	2.649583	-2.586327	6.166169	C	-6.182964	-1.124153	4.494829
H	1.404190	-2.901342	7.392619	N	-4.946037	-0.333223	4.767609
H	1.386568	-3.782557	5.863847	C	-4.680558	-0.288294	6.212555
H	0.126393	0.313174	5.918130	C	-4.709587	-5.955313	3.949836
H	1.850283	0.099138	5.715049	C	-4.944792	-5.795934	2.433839
H	2.852456	0.036289	9.177547	C	-8.360479	-4.686482	7.326355
H	2.863445	-1.423539	8.188716	C	-8.107141	-3.927007	8.643396
H	3.375588	0.122682	7.483857	O	-1.439493	-0.887109	4.994894
H	-2.389931	-4.399782	7.233445	C	-1.092777	-1.858643	5.806748
H	-2.949202	-2.700584	7.239412	O	-1.993842	-2.919527	5.680871
H	-2.868832	-3.601687	5.702501	C	-2.576800	-3.450917	6.872154
H	1.725567	2.039812	7.303751	C	-0.002132	-1.915720	6.612362
H	-0.008804	1.750495	7.593620	C	0.435583	-3.194311	7.279390
H	-2.929248	-0.532257	9.120525	C	0.868543	-0.691340	6.732637
H	-1.920023	-1.985792	9.435039	C	1.047354	-0.057529	8.152351
H	-1.711021	-0.534690	10.434300	C	-0.305368	-0.012148	8.857605
H	1.942534	3.685498	8.859106	O	-0.660331	-0.764519	9.737901
H	-0.037641	4.949361	9.721805	C	2.029268	-0.846868	9.024772
H	-0.525531	3.816392	8.459261	C	-3.204634	-5.848282	4.257090
H	-0.821244	3.418364	10.162809	C	-5.156028	-7.374381	4.334537
H	1.951864	4.380263	11.263692	C	-9.764613	-4.330204	6.798440
H	1.179905	2.843401	11.705744	C	-8.334227	-6.190009	7.633628
H	2.816537	2.846062	11.026123	C	-5.158996	1.022419	4.219248
YT3SS_NLBf.xyz				C	-3.920080	1.903451	4.259368
149				C	-6.241712	-2.188777	0.568404
scf done: -2856.882303				C	-6.685565	-1.322838	-1.714337
C	-5.301727	0.068185	-0.076127	C	-5.370769	4.638976	-1.556312
C	-4.299641	0.273339	0.911866	C	-7.479604	3.340123	-1.800250
C	-3.935604	1.600988	1.243267	C	1.076389	-2.309062	1.968922
C	-4.605989	2.686817	0.685973	C	1.218796	-1.434119	2.974788
C	-5.642625	2.516109	-0.234626	C	2.194646	-2.750646	1.067381
C	-5.943255	1.198678	-0.598680	O	-1.102447	0.972493	8.385412
O	-3.685533	-0.721352	1.542117	C	-2.350462	1.102223	9.066067
Y	-3.012038	-1.365805	3.483105	C	1.583017	1.367116	7.945717
O	-1.302830	-2.529593	2.318007	O	1.765429	1.983104	9.199789
C	-0.267175	-2.900728	1.762941	C	2.397197	3.256673	9.162468
O	-0.260252	-3.903773	0.899197	C	2.913651	3.521748	10.568520
				C	1.442784	4.351017	8.687393
				H	-5.966397	1.527515	4.778283

H	0.389807	-1.162594	3.624895
H	-1.294421	-5.341743	-0.071546
H	-1.920427	-4.971854	1.569996
H	-2.234203	-3.842597	0.228090
H	1.960461	-2.555334	0.015833
H	3.117029	-2.223020	1.320339
H	2.374641	-3.826586	1.157318
H	1.530601	-3.262466	7.271888
H	0.120899	-3.275848	8.327957
H	0.060560	-4.072039	6.745340
H	0.461331	0.075467	6.066163
H	1.888683	-0.914614	6.378717
H	2.225294	-0.306340	9.953126
H	1.639474	-1.831129	9.280888
H	2.978267	-0.969476	8.491084
H	-3.608181	-3.719283	6.632410
H	-2.048286	-4.347132	7.210359
H	-2.546689	-2.705908	7.674177
H	2.544133	1.304892	7.404344
H	0.880254	1.933498	7.319790
H	-2.857310	1.949891	8.603217
H	-2.949666	0.193874	8.962666
H	-2.189450	1.291350	10.130649
H	3.254781	3.205108	8.468200
H	1.946600	5.323149	8.678184
H	1.074596	4.159295	7.675224
H	0.580161	4.414520	9.358465
H	3.438546	4.480777	10.616163
H	2.079559	3.548117	11.277120
H	3.600563	2.730286	10.879848

149

scf done: -2856.878817

C	-5.612937	-0.338830	-0.043955
C	-4.552017	-0.186108	0.889851
C	-4.021228	1.110042	1.111635
C	-4.592393	2.228443	0.509200
C	-5.689538	2.118902	-0.348831
C	-6.150826	0.823791	-0.611657
O	-4.033929	-1.199034	1.569906
Y	-3.068879	-1.751491	3.411283
O	-1.391739	-2.668687	2.164141
C	-0.336230	-3.289655	1.865823
O	0.146735	-3.204600	0.618837
C	-0.598601	-2.424051	-0.317300
C	-2.745913	1.252958	1.893028
N	-2.730707	0.831088	3.327010
C	-1.406874	1.187669	3.862592
C	-6.304570	3.373883	-0.982961
C	-6.752049	4.347252	0.125327
C	-6.119183	-1.730437	-0.459836
C	-4.941840	-2.540841	-1.040827

O	-4.306581	-3.387026	3.944994	H	-8.158536	-2.219800	5.956417
C	-5.413337	-3.731867	4.604995	H	-6.974570	0.709153	-1.304669
C	-6.348616	-2.722196	4.945666	H	-4.151265	3.203747	0.710758
C	-7.472687	-3.028624	5.709764	H	-5.626996	0.088968	6.630020
C	-7.745018	-4.328528	6.139484	H	-4.859822	-1.512865	6.595473
C	-6.846527	-5.319597	5.732618	H	-3.856608	-0.061069	6.440418
C	-5.697395	-5.076590	4.969117	H	-1.260423	2.279561	3.879408
C	-6.214649	-1.334819	4.377760	H	-1.274022	0.783013	4.866189
N	-4.972350	-0.584572	4.719356	H	-0.632500	0.756943	3.223173
C	-4.817726	-0.507177	6.177218	H	-5.280246	-3.540359	-1.339318
C	-4.797154	-6.239456	4.518380	H	-4.529949	-2.044331	-1.926822
C	-4.683845	-6.240952	2.979883	H	-4.148264	-2.651725	-0.298915
C	-8.985313	-4.615874	6.996118	H	-7.100591	-3.462550	0.418224
C	-8.894852	-3.818173	8.312338	H	-5.955837	-2.669149	1.508572
O	-1.651028	-1.745608	5.202239	H	-7.543736	-1.930992	1.185017
C	-0.763572	-2.414218	5.853178	H	-7.505616	-2.672395	-1.821470
O	-1.163636	-3.110948	6.947600	H	-8.107450	-1.139290	-1.188017
C	-2.525396	-3.042177	7.339782	H	-6.855722	-1.154517	-2.448680
C	0.587565	-2.583873	5.520573	H	-7.942446	3.976216	-2.264668
C	-0.078707	-4.331026	4.007322	H	-7.272104	2.399940	-2.693078
C	0.434147	-4.108010	2.748980	H	-8.320397	2.563967	-1.270828
C	1.740078	-4.694439	2.275216	H	-7.190465	5.253464	-0.309306
C	1.466433	-3.415337	6.425449	H	-7.504148	3.882150	0.771556
C	1.212931	-1.628906	4.540856	H	-5.913565	4.656350	0.757410
C	2.370577	-0.699031	5.034096	H	-5.672379	4.974934	-2.328753
C	2.522129	0.417314	3.983537	H	-4.368565	4.360425	-1.303054
O	3.537305	1.304166	4.390413	H	-4.927529	3.403322	-2.680165
C	3.974366	2.228402	3.400988	H	-2.741905	-6.907214	4.801624
C	5.306018	2.779109	3.887342	H	-2.947044	-5.147263	4.878644
C	-3.399894	-6.101360	5.148498	H	-3.459605	-6.161497	6.240889
C	-5.353188	-7.610788	4.933603	H	-4.685257	-8.395106	4.561318
C	-10.254915	-4.190719	6.232448	H	-5.413144	-7.724044	6.021710
C	-9.119346	-6.103264	7.350230	H	-6.346572	-7.797433	4.511440
C	-5.092933	0.766713	4.139851	H	-4.025022	-7.053512	2.650177
C	-3.773218	1.519367	4.117397	H	-5.667405	-6.398890	2.523743
C	-6.711227	-2.489912	0.742168	H	-4.282772	-5.295883	2.611389
C	-7.208146	-1.656428	-1.540932	H	-10.010085	-6.257030	7.968970
C	-5.255522	4.068169	-1.874191	H	-9.227506	-6.727104	6.456563
C	-7.528624	3.050635	-1.850456	H	-8.256338	-6.465965	7.918730
C	3.712871	-1.427107	5.166847	H	-9.779842	-3.997611	8.934459
C	2.008712	-0.073545	6.379694	H	-8.010110	-4.112028	8.887309
O	2.563550	-0.295369	7.432012	H	-8.830130	-2.740982	8.128388
O	0.960295	0.776484	6.282938	H	-11.150086	-4.384473	6.835336
C	0.583171	1.396562	7.514014	H	-10.244531	-3.123867	5.988033
C	2.949861	3.336009	3.161567	H	-10.348878	-4.746319	5.293621
H	-5.833300	1.358715	4.705577	H	0.399459	-5.044244	4.669696
H	-5.469628	0.668689	3.119529	H	-1.125548	-4.135243	4.197623
H	-3.945398	2.533699	3.725792	H	-0.627541	-1.373719	-0.014591
H	-3.394826	1.637086	5.137797	H	-0.070677	-2.525945	-1.265456
H	-2.422962	2.306244	1.846263	H	-1.622207	-2.792799	-0.407893
H	-1.961686	0.657346	1.405494	H	2.224855	-5.239204	3.089610
H	-7.083699	-0.739597	4.704144	H	1.585905	-5.396671	1.447553
H	-6.248079	-1.379535	3.283502	H	2.439767	-3.932529	1.915018
H	-7.050911	-6.342476	6.021071	H	0.896700	-4.220331	6.894327

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H	1.615833	-2.185466	3.677598	C	-4.503259	-6.300541	3.193237
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H	-2.632856	-3.765399	8.149739	C	-0.814800	-2.331665	6.001182
H	-2.773831	-2.043467	7.712826	O	-1.324073	-3.176546	6.966289
H	-3.202446	-3.305511	6.523633	C	-2.568493	-2.835307	7.535976
H	2.779194	-0.047911	3.015228	C	0.540946	-2.312227	5.862927
H	1.565442	0.942086	3.863651	C	0.001762	-5.021803	3.399355
H	4.134449	1.680599	2.455216	C	-0.078769	-4.743465	2.090448
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H	0.278138	0.646255	8.248033	C	1.415712	-3.177261	6.733524
H	1.416099	1.971234	7.926906	C	1.173489	-1.529529	4.741512
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				C	-5.083570	-7.598785	5.224083
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YT3SS_NLFb.xyz				C	-9.033140	-6.262093	7.451492
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scf done: -2856.882537				C	-4.040427	1.554446	4.246302
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C	-5.416789	2.148314	-0.339053	C	3.696089	-1.294546	5.199496
C	-5.811939	0.845776	-0.663816	C	2.068135	0.153492	6.406081
O	-3.789299	-1.166379	1.623435	O	2.663118	-0.024047	7.444939
Y	-3.119894	-1.692186	3.640995	O	1.043015	1.029661	6.301969
O	-1.320357	-2.712335	2.458201	C	0.719559	1.707188	7.516963
C	-0.653818	-3.431726	1.710807	C	2.824971	3.342755	2.948745
O	-0.360300	-3.083585	0.467037	H	-6.138197	1.269674	4.615469
C	-0.823895	-1.800492	0.007107	H	-5.563394	0.577333	3.092811
C	-2.700940	1.337904	2.193420	H	-4.228151	2.539433	3.793374
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C	-1.648768	1.299292	4.337143	H	-2.408049	2.400921	2.191303
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C	-4.551202	-2.520512	-1.031671	H	-6.931990	-6.417193	6.166270
O	-4.354756	-3.370329	4.009932	H	-8.315841	-2.385609	5.895149
C	-5.442569	-3.764157	4.671511	H	-6.568473	0.721652	-1.427664
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C	-7.572053	-3.156086	5.697974	H	-5.949864	0.082193	6.619280
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C	-6.790972	-5.396712	5.834257	H	-4.168059	-0.021005	6.539290
C	-5.638925	-5.107118	5.092414	H	-1.549672	2.395024	4.390197
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H	-4.879502	-3.507095	-1.380158	H	-3.393164	-2.950429	6.825076
H	-4.061034	-2.012518	-1.870034	H	2.605533	-0.075259	3.001084
H	-3.823378	-2.664975	-0.231620	H	1.491992	1.009693	3.871419
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H	-5.728677	-2.637414	1.453785	H	-0.099656	2.384711	7.272981
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H	-7.696806	-1.117071	-1.381314	H	3.114072	4.004322	2.125562
H	-6.368319	-1.132922	-2.560471	H	1.825485	2.956385	2.727114
H	-7.474774	3.974172	-2.490807	H	2.766310	3.937240	3.866244
H	-6.672874	2.445021	-2.864008	H	5.582042	3.407215	2.602882
H	-7.921718	2.511767	-1.605438	H	5.236584	3.322175	4.342899
H	-7.077996	5.199695	-0.386399	H	5.949082	1.926729	3.515762
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H	-3.339052	-5.913107	6.455952	C	-4.056829	0.969260	0.576850
H	-4.342430	-8.345195	4.918088	C	-4.539048	2.106497	-0.067600
H	-5.158614	-7.642771	6.316094	C	-5.694952	2.073185	-0.851281
H	-6.047466	-7.898526	4.798511	C	-6.322050	0.829493	-0.989029
H	-3.768331	-7.067895	2.920198	O	-4.301573	-1.294535	1.185327
H	-5.461785	-6.576181	2.739365	Y	-3.139249	-1.832051	2.893158
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H	-9.935788	-6.455569	8.041138	C	-0.221871	-2.889417	1.463286
H	-9.036110	-6.960032	6.607550	O	0.207339	-2.481726	0.224277
H	-8.168862	-6.493075	8.083444	C	-0.778599	-2.480944	-0.798758
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H	-8.209607	-4.056939	8.873608	N	-2.666283	0.693471	2.725703
H	-9.125204	-2.840292	7.973487	C	-1.293067	0.964086	3.179849
H	-11.187978	-4.793104	6.693697	C	-6.205945	3.350879	-1.530812
H	-10.350915	-3.519439	5.794817	C	-6.534389	4.407455	-0.457292
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H	0.436218	-5.957342	3.739100	C	-5.573450	-2.681452	-1.243950
H	-0.329322	-4.317989	4.157725	O	-4.358811	-3.418057	3.645615
H	-0.155174	-1.022546	0.386535	C	-5.282654	-3.667630	4.567553
H	-0.764742	-1.842948	-1.079482	C	-6.106853	-2.604896	5.022900
H	-1.845390	-1.613266	0.343389	C	-7.040375	-2.816146	6.035792
H	0.798389	-6.580903	1.424603	C	-7.221086	-4.067490	6.628508
H	-0.377030	-5.892242	0.288513	C	-6.437548	-5.112800	6.128024
H	1.223781	-5.175847	0.427140	C	-5.486424	-4.967870	5.109989
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H	2.062404	-3.827830	6.125424	N	-4.779005	-0.516689	4.425304
H	2.077051	-2.584578	7.376804	C	-4.418867	-0.309976	5.830915
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H	1.578247	-2.215783	3.976794	C	-4.979321	-6.327601	3.054719
H	4.506033	-0.579838	5.355947	C	-8.259386	-4.252926	7.742971
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H	-2.721588	-3.532392	8.363222	C	-0.819410	-2.724299	5.452386

