

Supporting Information

The Role of Ligands in Controlling the Regioselectivity in Ruthenium-Catalyzed Addition of Carboxylic Acids to Terminal Alkynes: A DFT study

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Scheme S1. To quantify the steric interaction with exchange of *bi*-phosphine chelating ligands. The energy terms are ΔG_L^S in kcal/mol.

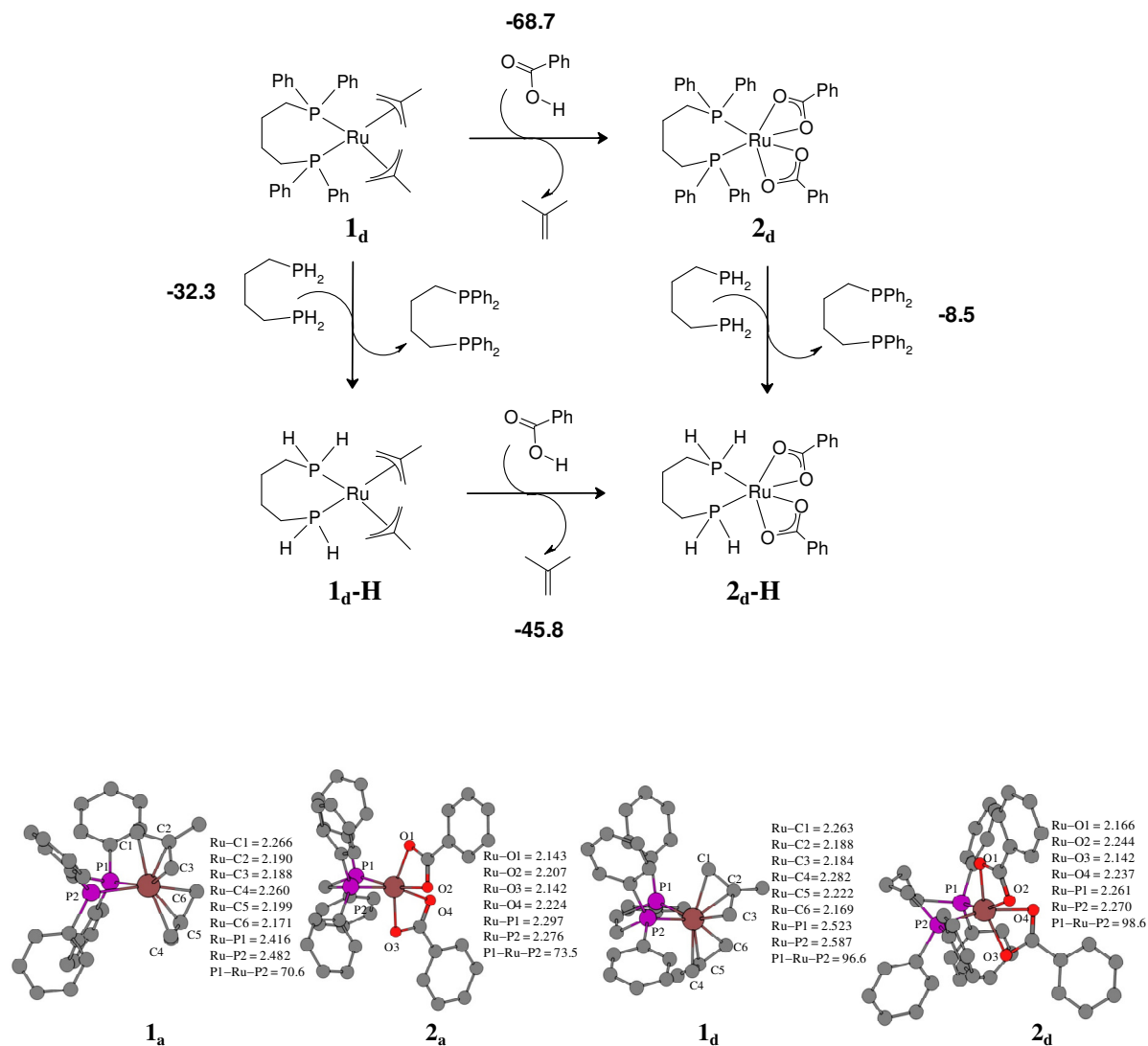


Figure S1. Optimized geometries of intermediates involve in ligand exchange step for $1_{a/d}$. Hydrogen atoms are omitted for clarity. All bond lengths are in angstrom (\AA) and angles in degree ($^\circ$).

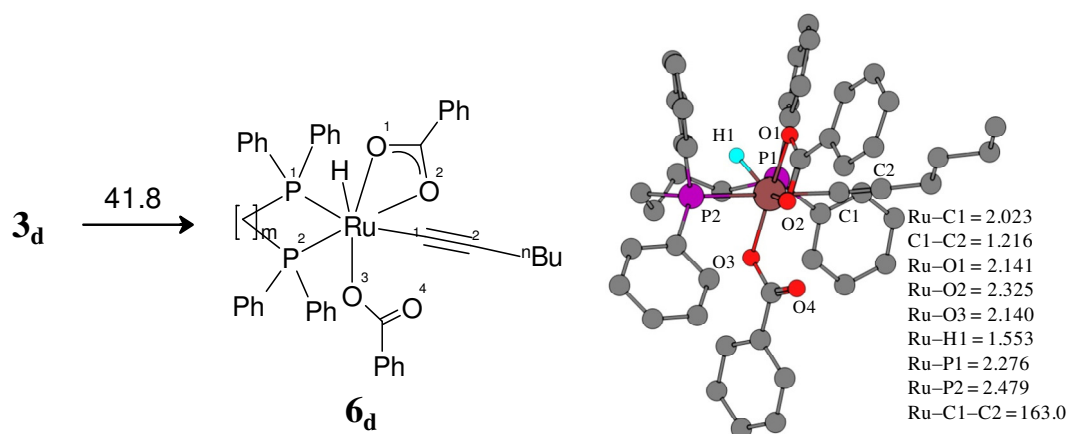


Figure S2. Optimized geometries of intermediates involve in oxidative addition step of **3_d** intermediate *via* C1–H activation. For other conventions see Figure 1 and Scheme S1.

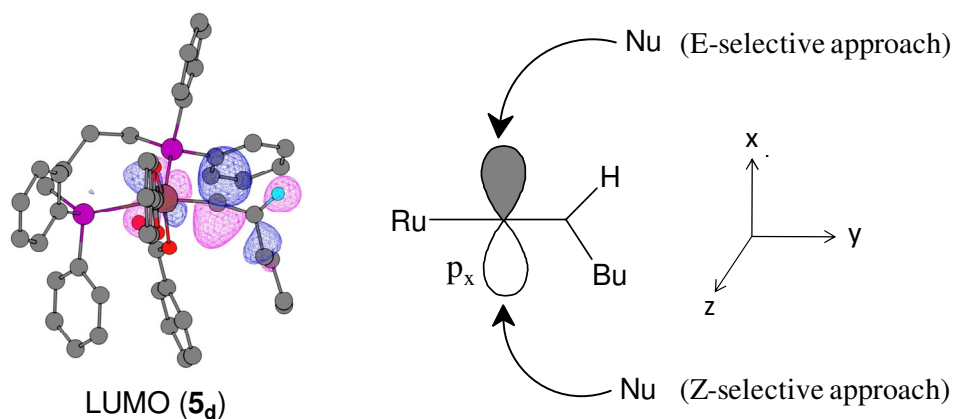


Figure S3. KS-LUMO of vinylidene **5_d** (left) and nucleophilic approach to the same intermediate (right).