O	-1.034267	-3.235392	6.654747	H	-8.549036	-0.903761	-1.237616
C	-2.323645	-3.038492	7.252970	H	-7.432475	-1.168611	-2.593977
C	0.523138	-3.116319	4.852976	H	-7.805982	4.043612	-2.815573
C	0.147168	-4.054514	3.595281	H	-7.300100	2.388315	-3.168345
C	0.604637	-3.652632	2.226636	H	-8.297901	2.729556	-1.741249
C	1.925059	-4.167166	1.724048	H	-6.889066	5.335003	-0.922448
C	1.351217	-3.960314	5.829869	H	-7.316322	4.046125	0.219356
C	1.254457	-1.839664	4.359055	H	-5.656941	4.654725	0.149079
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C	-3.210367	-6.022464	4.825066	H	-3.000484	-5.994179	5.900678
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C	-8.294799	-5.691781	8.276295	H	-6.222349	-7.706675	5.074643
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C	3.532207	-1.578911	5.539091	H	-8.666766	-3.426386	9.723089
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C	-0.265213	0.316574	7.822211	H	-9.715738	-2.875990	6.844347
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H	-3.830115	2.455245	3.005197	H	-1.646178	-1.870568	-0.532952
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H	-7.200202	0.769914	-1.619235	H	1.596302	-3.432578	6.753509
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H	-4.460204	-1.268071	6.348843	H	4.167475	-0.847840	6.042098
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H	-1.165616	0.651848	4.219318	H	-2.294821	-3.599009	8.186496
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H	-6.052180	-3.651852	-1.422625	H	-3.112424	-3.420707	6.601921
H	-5.198756	-2.307982	-2.203575	H	2.813377	0.224131	3.649547
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YT3RR_TRB.xyz
149

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149			
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149

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H	-0.059520	-2.551241	8.692165	C	-7.348544	-3.143187	6.350127
H	1.316095	-1.768744	7.897292	C	-6.548551	-4.286616	6.271778
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H	2.627525	-2.177424	5.465067	C	-5.614279	-0.979922	3.757606
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H	1.467068	-3.507297	5.384451	C	-3.948772	-0.108597	5.292014
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H	-0.167919	-5.088347	1.710293	C	-0.585764	-4.460888	1.495191
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Y	-2.727921	-2.087285	2.648490	C	1.145976	-2.299312	-0.365843
O	-1.176650	-1.962071	4.442358	O	0.598825	-1.222982	-0.208684
C	-0.116166	-2.300162	5.026780	O	0.788962	-3.154177	-1.330678
O	0.428628	-1.482827	5.949899	C	-0.306555	-2.734218	-2.152134
C	-0.309046	-0.336517	6.352757	C	5.499325	0.299502	0.650124
C	-2.196526	0.486182	0.547186	H	-4.759087	1.661641	3.612615
				H	-4.741422	0.670991	2.149247
				H	-2.841666	2.272722	2.241468

H	-2.267256	1.516940	3.723425	H	-1.273943	-0.626116	6.776998
H	-1.759146	1.458144	0.265206	H	0.300918	0.152004	7.113212
H	-1.567187	-0.284015	0.087113	H	1.862416	-3.575008	6.648007
H	-6.359400	-0.193263	3.961356	H	2.416754	-4.611831	5.324756
H	-5.725655	-1.266912	2.706018	H	2.671678	-2.861355	5.259593
H	-6.802798	-5.129739	6.900776	H	1.560248	-6.277092	0.668236
H	-7.570625	-1.158203	5.536832	H	2.409049	-5.915619	2.172652
H	-6.881140	0.092416	-1.975927	H	0.821440	-6.701436	2.199159
H	-3.483269	2.398442	-0.803565	H	1.055342	-2.516550	2.293765
H	-4.701723	0.563205	5.735283	H	2.467223	-3.533153	2.541135
H	-3.941117	-1.040370	5.859262	H	3.658600	-3.441112	-1.016679
H	-2.967945	0.360285	5.377677	H	3.870209	-4.273985	0.532288
H	-0.279849	1.563763	2.091722	H	2.524825	-4.712516	-0.536169
H	-0.367094	0.293003	3.343477	H	-2.843371	-6.594756	0.532586
H	0.007925	-0.132694	1.653635	H	-3.221600	-5.129093	1.469640
H	-5.779515	-4.310637	-1.429006	H	-2.618803	-4.979012	-0.197259
H	-4.962325	-3.055627	-2.379828	H	2.537577	-0.849750	1.387868
H	-4.404259	-3.423340	-0.733805	H	3.922369	-1.951374	1.600650
H	-7.330107	-3.681182	0.465900	H	3.448187	0.859351	0.295464
H	-5.946247	-2.919527	1.265099	H	-0.437762	-3.523985	-2.891698
H	-7.447852	-2.001791	1.009262	H	-1.210720	-2.617699	-1.550284
H	-7.931401	-3.196856	-1.806418	H	-0.076392	-1.785184	-2.642504
H	-8.232563	-1.509302	-1.385046	H	5.876431	1.326419	0.695538
H	-7.183933	-1.912709	-2.761271	H	5.332540	-0.036839	1.678146
H	-7.493395	3.258876	-3.442713	H	6.273953	-0.333160	0.204209
H	-7.084719	1.553524	-3.652129	H	4.781951	1.758173	-1.614757
H	-7.933944	2.092042	-2.190281	H	5.192507	0.102822	-2.108283
H	-6.361045	4.702994	-1.800591	H	3.507695	0.652930	-2.176737
H	-6.728651	3.571944	-0.483824				
H	-5.061496	4.090304	-0.769120				
H	-5.145398	3.901912	-3.879846	YT3RR_TRFb.xyz			
H	-3.817035	3.278422	-2.892407	149			
H	-4.643097	2.206394	-4.029288	scf done: -2856.910046			
H	-2.558109	-6.320842	5.809286	C	-5.194547	-0.857847	-0.681722
H	-2.725871	-4.643808	5.246509	C	-4.056803	-0.632691	0.142318
H	-3.161845	-5.068406	6.909173	C	-3.484511	0.665858	0.174105
H	-4.553971	-7.680426	6.315185	C	-4.071412	1.718217	-0.523884
H	-5.172322	-6.451663	7.421090	C	-5.223729	1.541543	-1.294748
H	-6.201397	-7.077156	6.114636	C	-5.739699	0.243053	-1.357175
H	-4.007759	-7.227536	3.972482	O	-3.502264	-1.584712	0.886078
H	-5.647578	-6.601119	3.716348	Y	-2.692052	-1.804182	2.893500
H	-4.248606	-5.608482	3.277914	O	-1.209408	-1.700645	4.466429
H	-9.666626	-4.170158	8.751565	C	-0.000600	-1.732178	4.967406
H	-8.961278	-5.176690	7.482669	O	0.394349	-0.568248	5.615752
H	-7.931481	-4.506628	8.762845	C	-0.304027	-0.333213	6.828186
H	-9.251707	-1.744423	8.900026	C	-2.165000	0.874429	0.867236
H	-7.494311	-1.987384	8.864512	N	-2.103097	0.672425	2.346781
H	-8.263532	-0.898031	7.702477	C	-0.713805	0.962801	2.759722
H	-10.718960	-2.701553	7.063994	C	-5.846415	2.730615	-2.038961
H	-9.756533	-1.882833	5.825007	C	-6.259109	3.814648	-1.023216
H	-10.000315	-3.631103	5.733855	C	-5.795002	-2.263774	-0.861069
H	0.545842	-5.530183	4.184743	C	-4.708227	-3.221066	-1.389613
H	-0.955218	-4.520201	3.855940	O	-4.089575	-3.173307	3.734883
H	-0.473955	0.349856	5.517754	C	-5.171840	-3.260452	4.504722

C	-6.026304	-2.135715	4.607371	H	-3.597772	2.697261	-0.467999
C	-7.157619	-2.173648	5.418531	H	-4.947957	0.600379	5.852651
C	-7.505949	-3.311082	6.149230	H	-4.174887	-1.000670	5.939333
C	-6.657746	-4.415967	6.024342	H	-3.197487	0.423709	5.551483
C	-5.504987	-4.437180	5.230033	H	-0.456883	2.014735	2.552894
C	-5.755941	-0.909822	3.780735	H	-0.582067	0.756007	3.822670
N	-4.421911	-0.271486	3.980937	H	-0.028014	0.326818	2.196442
C	-4.172142	-0.045810	5.411301	H	-5.120318	-4.230239	-1.514020
C	-4.634039	-5.699324	5.141656	H	-4.338321	-2.885171	-2.365121
C	-4.554843	-6.168970	3.675499	H	-3.869744	-3.267181	-0.692390
C	-8.768420	-3.313871	7.021219	H	-6.778703	-3.799579	0.328341
C	-8.677839	-2.187980	8.070059	H	-5.556581	-2.885236	1.225932
O	-1.273485	-3.488781	1.958438	H	-7.134120	-2.151096	0.859757
C	-0.451041	-4.407154	1.968107	H	-7.316473	-3.309862	-1.982615
O	-0.667941	-5.522273	1.290329	H	-7.799835	-1.671583	-1.542433
C	-1.888601	-5.603681	0.532252	H	-6.641589	-1.934292	-2.863143
C	0.853603	-4.383087	2.741595	H	-7.504040	3.212621	-3.346237
C	1.776148	-3.263583	2.182025	H	-6.860536	1.588476	-3.610731
C	2.016448	-3.068229	0.659014	H	-7.879213	1.923569	-2.197102
C	3.204776	-2.086340	0.558676	H	-6.692787	4.681502	-1.536353
O	3.390462	-1.741778	-0.793649	H	-7.005015	3.427435	-0.320752
C	4.211938	-0.599486	-1.022117	H	-5.403271	4.168305	-0.439470
C	3.972745	-0.184387	-2.464916	H	-5.245689	4.179200	-3.558937
C	1.540173	-5.757861	2.719078	H	-3.917943	3.673810	-2.505582
C	-3.222379	-5.392797	5.678957	H	-4.509322	2.577143	-3.760180
C	-5.195151	-6.867980	5.966103	H	-2.574793	-6.273003	5.578500
C	-10.006521	-3.080210	6.132646	H	-2.769869	-4.559387	5.139713
C	-8.961498	-4.641381	7.767504	H	-3.264963	-5.127183	6.741166
C	-4.416598	1.004924	3.239147	H	-4.536454	-7.736247	5.853425
C	-3.020317	1.581281	3.063148	H	-5.245775	-6.633119	7.034853
C	-6.342624	-2.803478	0.473745	H	-6.194192	-7.167691	5.631112
C	-6.952429	-2.282650	-1.872117	H	-3.898868	-7.044689	3.590617
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C	-7.092929	2.332045	-2.840893	H	-4.171739	-5.370479	3.037776
C	0.882569	-2.762661	4.893546	H	-9.869706	-4.593100	8.378091
C	0.471155	-4.063232	4.264735	H	-9.073088	-5.484847	7.077837
C	2.238932	-2.697101	5.542344	H	-8.123124	-4.856681	8.438733
C	2.362032	-4.336991	-0.125713	H	-9.578745	-2.169026	8.695046
C	0.832872	-2.301134	0.059098	H	-7.812158	-2.333988	8.724837
O	0.479694	-1.208600	0.461097	H	-8.578733	-1.203784	7.601555
O	0.233989	-2.933353	-0.953777	H	-10.921498	-3.070852	6.737248
C	-0.847710	-2.217600	-1.573213	H	-9.948403	-2.124715	5.601733
C	5.683469	-0.895172	-0.742854	H	-10.101837	-3.871652	5.381835
H	-5.051877	1.746445	3.754101	H	0.920154	-4.873573	4.851881
H	-4.860663	0.825527	2.256807	H	-0.611291	-4.178707	4.371622
H	-3.096906	2.545725	2.536380	H	-1.388703	-0.336645	6.675078
H	-2.579749	1.796183	4.041773	H	-0.052609	-1.094609	7.579289
H	-1.817418	1.899333	0.653513	H	0.008966	0.647678	7.194024
H	-1.419724	0.189455	0.448436	H	2.385524	-1.743515	6.051965
H	-6.536431	-0.162146	3.997665	H	2.369455	-3.503610	6.278626
H	-5.823987	-1.145968	2.711936	H	3.058157	-2.808469	4.817246
H	-6.906057	-5.313935	6.575399	H	1.772954	-6.111832	1.715219
H	-7.783658	-1.283924	5.465344	H	2.473821	-5.692405	3.286670
H	-6.614639	0.072666	-1.970932	H	0.909963	-6.511939	3.200385

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H	2.756102	-3.437884	2.641869
H	2.647433	-4.072825	-1.145681
H	3.211000	-4.842957	0.345453
H	1.525401	-5.035093	-0.178227
H	-1.866032	-6.584489	0.059615
H	-2.751900	-5.513395	1.192806
H	-1.913346	-4.812292	-0.217374
H	2.987864	-1.190897	1.159824
H	4.096811	-2.578078	0.978622
H	3.875386	0.211192	-0.353240
H	-1.183661	-2.851376	-2.393513
H	-1.655686	-2.049418	-0.857205
H	-0.492497	-1.258011	-1.956161
H	6.297485	-0.013010	-0.950915
H	5.852854	-1.174188	0.301617
H	6.031762	-1.715679	-1.378887
H	4.543480	0.717041	-2.707404
H	4.282118	-0.983256	-3.146542
H	2.911724	0.018650	-2.632408

YT3RR_TRFf.xyz

149

scf done: -2856.884620

C	-5.369501	-0.942700	-0.628909
C	-4.197920	-0.783425	0.160203
C	-3.510434	0.457343	0.122500
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C	-5.848640	0.180722	-1.317021
O	-3.715199	-1.747547	0.937166
Y	-2.657305	-2.053393	2.769963
O	-1.198544	-1.806101	4.776001
C	-0.202224	-2.093180	5.449896
O	0.243269	-1.280057	6.411675
C	-0.514116	-0.106586	6.707833
C	-2.136062	0.571805	0.727852
N	-1.977692	0.378579	2.205484
C	-0.546648	0.581612	2.502718
C	-5.780933	2.652520	-2.059737
C	-6.022342	3.806719	-1.066940
C	-6.056523	-2.311732	-0.781335
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O	-4.001837	-3.293522	3.860783
C	-5.110894	-3.310041	4.600524
C	-5.945435	-2.164432	4.609744
C	-7.105150	-2.133789	5.380660
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C	-6.671018	-4.341225	6.138037
C	-5.489207	-4.430135	5.392410
C	-5.620216	-0.979682	3.742888
N	-4.281276	-0.365373	3.972858
C	-4.087284	-0.104957	5.402507

C	-4.629424	-5.701951	5.446157
C	-4.465620	-6.287870	4.030629
C	-8.795700	-3.145955	6.987347
C	-8.702058	-1.980432	7.991961
O	-1.104485	-3.274514	1.903915
C	-0.467955	-4.416357	1.794852
O	-1.255887	-5.545339	1.919047
C	-2.282024	-5.658552	0.943347
C	0.876071	-4.585762	1.656896
C	1.790188	-3.390761	1.624978
C	2.228664	-2.849515	0.222273
C	3.269967	-1.749101	0.465359
O	3.671333	-1.212183	-0.774534
C	4.408165	0.001149	-0.700205
C	4.375530	0.608145	-2.094317
C	1.494200	-5.958773	1.637867
C	-3.251231	-5.354977	6.041054
C	-5.244442	-6.801227	6.326265
C	-9.995629	-2.910343	6.048819
C	-9.056395	-4.434781	7.779130
C	-4.211155	0.891587	3.206989
C	-2.780300	1.351061	2.974194
C	-6.577007	-2.835079	0.570459
C	-7.253819	-2.260506	-1.743662
C	-4.763813	3.107184	-3.125737
C	-7.109349	2.350807	-2.766683
C	0.627924	-3.308389	5.353747
C	0.134903	-4.373082	4.699274
C	1.958216	-3.318063	6.058943
C	2.830069	-3.940095	-0.667052
C	1.011204	-2.185926	-0.413592
O	0.589940	-1.091297	-0.083232
O	0.428112	-2.931294	-1.355776
C	-0.768455	-2.389174	-1.926275
C	5.835298	-0.230363	-0.206451
H	-4.770432	1.691668	3.722627
H	-4.696239	0.732306	2.241667
H	-2.790972	2.326732	2.462428
H	-2.280501	1.510201	3.936229
H	-1.732980	1.567848	0.480334
H	-1.466759	-0.159951	0.262818
H	-6.393251	-0.209602	3.903011
H	-5.653636	-1.253700	2.682290
H	-6.953684	-5.198983	6.734270
H	-7.711593	-1.229807	5.354355
H	-6.754934	0.065328	-1.897259
H	-3.475509	2.468898	-0.590118
H	-4.900618	0.518975	5.808018
H	-4.068333	-1.046808	5.952973
H	-3.141447	0.414857	5.561334
H	-0.243857	1.622706	2.305786
H	-0.350894	0.350978	3.552478
H	0.055529	-0.072720	1.867990
H	-5.497344	-4.308650	-1.456072

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H	-4.163941	-3.397791	-0.715229
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H	-6.405912	4.691875	-1.588371
H	-6.753508	3.517651	-0.304407
H	-5.100762	4.098332	-0.553184
H	-5.138196	3.984083	-3.667479
H	-3.801683	3.378264	-2.679446
H	-4.579024	2.310203	-3.853630
H	-2.597740	-6.235947	6.038488
H	-2.770819	-4.563092	5.465510
H	-3.355450	-5.014502	7.078009
H	-4.586944	-7.677387	6.314128
H	-5.351879	-6.488115	7.370727
H	-6.225602	-7.122227	5.959647
H	-3.834374	-7.184183	4.061668
H	-5.440888	-6.574537	3.620988
H	-4.007450	-5.562711	3.358841
H	-9.985199	-4.335799	8.351418
H	-9.166057	-5.302201	7.119654
H	-8.250903	-4.645763	8.490765
H	-9.622248	-1.905406	8.583807
H	-7.864496	-2.127302	8.682368
H	-8.553490	-1.020839	7.486642
H	-10.928565	-2.846595	6.621817
H	-9.889375	-1.980234	5.481620
H	-10.093080	-3.729051	5.328258
H	0.692774	-5.302250	4.651855
H	-0.846292	-4.370918	4.243983
H	-0.598695	0.537238	5.829382
H	-1.511691	-0.377873	7.059902
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H	1.839560	-3.189514	7.139473
H	2.469491	-4.266406	5.879010
H	2.607200	-2.507934	5.710274
H	2.024980	-6.179246	0.704191
H	2.240597	-6.061807	2.440814
H	0.737088	-6.731044	1.780477
H	1.325470	-2.556866	2.164128
H	2.721256	-3.641483	2.156212
H	3.205533	-3.507458	-1.596978
H	3.669212	-4.418646	-0.149910
H	2.090584	-4.702485	-0.912111
H	-2.823555	-6.579921	1.163917
H	-2.980831	-4.816074	0.981466
H	-1.852681	-5.721020	-0.065547

H	2.833344	-0.961793	1.098542
H	4.121453	-2.192521	1.006993
H	3.894080	0.683067	-0.000023
H	-1.061969	-3.087730	-2.709697
H	-1.551850	-2.317595	-1.168426
H	-0.578329	-1.399435	-2.348775
H	6.391518	0.712368	-0.179183
H	5.853080	-0.653686	0.802442
H	6.358396	-0.920725	-0.876397
H	4.895660	1.570854	-2.111015
H	4.863892	-0.061008	-2.810163
H	3.342498	0.760872	-2.417572

YT3RS_TLB.xyz

149

scf done: -2856.868097

C	-6.522200	-1.074449	-0.135757
C	-5.232041	-0.916903	0.439822
C	-4.500684	0.266672	0.164401
C	-5.073298	1.303135	-0.569412
C	-6.371043	1.211757	-1.078717
C	-7.046478	0.006032	-0.857367
O	-4.678446	-1.823808	1.231533
Y	-3.254745	-2.099522	2.806986
O	-1.378918	-2.007307	4.145058
C	-3.048431	0.339116	0.547794
N	-2.686885	0.295815	1.999798
C	-1.236074	0.536169	2.085876
C	-6.976284	2.380681	-1.867854
C	-6.976936	3.649988	-0.993336
C	-7.292479	-2.401485	-0.023323
C	-6.440783	-3.528010	-0.643960
O	-4.356801	-3.337476	4.117834
C	-5.209211	-3.324068	5.141164
C	-5.971962	-2.153626	5.377872
C	-6.856281	-2.089076	6.452603
C	-7.041971	-3.163833	7.323596
C	-6.291222	-4.314475	7.062366
C	-5.381560	-4.438787	6.005620
C	-5.905252	-0.997743	4.417259
N	-4.557541	-0.388103	4.213013
C	-3.961226	-0.035265	5.506755
C	-4.593947	-5.741623	5.796671
C	-4.871411	-6.308285	4.390034
C	-8.032846	-3.053225	8.490293
C	-7.616352	-1.891382	9.413716
O	-1.947201	-3.313742	1.388324
C	-0.719200	-3.549736	1.200787
O	0.083121	-2.448517	1.030855
C	0.646501	-2.259215	-0.265123
C	-0.110385	-4.813055	1.387059
C	-1.003643	-6.038168	1.310521
C	-1.314616	-6.674043	-0.082443

C	-1.972150	-5.642097	-1.007089	H	-6.547903	3.476291	-3.709150
O	-2.317960	-6.292455	-2.210866	H	-5.097300	2.883977	-2.886786
C	-3.195812	-5.561987	-3.061470	H	-6.122881	1.754666	-3.780115
C	-3.759611	-6.565311	-4.055537	H	-2.505297	-6.370725	5.781231
C	1.372857	-4.985394	1.154561	H	-2.750427	-4.680321	5.291098
C	-3.088514	-5.461557	5.973160	H	-2.875495	-5.135697	6.997870
C	-4.977972	-6.832262	6.809195	H	-4.392188	-7.734630	6.602388
C	-9.447936	-2.782628	7.941830	H	-4.766331	-6.535465	7.842513
C	-8.087430	-4.333831	9.334652	H	-6.036625	-7.105050	6.738124
C	-4.724071	0.805473	3.361791	H	-4.295142	-7.227337	4.229825
C	-3.411363	1.317139	2.785942	H	-5.933122	-6.555171	4.278790
C	-7.600774	-2.748212	1.445169	H	-4.606428	-5.594087	3.610235
C	-8.631441	-2.362890	-0.776159	H	-8.802751	-4.205471	10.154325
C	-6.135181	2.638725	-3.133978	H	-8.413072	-5.197014	8.744555
C	-8.422415	2.105568	-2.302911	H	-7.114731	-4.570811	9.778992
C	-0.085896	-7.286792	-0.761265	H	-8.317854	-1.791941	10.250841
C	-2.392814	-7.728118	0.209336	H	-6.616002	-2.061179	9.826083
O	-3.502953	-7.462490	0.616216	H	-7.599399	-0.935804	8.879960
O	-1.972447	-8.989466	0.008326	H	-10.171081	-2.698929	8.762103
C	-2.946372	-9.999623	0.284390	H	-9.488711	-1.852394	7.366374
C	-2.477695	-4.406864	-3.756485	H	-9.771971	-3.594977	7.282985
H	-5.204716	1.619437	3.932152	H	1.929190	-4.124408	1.534273
H	-5.397467	0.544055	2.542363	H	1.728297	-5.875477	1.685762
H	-3.617172	2.205723	2.170251	H	1.643199	-5.129189	0.102548
H	-2.752050	1.645510	3.596054	H	-1.968579	-5.797108	1.765606
H	-2.623892	1.263712	0.122567	H	-0.549528	-6.828502	1.925000
H	-2.513387	-0.503020	0.089215	H	-0.381658	-7.834251	-1.657093
H	-6.593694	-0.211813	4.769292	H	0.610149	-6.501655	-1.066741
H	-6.248664	-1.308380	3.424206	H	0.439552	-7.975483	-0.094250
H	-6.417565	-5.166703	7.717054	H	1.332134	-1.413805	-0.182651
H	-7.422027	-1.169655	6.595135	H	1.202276	-3.135828	-0.608090
H	-8.038980	-0.104006	-1.275186	H	-0.136763	-2.019114	-0.993755
H	-4.475268	2.194175	-0.755730	H	-2.861234	-5.221437	-0.518512
H	-4.593393	0.682813	6.054216	H	-1.258849	-4.821995	-1.185550
H	-3.853218	-0.934894	6.114869	H	-4.019574	-5.155928	-2.451542
H	-2.973917	0.405607	5.361446	H	-2.456002	-10.949700	0.071279
H	-0.969514	1.529699	1.690522	H	-3.263285	-9.956100	1.329639
H	-0.907892	0.464601	3.123294	H	-3.825005	-9.869785	-0.352332
H	-0.703600	-0.229341	1.518011	H	-3.161376	-3.878371	-4.428596
H	-6.963407	-4.488365	-0.561984	H	-2.094983	-3.676258	-3.037234
H	-6.257864	-3.330795	-1.706457	H	-1.635913	-4.785632	-4.346151
H	-5.479214	-3.615619	-0.134625	H	-4.476305	-6.083507	-4.727530
H	-8.187875	-3.672798	1.497722	H	-2.953920	-6.995733	-4.659427
H	-6.684515	-2.901434	2.016448	H	-4.266193	-7.378327	-3.528859
H	-8.189204	-1.953643	1.918846	C	-0.178335	-2.313266	4.430201
H	-9.121404	-3.338303	-0.686588	C	0.530083	-3.480876	4.074809
H	-9.316690	-1.613783	-0.363611	C	-0.156156	-4.537539	3.452699
H	-8.499898	-2.159114	-1.844476	O	0.539824	-1.467893	5.211833
H	-8.816350	2.971610	-2.845817	C	-0.157449	-0.439128	5.894720
H	-8.491067	1.240306	-2.970586	C	1.975201	-3.619613	4.490201
H	-9.077743	1.927060	-1.443673	H	0.290324	-5.524096	3.566190
H	-7.398182	4.499028	-1.544743	H	-1.242567	-4.534976	3.498072
H	-7.577398	3.499661	-0.089787	H	0.572563	0.016067	6.565912
H	-5.965366	3.927604	-0.680247	H	-0.536945	0.323625	5.207318

H -0.993130 -0.843406 6.473002
H 2.104868 -3.458701 5.566306
H 2.341886 -4.623188 4.255036
H 2.633230 -2.901672 3.985571

YT3RS_TLBb.xyz
149

scf done: -2856.878596

C -6.455379 -1.173536 -0.169932
C -5.176723 -1.019266 0.431994
C -4.417543 0.142549 0.137299
C -4.953106 1.161809 -0.647233
C -6.237910 1.074575 -1.188363
C -6.940846 -0.110277 -0.942394
O -4.662393 -1.910214 1.268930
Y -3.213252 -2.152338 2.814381
O -1.376776 -1.902939 4.492421
C -2.977308 0.216317 0.566186
N -2.676934 0.229268 2.033301
C -1.231562 0.472290 2.183205
C -6.800741 2.224374 -2.034613
C -6.794824 3.525800 -1.208724
C -7.253481 -2.482403 -0.035592
C -6.414604 -3.639144 -0.615623
O -4.251849 -3.399376 4.189092
C -5.111073 -3.379943 5.206001
C -5.907418 -2.224184 5.411369
C -6.788742 -2.151364 6.488253
C -6.942596 -3.202650 7.392970
C -6.170481 -4.344233 7.156199
C -5.264440 -4.477669 6.097324
C -5.881812 -1.095436 4.416655
N -4.562739 -0.426019 4.221154
C -4.029519 0.008934 5.514683
C -4.466510 -5.777907 5.910594
C -4.747205 -6.374201 4.516875
C -7.924232 -3.077812 8.566040
C -7.520552 -1.881741 9.450883
O -1.739504 -3.152361 1.597817
C -0.555942 -3.449286 1.129056
O 0.278582 -2.336671 0.990351
C 0.533133 -1.958881 -0.354428
C -0.076010 -4.692448 0.849634
C -0.984732 -5.887583 0.980839
C -1.459552 -6.591543 -0.334347
C -2.109763 -5.555566 -1.258369
O -2.598414 -6.226052 -2.402686
C -3.383464 -5.426484 -3.277925
C -4.186586 -6.391194 -4.137251
C 1.380103 -4.903856 0.524683
C -2.962590 -5.483802 6.069020
C -4.834295 -6.851241 6.947455
C -9.349983 -2.849967 8.026006

C -7.945323 -4.334185 9.447453
C -4.758940 0.726119 3.321282
C -3.451563 1.262160 2.753865
C -7.590429 -2.789722 1.435331
C -8.580784 -2.436506 -0.808574
C -5.925705 2.416868 -3.289422
C -8.241960 1.961361 -2.492563
C -0.326096 -7.317380 -1.064246
C -2.576935 -7.547774 0.095012
O -3.616469 -7.188596 0.606073
O -2.283833 -8.844935 -0.115649
C -3.303793 -9.763435 0.280659
C -2.514777 -4.494349 -4.121195
H -5.284002 1.542387 3.847880
H -5.402542 0.406574 2.498902
H -3.672536 2.113482 2.093600
H -2.823983 1.649213 3.563276
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H -7.378274 -1.243438 6.605649
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H -4.335208 2.036073 -0.847367
H -4.717065 0.712064 6.013504
H -3.896682 -0.859019 6.162894
H -3.065467 0.501579 5.379806
H -0.937748 1.440565 1.746711
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H -0.670404 -0.330304 1.696768
H -6.955957 -4.587603 -0.519720
H -6.212018 -3.470801 -1.679353
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H -9.092272 -3.398654 -0.699011
H -9.255539 -1.661625 -0.427326
H -8.430314 -2.266585 -1.880257
H -8.606573 2.814030 -3.075585
H -8.312971 1.073460 -3.129544
H -8.919552 1.826977 -1.642564
H -7.189044 4.360914 -1.799913
H -7.415626 3.420788 -0.312518
H -5.784580 3.796882 -0.885803
H -6.306933 3.239895 -3.905956
H -4.888710 2.650159 -3.027268
H -5.917035 1.508621 -3.901108
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H -2.638851 -4.722816 5.358348
H -2.744596 -5.126175 7.082371
H -4.243933 -7.753320 6.752815
H -4.616453 -6.533368 7.973327

H	-5.891391	-7.132891	6.890520
H	-4.165283	-7.292497	4.373297
H	-5.807672	-6.630226	4.415970
H	-4.489638	-5.675371	3.720953
H	-8.653859	-4.195541	10.271327
H	-8.261343	-5.219766	8.886056
H	-6.963510	-4.540393	9.887090
H	-8.215560	-1.770522	10.291920
H	-6.513318	-2.021313	9.858021
H	-7.526396	-0.942237	8.888981
H	-10.065360	-2.754044	8.851740
H	-9.414592	-1.938949	7.422695
H	-9.666151	-3.688146	7.396423
H	1.990877	-4.078201	0.901509
H	1.741287	-5.828858	0.992579
H	1.594296	-5.006348	-0.548390
H	-1.888857	-5.589269	1.518317
H	-0.486016	-6.661724	1.585884
H	-0.712137	-7.861634	-1.927536
H	0.411453	-6.595575	-1.423311
H	0.179675	-8.029310	-0.406087
H	1.098975	-1.023491	-0.319740
H	1.127057	-2.708877	-0.888416
H	-0.401351	-1.790912	-0.905737
H	-2.928616	-5.051058	-0.725988
H	-1.354205	-4.800883	-1.520329
H	-4.078736	-4.819133	-2.674702
H	-2.917501	-10.755562	0.044997
H	-3.510632	-9.676102	1.350657
H	-4.229020	-9.572158	-0.268974
H	-3.135076	-3.890376	-4.791718
H	-1.936309	-3.805816	-3.497695
H	-1.814632	-5.077583	-4.728888
H	-4.839761	-5.847108	-4.826616
H	-3.513770	-7.024559	-4.724920
H	-4.803040	-7.037835	-3.507219
C	-0.309773	-2.230289	5.021617
C	0.485246	-3.448436	4.764114
C	-0.049805	-4.415079	4.002750
O	0.265948	-1.471811	5.957631
C	-0.415541	-0.292185	6.382953
C	1.842218	-3.561204	5.405182
H	0.490203	-5.338791	3.823333
H	-1.032922	-4.323969	3.559025
H	0.215323	0.146236	7.155584
H	-0.532028	0.409371	5.553303
H	-1.396575	-0.543640	6.790373
H	1.774054	-3.534498	6.497319
H	2.317369	-4.499823	5.111548
H	2.497160	-2.736829	5.104989

scf done: -2856.888557		
C	-6.596984	-1.182050 -0.158705
C	-5.302854	-1.005868 0.403350
C	-4.595875	0.192258 0.124904
C	-5.192630	1.219422 -0.602589
C	-6.492390	1.106630 -1.102179
C	-7.145825	-0.109986 -0.874569
O	-4.726690	-1.906625 1.185918
Y	-3.328053	-2.123748 2.805433
O	-1.406196	-2.129438 3.864872
C	-3.143077	0.290697 0.499287
N	-2.775188	0.254291 1.949292
C	-1.323980	0.499782 2.030370
C	-7.122555	2.264494 -1.888098
C	-7.137852	3.535066 -1.015558
C	-7.347739	-2.519063 -0.034653
C	-6.489288	-3.637467 -0.660090
O	-4.430942	-3.366271 4.119118
C	-5.250908	-3.337474 5.166659
C	-6.011099	-2.165444 5.402982
C	-6.862397	-2.081378 6.502295
C	-7.016488	-3.138705 7.400581
C	-6.268152	-4.291559 7.140942
C	-5.390456	-4.434005 6.059664
C	-5.965393	-1.028223 4.420048
N	-4.620421	-0.419281 4.186521
C	-4.002783	-0.049924 5.466884
C	-4.599491	-5.735060 5.853523
C	-4.924725	-6.337639 4.472117
C	-7.971734	-3.006091 8.594575
C	-7.531811	-1.823266 9.479825
O	-1.946182	-3.334889 1.291635
C	-0.740072	-3.529226 1.127556
O	-0.095459	-2.534549 0.522127
C	1.320694	-2.301523 0.523290
C	-0.125398	-4.836093 1.629651
C	-1.137819	-5.995062 1.384078
C	-1.410071	-6.589131 -0.032685
C	-1.737986	-5.489332 -1.052794
O	-2.063050	-6.109394 -2.275959
C	-2.781416	-5.289899 -3.195728
C	-3.342211	-6.228958 -4.251704
C	1.272333	-5.197148 1.115434
C	-3.090398	-5.440122 5.964519
C	-4.935692	-6.803085 6.906367
C	-9.403954	-2.751689 8.084236
C	-7.996204	-4.268316 9.467550
C	-4.801772	0.764803 3.323142
C	-3.495976	1.278357 2.733974
C	-7.636038	-2.862438 1.438888
C	-8.695145	-2.500693 -0.773228
C	-6.294872	2.534600 -3.160545
C	-8.567045	1.965174 -2.312645
C	-0.288200	-7.491304 -0.563620

C	-2.720773	-7.380882	0.143997	H	-6.519084	-1.981209	9.865787
O	-3.787219	-6.864623	0.396708	H	-7.534110	-0.879374	8.925418
O	-2.560928	-8.708656	0.025966	H	-10.101009	-2.648530	8.924676
C	-3.755781	-9.477940	0.195198	H	-9.465083	-1.836323	7.487177
C	-1.893139	-4.205287	-3.800285	H	-9.746676	-3.580921	7.456610
H	-5.285128	1.579669	3.889464	H	2.051469	-4.571153	1.548361
H	-5.478353	0.488574	2.510836	H	1.489900	-6.226553	1.414327
H	-3.710936	2.161517	2.113457	H	1.354019	-5.152764	0.026557
H	-2.830760	1.615259	3.535561	H	-2.100315	-5.668942	1.783853
H	-2.735677	1.221832	0.071263	H	-0.796968	-6.822524	2.019844
H	-2.596608	-0.542884	0.039095	H	-0.615573	-7.999323	-1.471364
H	-6.649173	-0.236633	4.767722	H	0.600164	-6.908929	-0.814074
H	-6.322674	-1.357571	3.437526	H	-0.008740	-8.251029	0.171218
H	-6.369620	-5.129797	7.817743	H	1.426754	-1.267792	0.192591
H	-7.426642	-1.160944	6.644000	H	1.716846	-2.404473	1.533659
H	-8.140657	-0.236360	-1.282208	H	1.833193	-2.958610	-0.179785
H	-4.610978	2.120608	-0.792299	H	-2.579306	-4.887726	-0.685539
H	-4.631395	0.667085	6.019269	H	-0.862966	-4.826986	-1.168509
H	-3.874413	-0.942309	6.081777	H	-3.615929	-4.810637	-2.657849
H	-3.023525	0.401908	5.298892	H	-3.457097	-10.518639	0.068824
H	-1.071026	1.511927	1.674737	H	-4.180974	-9.316840	1.189006
H	-0.968537	0.368848	3.053266	H	-4.500442	-9.198204	-0.553964
H	-0.803618	-0.226333	1.402405	H	-2.456354	-3.609316	-4.525617
H	-7.001414	-4.602975	-0.573430	H	-1.514472	-3.519271	-3.036162
H	-6.316888	-3.439925	-1.724410	H	-1.038395	-4.657961	-4.314561
H	-5.523516	-3.717619	-0.158307	H	-3.948134	-5.677218	-4.976544
H	-8.205210	-3.797592	1.502663	H	-2.528937	-6.728352	-4.788530
H	-6.711741	-2.993974	2.002773	H	-3.967628	-6.994719	-3.785388
H	-8.235341	-2.075852	1.912537	C	-0.122545	-2.291866	4.028023
H	-9.170984	-3.482423	-0.675849	C	0.613512	-3.403886	3.730125
H	-9.386323	-1.759579	-0.356046	C	-0.083728	-4.629795	3.192514
H	-8.577143	-2.298341	-1.843438	O	0.556577	-1.194667	4.536551
H	-8.979105	2.824029	-2.853614	C	0.058775	-0.724736	5.779925
H	-8.625995	1.098104	-2.978915	C	2.064701	-3.512579	4.127832
H	-9.213196	1.776650	-1.448595	H	0.399003	-5.531475	3.594782
H	-7.575447	4.376731	-1.565635	H	-1.120242	-4.643133	3.545265
H	-7.730455	3.376764	-0.108189	H	0.620056	0.180252	6.022919
H	-6.128866	3.828680	-0.708834	H	-1.008886	-0.492364	5.724629
H	-6.724859	3.364922	-3.733669	H	0.215736	-1.469383	6.572191
H	-5.259250	2.796222	-2.920837	H	2.365701	-2.658776	4.736895
H	-6.273192	1.649974	-3.805677	H	2.240821	-4.427672	4.710845
H	-2.508894	-6.352327	5.780735	H	2.765414	-3.557821	3.279625
H	-2.782934	-4.678374	5.246552				
H	-2.842305	-5.080665	6.969770				
H	-4.349580	-7.705659	6.700934	YT3RS_TLF.xyz			
H	-4.688509	-6.477840	7.923070	149			
H	-5.993723	-7.086388	6.882283	scf done: -2856.876884			
H	-4.344664	-7.255444	4.314452	C	-6.407990	-2.907973	4.720810
H	-5.987260	-6.597304	4.407553	C	-5.469331	-3.896422	4.337525
H	-4.696921	-5.639266	3.666412	C	-5.695395	-5.245303	4.722996
H	-8.687213	-4.124289	10.305301	C	-6.837089	-5.524114	5.484692
H	-8.336522	-5.144878	8.906119	C	-7.767753	-4.561337	5.889368
H	-7.009894	-4.492900	9.887625	C	-7.521430	-3.247797	5.486380
H	-8.208647	-1.708155	10.335012	O	-4.401484	-3.525590	3.629555

Y	-3.141975	-1.912243	3.137801	C	-2.195509	-6.348976	-1.930026
O	-1.518377	-2.829631	1.875625	O	-0.950642	-7.598730	2.899873
C	-0.310134	-2.692978	1.481482	C	-1.894221	-8.771056	-1.262018
C	0.797219	-3.435510	1.914949	H	-5.785141	1.141040	4.839329
C	2.142306	-3.131381	1.294892	H	-5.455903	0.618058	3.183289
C	-4.722895	-6.363925	4.319741	H	-3.878207	2.367670	3.984047
C	-3.336893	-6.096532	4.938870	H	-3.339561	1.301181	5.274894
C	-9.007984	-4.890777	6.730999	H	-2.415531	2.355741	2.094079
C	-10.279176	-4.482654	5.960604	H	-1.952229	0.784917	1.440169
C	-6.250399	-1.490872	4.242592	H	-7.096156	-0.895063	4.624344
N	-4.978078	-0.813776	4.629349	H	-6.295452	-1.449612	3.148281
C	-5.066882	0.593911	4.203467	H	-7.006074	-6.552442	5.777014
C	-3.727861	1.310382	4.251818	H	-8.215417	-2.454998	5.761111
N	-2.705866	0.700380	3.373736	H	-6.987906	1.214164	-1.212777
C	-1.372331	0.984389	3.932354	H	-4.104578	3.395496	1.061729
O	-4.082331	-1.080556	1.402211	H	-5.570971	-0.355032	6.623276
C	-4.581870	0.019954	0.851548	H	-4.818380	-1.947096	6.385017
C	-4.018331	1.267600	1.220452	H	-3.809520	-0.490432	6.359680
C	-4.565755	2.459380	0.750830	H	-1.220016	2.066075	4.076662
C	-5.663948	2.474333	-0.112434	H	-1.246726	0.468755	4.886051
C	-6.159046	1.229727	-0.517102	H	-0.602109	0.628605	3.243485
C	-5.651331	-0.002494	-0.083663	H	-5.440624	-3.056766	-1.721116
C	-2.735026	1.303732	2.006704	H	-4.640372	-1.534204	-2.151138
C	-6.204517	-1.326296	-0.640397	H	-4.265623	-2.331228	-0.606609
C	-6.814328	-2.187857	0.481817	H	-7.238369	-3.108117	0.062487
C	-6.252521	3.808646	-0.589992	H	-6.061042	-2.471829	1.217841
C	-5.171415	4.616848	-1.334561	H	-7.624202	-1.651666	0.990086
O	-1.716929	-2.023497	4.955685	H	-7.636687	-2.072432	-2.073284
C	-0.749351	-2.645219	5.488811	H	-8.176680	-0.591763	-1.278923
C	0.579529	-2.770799	4.988296	H	-6.937416	-0.522679	-2.550563
C	1.576800	-3.583825	5.777748	H	-7.832388	4.592915	-1.846694
O	-0.921176	-3.238763	6.681358	H	-7.154686	3.077931	-2.450490
C	-2.203581	-3.159758	7.296322	H	-8.260901	3.068059	-1.063190
C	-7.300323	-1.101643	-1.694309	H	-7.157984	5.581879	0.308769
C	-5.062104	-2.109383	-1.319118	H	-7.522464	4.074392	1.169699
C	-7.441954	3.616261	-1.540970	H	-5.928681	4.825074	1.330546
C	-6.741959	4.618614	0.627183	H	-5.576178	5.575634	-1.679678
C	-5.178931	-7.747690	4.807593	H	-4.310746	4.832103	-0.693359
C	-4.609893	-6.436492	2.783250	H	-4.806525	4.066670	-2.208149
C	-4.781495	-0.900899	6.080641	H	-2.623198	-6.862553	4.620774
C	-9.111506	-6.386306	7.060577	H	-2.951396	-5.124889	4.624937
C	-8.949672	-4.112596	8.060628	H	-3.399885	-6.112288	6.033847
O	-0.013124	-1.658071	0.644083	H	-4.451266	-8.497536	4.480127
C	-1.026951	-1.247715	-0.274617	H	-5.239313	-7.803902	5.900374
C	0.571703	-4.770480	2.579887	H	-6.152982	-8.029828	4.392899
C	0.471199	-6.041251	1.663896	H	-3.868656	-7.191589	2.499887
C	1.772216	-6.326793	0.898964	H	-5.574234	-6.713732	2.341873
C	0.933273	-2.128655	3.814151	H	-4.304416	-5.476684	2.364288
C	0.156984	-7.191764	2.622999	H	-10.007182	-6.570478	7.663787
O	1.272160	-7.686695	3.199651	H	-9.191185	-6.998503	6.156008
C	1.051058	-8.730225	4.149980	H	-8.248574	-6.737442	7.636386
C	-0.697415	-5.919074	0.684885	H	-9.836425	-4.322496	8.670732
O	-0.721398	-7.077181	-0.123177	H	-8.064061	-4.395378	8.639921
C	-1.954939	-7.328858	-0.783168	H	-8.908489	-3.031246	7.895198

H	-11.176354	-4.707600	6.549631	C	-10.171058	-4.438985	6.337425
H	-10.290400	-3.411888	5.734008	C	-6.278524	-1.486042	4.270219
H	-10.349143	-5.023954	5.011423	N	-5.033767	-0.744984	4.625016
H	1.985620	-2.023410	3.571717	C	-5.131467	0.618749	4.076295
H	0.285271	-1.360654	3.411185	C	-3.802269	1.357179	4.106036
H	-2.981762	-3.551098	6.637719	N	-2.755937	0.679170	3.311583
H	-2.132673	-3.773594	8.194579	C	-1.430366	0.952196	3.893154
H	-2.438479	-2.128022	7.571595	O	-4.082173	-1.196851	1.373517
H	2.545072	-3.587727	5.269706	C	-4.554034	-0.116054	0.764588
H	1.726997	-3.172770	6.782817	C	-3.980958	1.139496	1.088792
H	1.260230	-4.624066	5.907327	C	-4.500117	2.315808	0.553091
H	2.370845	-2.061208	1.333356	C	-5.580496	2.306456	-0.332817
H	2.935527	-3.666902	1.826635	C	-6.087921	1.051582	-0.688159
H	2.205754	-3.419395	0.238904	C	-5.606897	-0.165795	-0.187883
H	-0.344958	-4.715260	3.177163	C	-2.717584	1.186629	1.903900
H	1.393490	-4.960197	3.280567	C	-6.167685	-1.507124	-0.689567
H	1.713163	-7.297900	0.403377	C	-6.800692	-2.308337	0.464344
H	1.930080	-5.572699	0.124803	C	-6.136614	3.625731	-0.885566
H	2.636024	-6.329200	1.567523	C	-5.029630	4.373959	-1.654490
H	-0.703655	-0.284557	-0.672994	O	-1.958555	-2.068590	5.307342
H	-1.095541	-1.969186	-1.097172	C	-1.146470	-2.766106	5.931657
H	-2.005648	-1.155884	0.200408	C	0.304564	-2.872255	5.662499
H	-1.638160	-5.812762	1.240843	C	1.096378	-3.902695	6.419001
H	-0.552984	-5.013589	0.076627	O	-1.504882	-3.499829	6.975568
H	-2.772863	-7.227875	-0.050382	C	-2.880762	-3.484812	7.380766
H	2.040433	-9.033125	4.493905	C	-7.247759	-1.320782	-1.766433
H	0.449082	-8.370243	4.988823	C	-5.023496	-2.330600	-1.316226
H	0.532732	-9.572709	3.685084	C	-7.316999	3.407804	-1.842153
H	-3.135337	-6.578386	-2.443049	C	-6.626408	4.505957	0.281618
H	-2.259388	-5.317064	-1.571494	C	-5.223198	-7.739567	4.846584
H	-1.379812	-6.411380	-2.658572	C	-4.823480	-6.415289	2.787872
H	-2.831565	-9.059098	-1.747818	C	-4.879960	-0.700027	6.082557
H	-1.078098	-8.899056	-1.980957	C	-8.925556	-6.302912	7.419808
H	-1.716502	-9.441498	-0.417005	C	-8.718270	-3.998849	8.339122
YT3RS_TLFb.xyz				O	-0.028969	-1.168834	1.309585
149				C	-0.435528	-1.060193	-0.051775
scf done: -2856.884812				C	0.789594	-4.666459	2.427686
C	-6.387598	-2.883029	4.819924	C	0.572283	-5.877285	1.460884
C	-5.462852	-3.879015	4.414056	C	1.652343	-5.973035	0.380620
C	-5.678557	-5.223673	4.826443	C	0.843968	-2.033496	4.765027
C	-6.767628	-5.482758	5.668283	C	0.538427	-7.113198	2.361367
C	-7.667656	-4.508585	6.113907	O	1.537973	-7.982074	2.118642
C	-7.453578	-3.206539	5.657204	C	1.541799	-9.144211	2.948560
O	-4.428357	-3.527475	3.655486	C	-0.810665	-5.764741	0.808386
Y	-3.163026	-1.894482	3.167248	O	-0.998469	-6.891922	-0.025017
O	-1.371413	-2.718703	2.294125	C	-2.244246	-6.926988	-0.711969
C	-0.179343	-2.463112	1.816878	C	-2.225360	-6.025450	-1.944841
C	0.898578	-3.292372	1.818709	O	-0.276561	-7.293116	3.243147
C	2.245727	-2.822131	1.334381	C	-2.497281	-8.383208	-1.072910
C	-4.775074	-6.364151	4.328595	H	-5.880742	1.206040	4.636227
C	-3.322845	-6.151461	4.797519	H	-5.481535	0.549553	3.043755
C	-8.852116	-4.817656	7.039695	H	-3.954602	2.384477	3.742263
				H	-3.445420	1.440608	5.137556
				H	-2.363152	2.230453	1.933160

H	-1.940002	0.596163	1.407322	H	2.146304	-3.864213	6.120131
H	-7.148809	-0.902357	4.614660	H	1.036152	-3.741007	7.499773
H	-6.319137	-1.509778	3.175179	H	0.719486	-4.911350	6.222718
H	-6.924105	-6.505822	5.985335	H	2.247024	-1.744516	1.157837
H	-8.138568	-2.409932	5.943804	H	3.022174	-3.045028	2.080922
H	-6.903918	1.014992	-1.398472	H	2.572187	-3.312270	0.408891
H	-4.030079	3.258313	0.829857	H	-0.032712	-4.684616	3.149277
H	-5.671333	-0.088434	6.547642	H	1.714286	-4.872058	2.988119
H	-4.956246	-1.712372	6.478024	H	1.522023	-6.878254	-0.213762
H	-3.906851	-0.289979	6.359630	H	1.574405	-5.114003	-0.291552
H	-1.232740	2.034421	3.955792	H	2.656060	-5.984748	0.814714
H	-1.363757	0.522733	4.895929	H	-0.255626	-0.026842	-0.360234
H	-0.663159	0.501785	3.257267	H	0.155829	-1.730409	-0.687829
H	-5.402822	-3.297133	-1.669185	H	-1.500854	-1.292706	-0.169741
H	-4.593109	-1.803164	-2.174981	H	-1.585793	-5.726987	1.586204
H	-4.231754	-2.515511	-0.587655	H	-0.849675	-4.824390	0.240357
H	-7.228654	-3.243380	0.083205	H	-3.038215	-6.584106	-0.027963
H	-6.060010	-2.562911	1.223704	H	2.396239	-9.738458	2.623306
H	-7.612102	-1.739745	0.933748	H	1.644886	-8.869784	4.002024
H	-7.589229	-2.304350	-2.105874	H	0.614024	-9.708850	2.825445
H	-8.123895	-0.784226	-1.385261	H	-3.187125	-6.064604	-2.466810
H	-6.868661	-0.784130	-2.642979	H	-2.036756	-4.981350	-1.678715
H	-7.684769	4.374899	-2.201744	H	-1.441711	-6.351005	-2.637094
H	-7.028310	2.819184	-2.719429	H	-3.452410	-8.494792	-1.595534
H	-8.151964	2.899136	-1.348542	H	-1.700346	-8.753837	-1.726257
H	-7.020610	5.459039	-0.090809	H	-2.516095	-9.002327	-0.171869
H	-7.423539	4.003827	0.840332				
H	-5.818284	4.733323	0.984301				
H	-5.409303	5.322907	-2.051679	YT3RS_TLff.xyz			
H	-4.172241	4.601884	-1.013197	149			
H	-4.665752	3.773898	-2.495046	scf done: -2856.899598			
H	-2.661064	-6.915786	4.378552	C	-6.554698	-2.930400	4.775392
H	-2.946878	-5.178905	4.476256	C	-5.637607	-3.913139	4.331941
H	-3.259573	-6.213470	5.890794	C	-5.849058	-5.268861	4.698227
H	-4.547235	-8.505877	4.452823	C	-6.955917	-5.559775	5.505156
H	-5.186691	-7.802955	5.940073	C	-7.864184	-4.602842	5.971280
H	-6.237362	-7.994705	4.520027	C	-7.633879	-3.281648	5.583422
H	-4.176930	-7.220054	2.419223	O	-4.604966	-3.525929	3.583714
H	-5.844254	-6.612851	2.441269	Y	-3.297638	-1.918262	3.220252
H	-4.489118	-5.472057	2.352819	O	-1.659892	-2.939506	1.811494
H	-9.779975	-6.472863	8.083958	C	-0.529527	-2.880933	1.314868
H	-9.059371	-6.942149	6.540755	C	0.736470	-3.260816	2.049682
H	-8.025400	-6.633539	7.949054	C	1.978037	-3.012554	1.185826
H	-9.564598	-4.194178	9.008523	C	-4.897983	-6.378982	4.225542
H	-7.797427	-4.259717	8.872172	C	-3.485008	-6.131422	4.790611
H	-8.694371	-2.922973	8.138444	C	-9.066553	-4.947243	6.860687
H	-11.028602	-4.646298	6.988659	C	-10.370445	-4.530947	6.151550
H	-10.201281	-3.376500	6.076570	C	-6.412857	-1.509366	4.304960
H	-10.298109	-5.011878	5.413054	N	-5.126679	-0.833010	4.650738
H	1.905026	-2.058506	4.541240	C	-5.221290	0.569890	4.204498
H	0.243006	-1.300787	4.244279	C	-3.895529	1.311375	4.276078
H	-3.535297	-3.732282	6.543819	N	-2.817153	0.663848	3.495549
H	-2.958553	-4.242183	8.159338	C	-1.529227	0.901418	4.171771
H	-3.136264	-2.502349	7.783698	O	-4.084335	-1.068056	1.377222

C	-4.555899	0.064850	0.869572	H	-4.921220	-1.954510	6.410806
C	-3.953964	1.282083	1.280550	H	-3.913101	-0.500172	6.352209
C	-4.445446	2.508045	0.838496	H	-1.352643	1.978050	4.325299
C	-5.534748	2.591699	-0.031387	H	-1.507313	0.380047	5.129378
C	-6.085534	1.379183	-0.460594	H	-0.712144	0.507995	3.562987
C	-5.634283	0.114985	-0.057553	H	-5.649587	-2.923115	-1.747005
C	-2.708474	1.239547	2.120734	H	-4.732562	-1.457749	-2.143330
C	-6.276460	-1.164394	-0.624601	H	-4.429175	-2.313980	-0.611963
C	-6.924234	-1.997076	0.497603	H	-7.413691	-2.883368	0.076432
C	-6.057908	3.960810	-0.485943	H	-6.179209	-2.337574	1.218412
C	-4.938182	4.725572	-1.219164	H	-7.689453	-1.414297	1.023241
O	-1.770144	-2.143455	4.735467	H	-7.770108	-1.803903	-2.046869
C	-0.686946	-2.653379	5.262638	H	-8.207631	-0.302132	-1.230746
C	0.549276	-2.748846	4.693165	H	-6.982050	-0.294530	-2.516705
C	1.695571	-3.326940	5.489061	H	-7.597999	4.842080	-1.727652
O	-0.793009	-3.150120	6.538504	H	-6.995612	3.305658	-2.356853
C	-2.008533	-2.953324	7.228427	H	-8.100724	3.327618	-0.968724
C	-7.369212	-0.860058	-1.662055	H	-6.874799	5.761982	0.441754
C	-5.199768	-2.016757	-1.324371	H	-7.310587	4.260728	1.280377
C	-7.255861	3.842548	-1.438414	H	-5.681862	4.930985	1.448590
C	-6.505581	4.774879	0.744418	H	-5.293895	5.709169	-1.548121
C	-5.339993	-7.773299	4.696007	H	-4.067470	4.885807	-0.575493
C	-4.852232	-6.410607	2.683910	H	-4.602163	4.171948	-2.102162
C	-4.892296	-0.909744	6.098898	H	-2.787863	-6.888810	4.416929
C	-9.153465	-6.447458	7.173306	H	-3.109058	-5.150217	4.497481
C	-8.953148	-4.188092	8.197680	H	-3.496216	-6.182759	5.885783
O	-0.337970	-2.408583	0.092804	H	-4.630423	-8.517843	4.319829
C	-1.499502	-2.036664	-0.674414	H	-5.354200	-7.857223	5.788459
C	0.626871	-4.709351	2.594499	H	-6.332155	-8.041198	4.316073
C	0.677020	-5.962202	1.665716	H	-4.140328	-7.172766	2.346950
C	2.075668	-6.256497	1.095902	H	-5.838874	-6.658813	2.275803
C	0.810628	-2.248646	3.309005	H	-4.546421	-5.445050	2.278420
C	0.253657	-7.112963	2.592411	H	-10.022172	-6.641804	7.811775
O	1.269491	-7.524940	3.373245	H	-9.271177	-7.047429	6.264685
C	0.938288	-8.550706	4.313588	H	-8.266005	-6.804613	7.706582
C	-0.356976	-5.903676	0.537082	H	-9.811630	-4.410975	8.842616
O	-0.253222	-7.080906	-0.233983	H	-8.041883	-4.475137	8.733252
C	-1.478004	-7.574542	-0.767099	H	-8.923718	-3.104310	8.046604
C	-1.984356	-6.701279	-1.912323	H	-11.240939	-4.763191	6.776733
O	-0.862724	-7.578036	2.669710	H	-10.391416	-3.457535	5.938404
C	-1.203076	-9.002539	-1.210276	H	-10.482570	-5.060717	5.199814
H	-5.962813	1.113935	4.815669	H	1.830685	-1.846377	3.275144
H	-5.587289	0.573215	3.174719	H	0.149156	-1.403349	3.084414
H	-4.052119	2.344944	3.933805	H	-2.860066	-3.386502	6.694410
H	-3.564578	1.375761	5.316842	H	-1.889375	-3.462452	8.187488
H	-2.311505	2.264460	2.207705	H	-2.207395	-1.890225	7.413479
H	-1.938799	0.645426	1.608189	H	2.656945	-3.012852	5.064515
H	-7.242560	-0.914272	4.720874	H	1.668568	-2.991971	6.531053
H	-6.497094	-1.460877	3.213288	H	1.704903	-4.426540	5.522010
H	-7.114908	-6.593244	5.784728	H	2.102889	-1.942382	0.992580
H	-8.313541	-2.493333	5.903358	H	2.865773	-3.364443	1.719366
H	-6.916651	1.417569	-1.152368	H	1.934502	-3.513772	0.217792
H	-3.948862	3.415380	1.179182	H	-0.296938	-4.747338	3.181048
H	-5.667132	-0.358810	6.656598	H	1.440503	-4.827230	3.314902

H	2.089239	-7.247845	0.638365
H	2.345177	-5.537610	0.320294
H	2.835244	-6.226425	1.880224
H	-1.118160	-1.450760	-1.509590
H	-1.990019	-2.940986	-1.041650
H	-2.207105	-1.465617	-0.071471
H	-1.360875	-5.807657	0.971291
H	-0.158744	-5.020735	-0.090177
H	-2.227578	-7.586744	0.039928
H	1.865515	-8.781037	4.838389
H	0.178733	-8.198498	5.016193
H	0.558039	-9.436523	3.798789
H	-2.915013	-7.103947	-2.325356
H	-2.189097	-5.679769	-1.575780
H	-1.239571	-6.656735	-2.714182
H	-2.113014	-9.468754	-1.600127
H	-0.441636	-9.018042	-1.997130
H	-0.840213	-9.595440	-0.366707

YT3SR_TRB.xyz

149

scf done: -2856.881844

C	-6.969552	-5.519816	5.137813
C	-6.498923	-4.273344	4.635161
C	-7.062246	-3.082078	5.161584
C	-7.995644	-3.131125	6.194925
C	-8.438666	-4.337039	6.739343
C	-7.911120	-5.501395	6.174677
O	-5.561542	-4.184436	3.688925
Y	-4.174361	-2.830859	2.780229
O	-2.966352	-3.946047	1.295651
C	-2.020853	-4.758209	0.979175
C	-0.756578	-4.407337	0.513266
C	-0.530454	-3.024633	-0.030379
C	-0.534716	-2.879580	-1.584381
C	0.792028	-3.406387	-2.134248
O	0.645886	-4.308700	-3.118465
C	1.867388	-4.791389	-3.681175
C	-6.750216	-1.748484	4.540289
N	-5.321174	-1.327484	4.555847
C	-5.255164	0.044738	4.021382
C	-3.840324	0.475862	3.677241
N	-3.197378	-0.397396	2.671122
C	-1.740899	-0.375289	2.889954
C	-9.470401	-4.343102	7.874940
C	-9.817854	-5.763620	8.340384
C	-6.495608	-6.857888	4.547913
C	-7.205289	-8.069980	5.172862
O	-5.391815	-1.916237	1.286459
C	-5.751482	-0.763245	0.737719
C	-6.993694	-0.579591	0.073555
C	-7.313562	0.714844	-0.356879
C	-6.474687	1.825395	-0.209401

C	-5.224803	1.592612	0.369683
C	-4.853057	0.330006	0.826280
C	-7.927298	-1.766752	-0.217257
C	-9.175775	-1.345967	-1.008767
C	-3.437935	0.091062	1.277117
C	-6.857804	3.236254	-0.676275
C	-8.270861	3.290770	-1.272752
O	-2.458565	-3.251775	4.315070
C	-1.683904	-4.211696	4.597722
C	-0.545686	-4.654906	3.848817
C	0.195961	-5.886198	4.304326
O	-1.863192	-4.896063	5.737401
C	-2.909334	-4.478376	6.612217
C	-6.807728	4.205247	0.521632
C	-5.864870	3.713083	-1.754903
C	-7.165503	-2.805520	-1.066894
C	-8.412589	-2.429554	1.085933
C	-4.789396	-1.375160	5.922626
C	-6.802585	-6.887677	3.037002
C	-4.987710	-7.037957	4.805417
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C	-10.769193	-3.665989	7.394027
O	-2.220103	-6.083176	1.180543
C	-3.553336	-6.518637	1.408678
C	0.234145	-5.482656	0.149263
C	-0.523975	-1.371289	-1.888977
O	-0.404007	-1.187088	-3.280283
C	-0.173291	0.154752	-3.696429
C	-1.440283	1.002311	-3.601294
C	-1.764101	-3.532374	-2.216164
C	0.356381	0.075284	-5.119773
O	1.877107	-3.039390	-1.731674
C	-0.127240	-3.905357	2.772945
H	-5.678787	0.758388	4.749670
H	-5.876614	0.090934	3.124869
H	-3.859036	1.517999	3.323950
H	-3.219078	0.461275	4.578369
H	-2.870900	1.027214	1.144748
H	-2.978993	-0.658716	0.618842
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H	-8.254649	-6.453914	6.556399
H	-8.394238	-2.188440	6.566299
H	-8.270530	0.861540	-0.840791
H	-4.505817	2.405853	0.458550
H	-5.288635	-0.635452	6.570018
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H	-1.348536	0.654197	2.876134
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H	-1.241475	-0.933199	2.095007
H	-7.806994	-3.671495	-1.270740
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H	-6.269090	-3.152051	-0.548895

H	-9.111561	-3.242535	0.855658	H	1.576457	-5.500543	-4.456368
H	-7.580300	-2.852168	1.650335	H	2.476310	-5.284850	-2.919071
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H	-9.785834	-2.232229	-1.213148	H	0.603901	0.595508	-3.047779
H	-9.801494	-0.640246	-0.450844	H	-1.246956	2.022230	-3.949644
H	-8.921222	-0.893790	-1.973541	H	-1.812707	1.069457	-2.574692
H	-8.503980	4.316277	-1.579128	H	-2.230882	0.569014	-4.222447
H	-8.363938	2.653923	-2.158821	H	0.591509	1.072957	-5.502795
H	-9.030999	2.981100	-0.547528	H	-0.391794	-0.380188	-5.776529
H	-7.068997	5.222671	0.207294	H	1.261931	-0.536099	-5.155635
H	-7.513338	3.898349	1.301125				
H	-5.810024	4.242790	0.970809				
H	-6.120365	4.723701	-2.095246	YT3SR_TRBb.xyz			
H	-4.837883	3.740076	-1.377122	149			
H	-5.882584	3.046420	-2.623320	scf done: -2856.915090			
H	-4.620430	-7.954929	4.328831	C	-7.003789	-5.658939	5.081197
H	-4.415395	-6.193765	4.418642	C	-6.633255	-4.357416	4.644955
H	-4.792516	-7.121221	5.880449	C	-7.386354	-3.250297	5.105896
H	-6.839691	-8.984677	4.693432	C	-8.444389	-3.426145	5.994617
H	-7.005102	-8.162696	6.245972	C	-8.818601	-4.689358	6.455505
H	-8.290011	-8.033653	5.025857	C	-8.077664	-5.772953	5.972368
H	-6.428285	-7.816933	2.589895	O	-5.612471	-4.137770	3.819237
H	-7.884684	-6.849037	2.870440	Y	-4.155033	-2.689293	3.251677
H	-6.352339	-6.038856	2.521067	O	-3.019644	-4.167858	1.748096
H	-10.549832	-5.717312	9.153898	C	-1.971145	-4.665765	1.329489
H	-10.258770	-6.359742	7.534354	C	-0.729829	-3.856172	0.997058
H	-8.937441	-6.295290	8.716994	C	-1.080412	-2.758276	-0.044500
H	-9.642664	-3.548980	9.902102	C	-1.247971	-3.112561	-1.542305
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H	-8.677434	-2.529446	8.826493	O	0.207776	-4.469977	-2.894299
H	-11.519015	-3.656323	8.194111	C	1.467477	-4.692354	-3.533375
H	-10.596133	-2.629635	7.087664	C	-7.094017	-1.877516	4.571700
H	-11.192215	-4.199830	6.536700	N	-5.708275	-1.371164	4.798820
H	0.856553	-4.078495	2.350528	C	-5.667452	0.025061	4.324727
H	-0.570045	-2.934531	2.596130	C	-4.269822	0.619473	4.334622
H	-2.896887	-5.189349	7.438360	N	-3.290182	-0.192539	3.578242
H	-3.878485	-4.506568	6.110157	C	-1.990927	-0.141480	4.273633
H	-2.716959	-3.469206	6.986806	C	-9.996923	-4.841881	7.426455
H	0.552791	-5.787005	5.335272	C	-10.232669	-6.302867	7.833684
H	1.061453	-6.060833	3.660032	C	-6.263171	-6.908450	4.581362
H	-0.432972	-6.782116	4.269485	C	-6.852698	-8.211516	5.143011
H	1.258482	-5.097803	0.221906	O	-4.875618	-1.696018	1.488033
H	0.104385	-5.842748	-0.880777	C	-5.108434	-0.505305	0.950893
H	0.143396	-6.349440	0.807108	C	-6.148280	-0.278876	0.007306
H	-1.321668	-2.368326	0.349164	C	-6.346543	1.032926	-0.442497
H	0.433469	-2.627714	0.321422	C	-5.579082	2.130609	-0.037122
H	-1.802490	-3.323403	-3.286670	C	-4.539621	1.868489	0.858468
H	-2.670398	-3.135114	-1.747252	C	-4.291475	0.585845	1.343579
H	-1.759173	-4.615133	-2.074033	C	-7.013298	-1.435223	-0.523486
H	-3.488046	-7.596373	1.563294	C	-8.033972	-0.969079	-1.573199
H	-4.185837	-6.309902	0.539128	C	-3.077985	0.343409	2.199248
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H	-1.457028	-0.930778	-1.502119	O	-2.406222	-3.176926	4.410242

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O	-1.130596	-4.599354	5.651487	H	-5.261094	4.508443	1.353755
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C	-6.099151	4.491929	0.649891	H	-3.685903	4.059526	-0.654753
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C	-6.111169	-2.491750	-1.191702	H	-4.243111	-7.729796	4.650170
C	-7.802499	-2.093063	0.624727	H	-4.297041	-5.950506	4.637520
C	-5.353303	-1.468342	6.221527	H	-4.707420	-6.846285	6.109855
C	-6.365555	-6.983232	3.044730	H	-6.291775	-9.062388	4.740765
C	-4.786164	-6.849359	5.016921	H	-6.781651	-8.260761	6.235048
C	-9.723720	-4.028191	8.706648	H	-7.901913	-8.346384	4.858801
C	-11.283727	-4.317962	6.757953	H	-5.824391	-7.861873	2.670605
O	-1.855623	-5.965570	1.133557	H	-7.412120	-7.080208	2.735388
C	-2.995053	-6.779548	1.457972	H	-5.954187	-6.085258	2.580643
C	0.440067	-4.734529	0.547715	H	-11.076896	-6.361714	8.529071
C	-1.771153	-1.827118	-2.220099	H	-10.472549	-6.932966	6.970614
O	-1.812291	-2.037311	-3.612442	H	-9.359004	-6.730421	8.337268
C	-1.990395	-0.860680	-4.396373	H	-10.561389	-4.119262	9.408429
C	-3.419189	-0.330099	-4.309084	H	-8.818377	-4.384813	9.209254
C	-2.235381	-4.253643	-1.797183	H	-9.587945	-2.963873	8.489850
C	-1.602021	-1.234166	-5.818336	H	-12.139426	-4.413118	7.437257
O	1.062561	-2.577596	-2.034305	H	-11.194882	-3.262752	6.480755
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H	-4.321123	1.640547	3.931250	H	-1.662014	-4.956665	7.553727
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H	-2.519595	1.290594	2.281344	H	-1.816699	-3.243741	7.084147
H	-2.410168	-0.370872	1.698434	H	1.164425	-4.713508	4.983568
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H	-7.254017	-1.848548	3.486779	H	0.996183	-5.695532	3.537693
H	-8.351127	-6.765801	6.305532	H	1.310850	-4.099653	0.360182
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H	-7.145007	1.205354	-1.152690	H	0.704701	-5.461969	1.316159
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H	-2.070022	-0.618251	5.251989	H	-2.699354	-7.798492	1.212295
H	-1.237677	-0.689265	3.706360	H	-3.859233	-6.473058	0.865757
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149

scf done: -2856.885757

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H	-9.617468	-6.109822	9.812312	C	-0.229378	-3.012420	2.121170
H	-9.575379	-6.728494	8.158453	C	1.032996	-3.067035	2.721066
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H	-7.195634	-4.234637	9.687022	C	-3.192345	-6.057302	5.200738
H	-8.088150	-2.785855	9.201254	C	-9.088683	-5.216105	6.269084
H	-10.902071	-4.130411	9.064338	C	-10.266208	-4.870883	5.335887
H	-10.272840	-3.036884	7.824244	C	-6.251900	-1.580485	4.262988
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H	-1.093172	-3.425446	2.703549	C	-3.933433	1.365377	4.630403
H	-3.446452	-5.140241	7.769999	N	-2.793544	0.797774	3.878386
H	-4.283437	-4.606302	6.278959	C	-1.538228	1.096001	4.592446
H	-3.474376	-3.407994	7.334927	O	-3.977561	-0.949674	1.728743
H	0.473760	-4.697341	6.358232	C	-4.412821	0.170304	1.164491
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H	-0.116193	-6.176863	5.612232	C	-4.366486	2.614938	1.143263
H	0.472130	-5.820657	-0.267741	C	-5.388901	2.671686	0.193143
H	-0.671632	-5.854308	-1.602608	C	-5.855914	1.446276	-0.293927
H	-1.065323	-6.692822	-0.095790	C	-5.394874	0.194547	0.135825
H	-1.123326	-2.448613	0.298397	C	-2.664853	1.394986	2.511551
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H	-1.842827	-2.518831	-3.442625	C	-6.579577	-2.031480	0.475232
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H	-2.222924	-3.948289	-2.461472	C	-4.777799	4.836319	-0.930993
H	-4.482098	-7.082772	0.766398	O	-1.866517	-2.071733	5.516740
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H	-4.903158	-5.357453	0.680885	C	0.141565	-3.399136	5.764685
H	0.897558	-1.250765	-1.196282	C	1.320852	-3.638000	6.676213
H	-0.805614	-0.712118	-1.241345	O	-0.688261	-2.041917	7.439659
H	0.726235	-5.359879	-5.123069	C	-1.708569	-1.254934	8.037300
H	1.624322	-5.708849	-3.609306	C	-6.897266	-0.822533	-1.665390
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H	0.558330	2.442534	-3.030986	C	-6.490031	4.813655	0.907773
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				O	-0.481001	-4.003652	1.230596
				C	-1.732250	-3.984241	0.552407
				C	1.558259	-1.856985	3.444301
				C	2.413752	-0.827989	2.628790
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149							
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149

scf done: -2856.884082

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O	-1.075740	-2.322317	2.777228

C	-0.163800	-3.171052	2.363561	C	1.520510	2.785448	-0.799499
C	1.187677	-3.026364	2.457354	H	-5.960088	1.038664	5.089758
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C	-3.302517	-6.153270	5.301654	H	-3.611871	1.253096	5.877039
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C	-10.358066	-4.814239	5.095360	H	-1.671214	0.754931	2.274803
C	-6.215760	-1.598116	4.264416	H	-7.147200	-1.055736	4.498387
N	-5.076510	-0.890091	4.914838	H	-6.051871	-1.508974	3.184888
C	-5.144127	0.534335	4.542575	H	-7.032245	-6.742255	5.450372
C	-3.840921	1.274384	4.806363	H	-8.374500	-2.689127	5.360879
N	-2.685887	0.693921	4.088676	H	-6.255981	1.493829	-1.034800
C	-1.450439	0.954256	4.851908	H	-3.674475	3.485425	1.724880
O	-3.810321	-0.999955	1.854821	H	-6.106222	-0.661636	6.765024
C	-4.193575	0.136421	1.287082	H	-5.080722	-2.108938	6.625020
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C	-4.111904	2.578912	1.308819	H	-1.323674	2.030232	5.048824
C	-5.081146	2.665064	0.306447	H	-1.485209	0.423654	5.806079
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C	-5.114613	0.190221	0.205267	H	-4.640368	-2.735611	-1.590468
C	-2.494396	1.313443	2.738396	H	-3.840363	-1.171289	-1.834888
C	-5.580379	-1.085670	-0.517006	H	-3.629312	-2.042768	-0.303975
C	-6.321892	-2.038339	0.439401	H	-6.679167	-2.918087	-0.109339
C	-5.569939	4.034449	-0.183792	H	-5.667138	-2.383597	1.240195
C	-4.384368	4.831197	-0.763914	H	-7.195860	-1.546510	0.881911
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C	-1.029699	-2.571498	6.619671	H	-7.458342	-0.307255	-1.354468
C	0.092056	-3.470150	6.282239	H	-6.063979	-0.141471	-2.443003
C	1.257317	-3.538251	7.233014	H	-6.968803	4.914362	-1.583831
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C	-5.035112	-7.844228	4.769543	H	-3.597546	4.989130	-0.019524
C	-4.156591	-6.421998	2.939063	H	-3.937755	4.302335	-1.612421
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C	-1.579894	-4.249687	0.804369	H	-5.288748	-7.953928	5.829787
C	1.760098	-1.814682	3.142502	H	-5.908743	-8.131728	4.174393
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C	3.686495	-1.124342	1.571949	H	-5.027121	-6.660132	2.317528
C	-0.003385	-4.229075	5.179072	H	-3.774566	-5.446580	2.637479
C	2.581051	0.515921	3.162058	H	-10.310585	-6.937256	6.777073
O	3.856468	0.926077	3.246970	H	-9.207637	-7.284555	5.441347
C	4.079274	2.059485	4.087252	H	-8.571025	-7.026689	7.077298
C	1.356820	-0.267010	1.186650	H	-10.436680	-4.720552	7.846925
O	1.882144	0.829691	0.467527	H	-8.687202	-4.702283	8.142722
C	1.003101	1.385803	-0.503977	H	-9.455559	-3.361606	7.281949
C	0.932319	0.522553	-1.761911	H	-11.339134	-5.086255	5.503106
O	1.685922	1.054694	3.786305	H	-10.370676	-3.740054	4.885929

H	-10.228090	-5.336762	4.141925	N	-5.190257	-0.832132	4.995573
H	0.778201	-4.936005	4.921899	C	-5.325863	0.613851	4.732113
H	-0.868339	-4.200662	4.530063	C	-4.081658	1.402264	5.108516
H	-2.079543	-0.419574	7.892832	N	-2.867320	0.949200	4.399203
H	-1.799203	-1.228342	9.461645	C	-1.687736	1.222865	5.245873
H	-2.986178	-1.902247	8.301186	O	-3.590167	-0.679840	1.970846
H	2.021697	-4.211987	6.839440	C	-4.090895	0.441324	1.467585
H	0.949725	-3.902075	8.218475	C	-3.752450	1.670387	2.089092
H	1.712727	-2.553842	7.382729	C	-4.327761	2.863717	1.659484
H	1.586075	-5.056467	1.847952	C	-5.232149	2.906545	0.594986
H	2.928306	-4.272413	2.706923	C	-5.499037	1.692730	-0.047389
H	2.605835	-3.881859	1.025838	C	-4.950394	0.461514	0.335066
H	0.973713	-1.347101	3.740798	C	-2.660123	1.699886	3.122881
H	2.551986	-2.131263	3.839403	C	-5.229728	-0.815139	-0.475571
H	4.114543	-0.301394	0.997255	C	-5.946150	-1.871537	0.387069
H	3.494074	-1.953029	0.887102	C	-5.855876	4.241033	0.164480
H	4.425175	-1.452962	2.308418	C	-4.744134	5.221964	-0.257405
H	-1.851477	-5.266752	0.516225	O	-1.738482	-1.919668	5.536817
H	-1.130501	-3.736218	-0.056158	C	-0.653729	-2.062486	6.257650
H	-2.486284	-3.711793	1.101973	C	0.401017	-2.865844	5.962748
H	0.413434	0.010009	1.678894	C	1.602725	-2.987222	6.858552
H	1.153634	-1.128920	0.536358	O	-0.596552	-1.282869	7.402098
H	-0.007305	1.461834	-0.066325	C	-1.582634	-1.610634	8.368139
H	5.150853	2.255049	4.042314	C	-6.113212	-0.549846	-1.704210
H	3.771447	1.847946	5.114832	C	-3.890747	-1.388776	-0.982135
H	3.517503	2.923885	3.724107	C	-6.820823	4.081521	-1.018316
H	0.265138	0.976282	-2.502045	C	-6.642821	4.845945	1.344215
H	0.550807	-0.479581	-1.545799	C	-4.866021	-7.728988	4.529947
H	1.927827	0.423321	-2.207156	C	-4.026651	-6.175611	2.789289
H	0.875434	3.293678	-1.522708	C	-5.229441	-1.110812	6.437516
H	2.532568	2.734149	-1.214522	C	-9.260494	-6.851177	6.067775
H	1.556850	3.380690	0.117070	C	-9.508642	-4.665538	7.232276
YT3SR_TRFf.xyz				O	-0.133982	-4.128223	1.413938
149				C	-1.246316	-4.263901	0.510200
scf done: -2856.906434				C	1.350882	-1.708836	3.530683
C	-6.453903	-2.995918	4.605341	C	2.073122	-0.906107	2.404472
C	-5.378700	-3.876971	4.335365	C	3.551862	-1.278940	2.234732
C	-5.566204	-5.268708	4.557306	C	0.335075	-3.737887	4.743287
C	-6.806873	-5.695724	5.045685	C	1.921910	0.563063	2.836873
C	-7.875818	-4.839716	5.330031	O	3.083226	1.158712	3.131036
C	-7.663755	-3.479531	5.096575	C	2.985490	2.525690	3.543375
O	-4.233216	-3.369717	3.887594	C	1.340300	-1.000481	1.058258
Y	-3.044669	-1.600349	3.843761	O	1.960576	-0.102989	0.165014
O	-1.290417	-2.589130	2.531679	C	1.273066	0.094462	-1.068601
C	-0.259568	-3.252931	2.399588	C	1.496746	-1.074284	-2.025452
C	0.921342	-3.188253	3.347518	O	0.850735	1.129772	2.931958
C	2.055415	-4.118690	2.902992	C	1.783182	1.408491	-1.638610
C	-4.442071	-6.275365	4.270585	H	-6.191648	1.021648	5.282550
C	-3.235152	-5.976920	5.181818	H	-5.529262	0.744718	3.666322
C	-9.226275	-5.329399	5.869959	H	-4.265427	2.470416	4.914104
C	-10.346028	-4.951453	4.880162	H	-3.894694	1.310561	6.183022
C	-6.312813	-1.530809	4.301945	H	-2.456177	2.752060	3.382379
				H	-1.735011	1.301113	2.689671
				H	-7.255745	-1.024843	4.566568

H	-6.152082	-1.374040	3.228430
H	-6.944115	-6.756225	5.213801
H	-8.460216	-2.762857	5.291359
H	-6.167622	1.703293	-0.898647
H	-4.041154	3.783156	2.167778
H	-6.183017	-0.782155	6.881208
H	-5.120808	-2.183535	6.605094
H	-4.411221	-0.596296	6.944239
H	-1.648434	2.287917	5.527430
H	-1.707769	0.604313	6.143825
H	-0.778178	0.991930	4.688294
H	-4.062859	-2.316542	-1.542285
H	-3.394917	-0.676331	-1.651052
H	-3.226514	-1.598585	-0.141278
H	-6.160674	-2.766487	-0.210179
H	-5.333467	-2.170976	1.238628
H	-6.902365	-1.485030	0.758141
H	-6.249579	-1.484880	-2.258578
H	-7.109375	-0.187221	-1.427385
H	-5.661004	0.175563	-2.389365
H	-7.247515	5.055441	-1.281651
H	-6.313121	3.693169	-1.907654
H	-7.652603	3.410313	-0.778999
H	-7.086976	5.807927	1.061276
H	-7.451658	4.177047	1.657460
H	-5.999210	5.019779	2.212581
H	-5.172777	6.184864	-0.560429
H	-4.040554	5.414127	0.558704
H	-4.173044	4.822096	-1.101802
H	-2.408772	-6.663650	4.959088
H	-2.885113	-4.951913	5.049890
H	-3.506916	-6.110955	6.234896
H	-4.027738	-8.395125	4.297617
H	-5.137561	-7.899542	5.577380
H	-5.710719	-8.031026	3.901146
H	-3.191727	-6.856676	2.580911
H	-4.861319	-6.454245	2.136323
H	-3.727993	-5.154169	2.546495
H	-10.240036	-7.151058	6.455829
H	-9.100030	-7.388117	5.126780
H	-8.504454	-7.185535	6.786240
H	-10.474623	-4.997239	7.631744
H	-8.732239	-4.924222	7.960145
H	-9.539867	-3.574349	7.152071
H	-11.321208	-5.287226	5.253004
H	-10.403075	-3.869202	4.727055
H	-10.175806	-5.416360	3.903440
H	0.883870	-4.664327	4.948652
H	-0.707132	-4.030247	4.584659
H	-2.591930	-1.565239	7.945174
H	-1.492946	-0.880723	9.176099
H	-1.416077	-2.618299	8.773057
H	1.751739	-4.024750	7.191269
H	1.498342	-2.357842	7.743960

H	2.535907	-2.692838	6.354339
H	1.727277	-5.161611	2.927928
H	2.900261	-4.014767	3.590225
H	2.405577	-3.914390	1.889270
H	0.451955	-1.155198	3.811085
H	2.002457	-1.680840	4.409033
H	4.035783	-0.592530	1.538715
H	3.656133	-2.288964	1.836198
H	4.083074	-1.230610	3.188869
H	-0.922805	-4.990777	-0.233531
H	-1.474209	-3.304056	0.044080
H	-2.125722	-4.625974	1.044491
H	0.282126	-0.733492	1.194095
H	1.396320	-2.035013	0.685683
H	0.194407	0.188626	-0.858455
H	4.009008	2.850560	3.729399
H	2.384928	2.611579	4.452370
H	2.527173	3.130441	2.757260
H	0.965925	-0.906297	-2.968030
H	1.134428	-2.018542	-1.607473
H	2.563911	-1.184376	-2.244429
H	1.280104	1.642397	-2.581637
H	2.860106	1.347626	-1.826693
H	1.601959	2.224700	-0.934380

YT3SS_TLB.xyz

149

scf done: -2856.872567

C	-6.180127	-0.017532	-0.012369
C	-4.977407	0.084824	0.739098
C	-4.345216	1.350398	0.846105
C	-4.941137	2.490668	0.312303
C	-6.161507	2.434123	-0.365222
C	-6.732158	1.165795	-0.520278
O	-4.419573	-0.948469	1.353478
Y	-3.115593	-1.497623	2.964898
O	-1.421077	-1.599182	4.556148
C	-0.251167	-1.916767	4.921202
O	0.296353	-1.284593	5.985806
C	-0.541321	-0.450562	6.770618
C	-2.954135	1.437023	1.413088
N	-2.737814	1.055817	2.844065
C	-1.334570	1.372210	3.162531
C	-6.797126	3.715912	-0.919948
C	-7.059350	4.701931	0.235812
C	-6.825857	-1.382683	-0.308415
C	-5.811564	-2.261082	-1.068951
O	-4.198640	-3.125050	3.788372
C	-5.135441	-3.437116	4.682146
C	-6.032737	-2.428330	5.113821
C	-7.010483	-2.708519	6.065892
C	-7.161407	-3.980587	6.620055
C	-6.276862	-4.965467	6.169241

C	-5.269815	-4.745489	5.221679	H	-1.135263	2.451714	3.067314
C	-6.002975	-1.063687	4.480874	H	-1.106442	1.054529	4.180775
N	-4.717857	-0.312671	4.592960	H	-0.674262	0.823307	2.487825
C	-4.290857	-0.247954	5.994965	H	-6.240371	-3.250733	-1.267980
C	-4.335322	-5.886426	4.790132	H	-5.556911	-1.805094	-2.032659
C	-4.413037	-6.087610	3.263133	H	-4.895523	-2.390154	-0.489114
C	-8.259531	-4.247587	7.657858	H	-7.738985	-3.046540	0.755096
C	-8.048203	-3.333285	8.881027	H	-6.373710	-2.318043	1.612956
O	-1.531404	-2.173272	1.527197	H	-7.947427	-1.486843	1.565025
C	-0.266775	-2.247117	1.398484	H	-8.480151	-2.258433	-1.385154
O	0.380649	-1.060026	1.569767	H	-8.874068	-0.682119	-0.695020
C	1.377873	-0.656617	0.622617	H	-7.865864	-0.792184	-2.153823
C	0.441050	-3.461059	1.296410	H	-8.552820	4.390775	-1.993997
C	1.948958	-3.494023	1.265476	H	-8.010652	2.784709	-2.490345
C	-0.314926	-4.653606	0.752221	H	-8.868457	2.998664	-0.951938
C	-0.190995	-4.972689	-0.776793	H	-7.503458	5.630835	-0.141473
C	-0.325178	-3.662564	-1.551215	H	-7.748320	4.269073	0.969044
O	0.612603	-2.972119	-1.901333	H	-6.135312	4.964990	0.760672
C	1.146624	-5.631862	-1.133325	H	-6.279277	5.291290	-2.341964
C	-2.892282	-5.547661	5.211365	H	-4.881418	4.633380	-1.481247
C	-4.700006	-7.229029	5.443078	H	-5.639043	3.693550	-2.773098
C	-9.638936	-3.951632	7.036486	H	-2.199499	-6.326842	4.869980
C	-8.260639	-5.702529	8.146683	H	-2.574891	-4.591429	4.793819
C	-4.934767	1.037866	4.039604	H	-2.816349	-5.485706	6.302941
C	-3.638387	1.784824	3.762232	H	-4.007778	-8.000304	5.087673
C	-7.241615	-2.097936	0.990540	H	-4.617775	-7.195887	6.535015
C	-8.081386	-1.257828	-1.185979	H	-5.713969	-7.552381	5.182990
C	-5.841493	4.371024	-1.936939	H	-3.730853	-6.889143	2.953467
C	-8.132643	3.447932	-1.627408	H	-5.427377	-6.376767	2.966112
C	0.595200	-2.921736	4.383881	H	-4.148461	-5.173815	2.729831
C	0.094997	-3.802713	3.426434	H	-9.058118	-5.844390	8.884094
C	1.984272	-3.085422	4.953666	H	-8.440191	-6.406468	7.327122
O	-1.601756	-3.312972	-1.758722	H	-7.314174	-5.971749	8.627721
C	-1.800225	-2.066220	-2.430020	H	-8.829721	-3.503492	9.631372
C	-1.337968	-5.936014	-1.117927	H	-7.077717	-3.527496	9.350201
O	-1.261831	-6.281888	-2.481066	H	-8.078571	-2.274377	8.605122
C	-2.226240	-7.237174	-2.911459	H	-10.438563	-4.131288	7.765191
C	-1.688032	-7.841495	-4.199419	H	-9.718667	-2.911785	6.704511
C	-3.601712	-6.602636	-3.104847	H	-9.819364	-4.592494	6.167169
H	-5.555063	1.639397	4.726876	H	0.630600	-4.740106	3.295386
H	-5.494188	0.932997	3.107346	H	-0.977261	-3.858885	3.266519
H	-3.880932	2.779440	3.359033	H	0.063044	-0.150144	7.627716
H	-3.097770	1.951236	4.699448	H	-0.855889	0.441699	6.220505
H	-2.591283	2.469768	1.280581	H	-1.428766	-0.991082	7.110913
H	-2.287242	0.784446	0.834371	H	1.961482	-3.253344	6.036446
H	-6.803508	-0.452935	4.930220	H	2.482216	-3.942573	4.491599
H	-6.215549	-1.137703	3.408572	H	2.616101	-2.205042	4.787125
H	-6.374954	-5.963479	6.576579	H	2.299232	-4.501334	1.516966
H	-7.678431	-1.902308	6.365478	H	2.368748	-3.244833	0.285399
H	-7.659558	1.089405	-1.072926	H	2.372285	-2.809160	2.005764
H	-4.421609	3.441856	0.419352	H	-1.376332	-4.514554	0.980160
H	-5.047273	0.254973	6.619371	H	0.011039	-5.562247	1.279140
H	-4.145611	-1.260078	6.376051	H	1.119581	-5.987881	-2.165374
H	-3.347889	0.294408	6.079251	H	1.981207	-4.939359	-1.033866

H 1.319736 -6.494040 -0.480092
H 2.381280 -0.763790 1.042519
H 1.296527 -1.231614 -0.302580
H 1.193531 0.400384 0.410659
H -1.236891 -6.837566 -0.487247
H -2.298163 -5.463286 -0.875139
H -2.877546 -1.965992 -2.552685
H -1.412790 -1.240964 -1.827807
H -1.295860 -2.069495 -3.399516
H -2.301644 -8.030739 -2.147164
H -4.327124 -7.352585 -3.437047
H -3.981383 -6.161636 -2.178736
H -3.548064 -5.813125 -3.861104
H -2.368458 -8.607909 -4.582969
H -1.577181 -7.064750 -4.962950
H -0.708287 -8.296405 -4.029892

YT3SS_TLBb.xyz

149

scf done: -2856.893850

C -6.137229 0.025243 -0.118294
C -4.927084 0.128861 0.622268
C -4.335334 1.408466 0.783521
C -4.968162 2.552263 0.302858
C -6.190747 2.488882 -0.370186
C -6.727375 1.212217 -0.571791
O -4.328698 -0.914451 1.178221
Y -3.122466 -1.479480 2.879844
O -1.409004 -1.590138 4.235675
C -0.146253 -1.650273 4.566075
O 0.283330 -0.646701 5.425884
C -0.311033 -0.709908 6.713747
C -2.952145 1.509803 1.365008
N -2.746524 1.084308 2.783241
C -1.348104 1.397183 3.131179
C -6.864187 3.773121 -0.871953
C -7.140458 4.711406 0.319571
C -6.755547 -1.343347 -0.453441
C -5.730481 -2.176848 -1.248476
O -4.265166 -3.124144 3.588012
C -5.176422 -3.458405 4.498432
C -6.050369 -2.455910 4.987734
C -6.995746 -2.753861 5.966392
C -7.136209 -4.039550 6.491794
C -6.280908 -5.019793 5.978046
C -5.308764 -4.782032 4.999157
C -6.025789 -1.077982 4.385535
N -4.732798 -0.338330 4.487286
C -4.273656 -0.304498 5.881497
C -4.412678 -5.920034 4.486802
C -4.571268 -6.066408 2.959767
C -8.194408 -4.325942 7.565372
C -7.932039 -3.440764 8.799913

O -1.451768 -2.246742 1.385699
C -0.212992 -2.235949 1.378551
O 0.318858 -1.040248 1.193610
C 1.711172 -0.705778 1.153985
C 0.523172 -3.541486 1.686970
C 2.015736 -3.635850 1.351127
C -0.263297 -4.715957 1.040780
C -0.274814 -4.962114 -0.501682
C -0.424397 -3.627322 -1.233044
O 0.486867 -2.824425 -1.343223
C 1.005201 -5.649043 -1.008762
C -2.944529 -5.615472 4.842042
C -4.764897 -7.278657 5.112517
C -9.595610 -4.010802 7.004875
C -8.182806 -5.791642 8.020672
C -4.950816 1.024853 3.964522
C -3.656347 1.784107 3.714342
C -7.145676 -2.104730 0.827425
C -8.020929 -1.219174 -1.316825
C -5.934405 4.487812 -1.872937
C -8.198972 3.496933 -1.577636
C 0.771198 -2.566637 4.144223
C 0.324601 -3.693601 3.246894
C 2.167706 -2.596377 4.711432
O -1.648369 -3.402126 -1.709708
C -1.839346 -2.136961 -2.355517
C -1.470698 -5.897390 -0.756811
O -1.478804 -6.305160 -2.102525
C -2.478514 -7.264932 -2.432384
C -2.033162 -7.917191 -3.732266
C -3.859491 -6.625283 -2.554539
H -5.577800 1.605433 4.663541
H -5.504806 0.939105 3.026601
H -3.903115 2.787116 3.334797
H -3.121475 1.930007 4.657928
H -2.610278 2.554106 1.270517
H -2.265442 0.891761 0.771414
H -6.812001 -0.471225 4.864354
H -6.260517 -1.128415 3.316147
H -6.373861 -6.028584 6.359308
H -7.645424 -1.950932 6.311522
H -7.658406 1.132239 -1.117852
H -4.476380 3.512970 0.449662
H -5.008019 0.199922 6.530229
H -4.135516 -1.325076 6.242307
H -3.319611 0.220274 5.951909
H -1.163129 2.483154 3.094553
H -1.105676 1.012961 4.122939
H -0.683399 0.907895 2.416227
H -6.142659 -3.166566 -1.479741
H -5.489002 -1.682328 -2.196601
H -4.810059 -2.307758 -0.676334
H -7.612600 -3.062923 0.568846
H -6.271616 -2.311522 1.446286

H	-7.871697	-1.531044	1.415272
H	-8.399395	-2.221647	-1.544553
H	-8.821881	-0.677431	-0.801393
H	-7.824114	-0.717762	-2.270727
H	-8.646148	4.441332	-1.906467
H	-8.068044	2.868276	-2.464809
H	-8.917033	3.004905	-0.912915
H	-7.610058	5.641724	-0.021859
H	-7.812775	4.236573	1.042219
H	-6.219084	4.978946	0.846718
H	-6.397142	5.412161	-2.239199
H	-4.976105	4.754747	-1.416196
H	-5.724742	3.846601	-2.735535
H	-2.283887	-6.396445	4.444879
H	-2.635331	-4.652583	4.433280
H	-2.810863	-5.582698	5.929170
H	-4.101910	-8.046688	4.698949
H	-4.630337	-7.282551	6.199792
H	-5.794853	-7.579741	4.891479
H	-3.915318	-6.863145	2.586982
H	-5.602924	-6.334541	2.705931
H	-4.324089	-5.135757	2.447169
H	-8.948865	-5.947019	8.788078
H	-8.400703	-6.476014	7.193839
H	-7.217835	-6.075413	8.454280
H	-8.684811	-3.625790	9.575665
H	-6.944859	-3.649086	9.226140
H	-7.968575	-2.375671	8.549903
H	-10.367050	-4.203423	7.760255
H	-9.683042	-2.963359	6.699598
H	-9.813151	-4.631069	6.129080
H	0.866379	-4.610952	3.517757
H	-0.737756	-3.891209	3.420348
H	0.008225	0.182027	7.258017
H	-1.403708	-0.730157	6.651206
H	0.027146	-1.602927	7.257111
H	2.275036	-1.868222	5.516988
H	2.406763	-3.591031	5.114136
H	2.954976	-2.372523	3.976118
H	2.330565	-4.670596	1.518827
H	2.218997	-3.386314	0.310061
H	2.630453	-3.014340	2.000401
H	-1.302247	-4.627076	1.371574
H	0.130886	-5.631585	1.498990
H	0.859325	-5.977606	-2.039716
H	1.868852	-4.987134	-0.975108
H	1.215272	-6.535192	-0.399959
H	2.185339	-0.933516	2.108783
H	2.204433	-1.207904	0.323188
H	1.726334	0.371985	0.989335
H	-1.366093	-6.775371	-0.094138
H	-2.400355	-5.382077	-0.482553
H	-2.861739	-2.151318	-2.728931
H	-1.710819	-1.324517	-1.637546

H	-1.126225	-2.015972	-3.174291
H	-2.506749	-8.031202	-1.637500
H	-4.607843	-7.378720	-2.821357
H	-4.179107	-6.159223	-1.618236
H	-3.848941	-5.855737	-3.332687
H	-2.741328	-8.692655	-4.039551
H	-1.974263	-7.168630	-4.529004
H	-1.045627	-8.371997	-3.615723

YT3SS_TLBf.xyz

149

scf done: -2856.879117

C	-6.037439	-0.141052	-0.104336
C	-4.864316	-0.043791	0.694454
C	-4.196385	1.206102	0.776451
C	-4.728222	2.337833	0.161972
C	-5.915542	2.288688	-0.571847
C	-6.523146	1.034136	-0.692807
O	-4.372060	-1.067538	1.379019
Y	-3.058489	-1.553499	2.995432
O	-1.465916	-1.594375	4.930081
C	-0.438060	-1.965927	5.505561
O	-0.064514	-1.437633	6.673806
C	-0.914664	-0.462648	7.276193
C	-2.837458	1.288620	1.418122
N	-2.726115	0.977804	2.879315
C	-1.351554	1.312446	3.292759
C	-6.479908	3.562194	-1.216014
C	-6.771499	4.606336	-0.119816
C	-6.727699	-1.493216	-0.359425
C	-5.732011	-2.444949	-1.052234
O	-4.082105	-3.210121	3.862007
C	-5.026864	-3.523794	4.745838
C	-5.961276	-2.530715	5.137758
C	-6.939532	-2.813311	6.089211
C	-7.058523	-4.072459	6.679355
C	-6.147460	-5.045843	6.257600
C	-5.140219	-4.824407	5.310693
C	-5.978528	-1.188432	4.456662
N	-4.737103	-0.370436	4.579041
C	-4.380518	-0.212399	5.990758
C	-4.193929	-5.961599	4.893732
C	-4.283339	-6.188408	3.370817
C	-8.155224	-4.340866	7.718284
C	-7.974238	-3.389281	8.917685
O	-1.355182	-2.086319	1.810714
C	-0.116532	-2.116364	1.388161
O	0.545066	-0.915280	1.611397
C	1.190791	-0.308193	0.496855
C	0.525448	-3.191298	0.853398
C	2.019030	-3.207852	0.656074
C	-0.273944	-4.414334	0.486331
C	-0.344012	-4.772807	-1.036975

C	-0.508752	-3.472904	-1.822183	H	-7.511883	4.227106	0.592785
O	0.367633	-2.925549	-2.458074	H	-5.868699	4.865109	0.442944
C	0.913782	-5.497730	-1.524839	H	-5.838825	5.056063	-2.674298
C	-2.750157	-5.601356	5.290936	H	-4.508690	4.394550	-1.714885
C	-4.537374	-7.296537	5.573262	H	-5.230679	3.421865	-3.002733
C	-9.538602	-4.098026	7.083011	H	-2.055679	-6.386411	4.966963
C	-8.120770	-5.781786	8.246041	H	-2.446920	-4.658455	4.835409
C	-4.985587	0.939783	3.947568	H	-2.663695	-5.503842	6.379460
C	-3.707649	1.727828	3.692160	H	-3.839359	-8.065969	5.225342
C	-7.205760	-2.133824	0.956579	H	-4.446920	-7.243166	6.663880
C	-7.954533	-1.359403	-1.275734	H	-5.549384	-7.636072	5.327059
C	-5.452545	4.141793	-2.208125	H	-3.593494	-6.985350	3.066651
C	-7.784240	3.300917	-1.981678	H	-5.296581	-6.495159	3.088356
C	0.514399	-3.008978	5.069944	H	-4.034521	-5.279852	2.820971
C	0.206741	-3.756659	3.999032	H	-8.917199	-5.924357	8.984443
C	1.769803	-3.205476	5.876705	H	-8.278924	-6.512071	7.445381
O	-1.746687	-2.960716	-1.698700	H	-7.169567	-6.013462	8.737230
C	-1.968003	-1.727557	-2.383573	H	-8.754892	-3.559495	9.668945
C	-1.567506	-5.679524	-1.236855	H	-7.001639	-3.546212	9.396501
O	-1.666324	-6.032111	-2.598463	H	-8.030415	-2.339273	8.613198
C	-2.628331	-7.035741	-2.896724	H	-10.337166	-4.281308	7.811934
C	-2.290162	-7.551201	-4.287516	H	-9.644922	-3.069384	6.724526
C	-4.057139	-6.502246	-2.814690	H	-9.696474	-4.765078	6.229184
H	-5.663057	1.547084	4.573239	H	0.869529	-4.552160	3.674427
H	-5.494611	0.763257	2.997510	H	-0.700042	-3.603920	3.427885
H	-3.969306	2.678102	3.204965	H	-0.425991	-0.187202	8.210270
H	-3.231466	1.985178	4.643631	H	-1.014791	0.415491	6.633551
H	-2.443483	2.305728	1.259500	H	-1.901322	-0.885829	7.474142
H	-2.150112	0.593530	0.918623	H	1.543701	-3.479779	6.911961
H	-6.823048	-0.603864	4.857998	H	2.377767	-3.997741	5.434277
H	-6.152741	-1.310745	3.382317	H	2.371333	-2.291404	5.912549
H	-6.225853	-6.036572	6.686345	H	2.414315	-4.207667	0.876709
H	-7.635584	-2.019898	6.357641	H	2.331415	-2.966092	-0.368335
H	-7.427538	0.962693	-1.283004	H	2.517399	-2.506944	1.332549
H	-4.182970	3.276230	0.252479	H	-1.296914	-4.272684	0.847750
H	-5.183476	0.293823	6.551979	H	0.129111	-5.306486	0.992632
H	-4.218703	-1.196728	6.433467	H	0.782667	-5.821385	-2.559344
H	-3.464383	0.372480	6.086118	H	1.793491	-4.856759	-1.478349
H	-1.143423	2.386690	3.162773	H	1.089630	-6.385324	-0.906729
H	-1.210706	1.051758	4.344211	H	2.280386	-0.364524	0.594273
H	-0.638543	0.731508	2.700891	H	0.898499	-0.793086	-0.439177
H	-6.189786	-3.430635	-1.199231	H	0.897651	0.747903	0.470462
H	-5.451273	-2.057818	-2.038063	H	-1.438867	-6.583320	-0.614360
H	-4.826684	-2.570997	-0.455168	H	-2.468902	-5.157318	-0.891333
H	-7.754179	-3.059892	0.746768	H	-2.979751	-1.420421	-2.123224
H	-6.360645	-2.381628	1.599287	H	-1.246012	-0.971575	-2.064868
H	-7.882181	-1.461768	1.497415	H	-1.872114	-1.867461	-3.464024
H	-8.386391	-2.352052	-1.442807	H	-2.513883	-7.860455	-2.170300
H	-8.736551	-0.732397	-0.832734	H	-4.775255	-7.287151	-3.074339
H	-7.695941	-0.946712	-2.256910	H	-4.303117	-6.147839	-1.809588
H	-8.153456	4.237295	-2.413692	H	-4.187474	-5.668396	-3.511968
H	-7.638498	2.593783	-2.805220	H	-2.972286	-8.355037	-4.581054
H	-8.569013	2.906987	-1.327077	H	-2.373348	-6.741834	-5.019988
H	-7.164993	5.530394	-0.559893	H	-1.265921	-7.932822	-4.315842

YT3SS_TLF.xyz
149

scf done: -2856.877088

C	-4.921461	-0.790780	0.043679
C	-4.163107	-0.420993	1.187231
C	-3.772386	0.933274	1.340376
C	-4.197030	1.902312	0.434253
C	-4.998684	1.581589	-0.663890
C	-5.320846	0.230313	-0.829078
O	-3.806262	-1.287473	2.129522
Y	-3.368563	-1.513389	4.215919
O	-2.629856	-1.020097	6.358330
C	-1.874765	-1.474238	7.271408
O	-2.416932	-1.933487	8.412579
C	-3.833532	-1.897227	8.553088
C	-2.784262	1.306194	2.411467
N	-3.167132	1.090071	3.840153
C	-2.085276	1.663115	4.659707
C	-5.454103	2.678613	-1.635617
C	-6.262209	3.744504	-0.869222
C	-5.254091	-2.262062	-0.259233
C	-3.940683	-3.058760	-0.394112
O	-4.622780	-3.140658	4.731193
C	-5.803501	-3.447248	5.266127
C	-6.859312	-2.505498	5.180210
C	-8.091629	-2.766991	5.774904
C	-8.346340	-3.958340	6.456903
C	-7.305075	-4.891445	6.493239
C	-6.046074	-4.689482	5.913615
C	-6.684635	-1.251934	4.367097
N	-5.612932	-0.323252	4.827443
C	-5.824333	0.032583	6.235142
C	-4.979846	-5.796944	5.942570
C	-4.604886	-6.180122	4.496751
C	-9.719959	-4.205255	7.094802
C	-10.026481	-3.090919	8.114793
O	-1.360876	-2.443184	3.831843
C	-0.139593	-2.064306	3.781386
O	0.176439	-1.056036	2.909317
C	-0.233252	-1.293853	1.554058
C	0.893397	-2.495535	4.619540
C	0.261147	-0.996416	6.209557
C	-0.451984	-1.529629	7.272700
C	0.246337	-2.138720	8.464933
C	2.294113	-2.007570	4.331323
C	0.698250	-3.778114	5.387475
C	1.113024	-5.117101	4.683730
C	0.596511	-6.260453	5.570595
O	0.988420	-7.494484	5.013880
C	0.806357	-8.627181	5.853400
C	1.661131	-9.738811	5.263425
C	-3.725880	-5.318492	6.698722

C	-5.474115	-7.072130	6.643000
C	-10.804198	-4.200947	5.998777
C	-9.790445	-5.551149	7.829041
C	-5.656345	0.881364	3.980706
C	-4.438671	1.772174	4.166417
C	-6.113332	-2.877912	0.861204
C	-6.031721	-2.426217	-1.574810
C	-4.220399	3.343290	-2.277978
C	-6.340348	2.129874	-2.762382
C	2.634038	-5.244102	4.533531
C	0.478220	-5.152893	3.294384
O	1.000440	-4.697183	2.296618
O	-0.746730	-5.697968	3.291876
C	-1.414941	-5.688961	2.027994
C	-0.662625	-9.030654	5.960190
H	-6.564899	1.469732	4.200215
H	-5.720753	0.565133	2.937342
H	-4.557686	2.673455	3.546498
H	-4.383258	2.111490	5.205368
H	-2.527629	2.371365	2.287389
H	-1.857645	0.739018	2.267766
H	-7.643144	-0.706573	4.349663
H	-6.439978	-1.508112	3.329971
H	-7.483013	-5.834119	6.994463
H	-8.872692	-2.013843	5.685185
H	-5.914705	-0.049180	-1.689380
H	-3.873852	2.930420	0.590732
H	-6.739040	0.635713	6.359552
H	-5.934739	-0.879406	6.821370
H	-4.971152	0.592090	6.622507
H	-2.023306	2.756200	4.535482
H	-2.245597	1.424409	5.712705
H	-1.129773	1.235409	4.345816
H	-4.157742	-4.114028	-0.599052
H	-3.335405	-2.671547	-1.221325
H	-3.354367	-2.997251	0.524602
H	-6.375880	-3.912529	0.609511
H	-5.578172	-2.888009	1.811601
H	-7.048709	-2.319720	0.985008
H	-6.218156	-3.491003	-1.751015
H	-7.005552	-1.924781	-1.544934
H	-5.473569	-2.044461	-2.436564
H	-6.650823	2.948771	-3.420339
H	-5.809367	1.396583	-3.378549
H	-7.247787	1.656203	-2.372795
H	-6.590848	4.541506	-1.546727
H	-7.151837	3.303049	-0.407283
H	-5.669175	4.208712	-0.074661
H	-4.525989	4.130649	-2.977413
H	-3.569166	3.800570	-1.526426
H	-3.625960	2.608375	-2.830726
H	-2.966441	-6.109370	6.708120
H	-3.292798	-4.435876	6.226312
H	-3.969310	-5.078788	7.740053

H	-4.680294	-7.826365	6.615945	C	-4.221517	1.791409	0.355751
H	-5.723583	-6.897145	7.695513	C	-5.019742	1.437091	-0.734632
H	-6.351178	-7.502396	6.147546	C	-5.354277	0.083348	-0.851248
H	-3.827814	-6.953768	4.500737	O	-3.879889	-1.335716	2.172386
H	-5.478271	-6.577564	3.967722	Y	-3.402540	-1.444892	4.248526
H	-4.232075	-5.313934	3.948130	O	-2.832808	-0.944079	6.602785
H	-10.782495	-5.676617	8.276070	C	-2.178086	-1.312128	7.586699
H	-9.626504	-6.395134	7.150736	O	-2.752932	-1.849973	8.655008
H	-9.053088	-5.613073	8.636731	C	-4.178510	-2.009682	8.655063
H	-11.010745	-3.246696	8.572245	C	-2.821490	1.251626	2.360352
H	-9.278385	-3.077446	8.914764	N	-3.219888	1.110609	3.796325
H	-10.032114	-2.101638	7.646478	C	-2.129631	1.693043	4.597943
H	-11.796232	-4.368326	6.435201	C	-5.458958	2.501649	-1.749096
H	-10.833639	-3.247647	5.461673	C	-6.268388	3.598413	-1.029084
H	-10.617736	-4.990339	5.263197	C	-5.310873	-2.386743	-0.183111
H	1.322806	-0.810889	6.337147	C	-4.001191	-3.197022	-0.270763
H	-0.238385	-0.336940	5.511406	O	-4.626578	-3.087834	4.836128
H	-4.326878	-2.427422	7.735476	C	-5.796122	-3.382264	5.392549
H	-4.044061	-2.396428	9.499341	C	-6.854696	-2.440115	5.316528
H	-4.192425	-0.865153	8.593561	C	-8.069361	-2.690188	5.951825
H	1.330819	-2.089066	8.332741	C	-8.305957	-3.868961	6.662571
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149

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