Table S1. Absolute energies (hartrees) of all intermediates and transition states we have discussed in our study. E_e = Electronic energy, H_{298} = enthalpy at 298 K, G_{298} = Gibbs free energy and E_L^S = Electronic energy at SMD solvation model. First three energy terms (E_e , H_{298} and G_{298}) are from ONIOM{M06-2X/LANL2DZ(Ru)/6-31G*(H, C, O and P):HF/STO-3G} in gas phase and last one (E_L^S) from M06-2X/LANL2TZ(f)(Ru)/TZVP(H, C, O and P)//ONIOM{M06-2X/LANL2DZ(Ru)/6-31G*(H, C, O and P):HF/STO-3G} level of theory in solution.

Molecule	E_e	H_{298}	G_{298}	E_L^S
1_a	-2038.176303	-2037.488197	-2037.590374	-2055.515513

1_b	-2077.467566	-2076.748468	-2076.850838	-2094.824551
1_c	-2116.752727	-2116.002737	-2116.107301	-2134.126724
1_d	-2156.040429	-2155.259699	-2155.366	-2173.429832
1_e	-2453.55952	-2452.679442	-2452.803261	-2479.46211367
2_a	-2565.257675	-2564.551129	-2564.673258	-2582.799886
2_b	-2604.572035	-2603.83467	-2603.956288	-2622.130054
2_c	-2643.869328	-2643.101334	-2643.225176	-2661.438327
2_d	-2683.156616	-2682.358202	-2682.484121	-2700.744389
2_e	-2980.671079	-2979.772529	-2979.91036	-3006.768125
3_a	-2799.74725	-2798.885992	-2799.021438	-2817.375260
3_b	-2839.05786	-2838.165713	-2838.301725	-2856.704059
3_c	-2878.357507	-2877.43453	-2877.571097	-2896.015022
3_d	-2917.638795	-2916.685729	-2916.82585	-2935.320687
3_e	-3215.139062	-3214.086357	-3214.242997	-3241.328988
3'_a	-2799.743155	-2798.882077	-2799.021584	-2817.373337
3'_b	-2839.048263	-2838.156098	-2838.294215	-2856.694635
3'_c	-2878.352501	-2877.429713	-2877.572141	-2896.014422
3'_d	-2917.629132	-2916.676151	-2916.819454	-2935.306147
3'_e	-3215.149456	-3214.096407	-3214.250729	-3241.335867
[3_a-4_a][‡]	-3220.350717	-3219.366553	-3219.534406	-3238.141680
[3_d-4_d][‡]	-3338.24469	-3337.168941	-3337.332584	-3356.064745
4_a	-3220.411693	-3219.421866	-3219.577992	-3238.209448

4_d	-3338.308497	-3337.226762	-3337.388121	-3356.133597
[3_a-5_a][‡]	-2799.681032	-2798.83286	-2798.956017	-2817.309423
[3_a-5_d][‡]	-2917.585611	-2916.629134	-2916.768957	-2935.271300
5_a	-2799.734713	-2798.873331	-2799.010712	-2817.353181
5_d	-2917.614833	-2916.661656	-2916.803835	-2935.290770
[3'_a-6_a][‡]	-2799.730356	-2798.870447	-2799.008039	-2817.353242
[3'_a-6_d][‡]	-2917.616325	-2916.668114	-2916.807282	-2935.295118
6'_a	-2799.736621	-2798.874761	-2799.018939	-2817.363993
6'_d	-2917.617827	-2916.661492	-2916.809174	-2935.295488
7'_a	-2800.145491	-2799.271398	-2799.411563	-2817.796697
7'_d	-2918.025518	-2917.059477	-2917.203848	-2935.722343
8_d-E	-3338.270645	-3337.190746	-3337.355457	-3356.109336
[8_d-9_d-E][‡]	-3338.261099	-3337.182923	-3337.342070	-3356.096157
9_d-E	-3338.292847	-3337.211368	-3337.371547	-3356.122868
8_d-Z	-3338.283345	-3338.283345	-333.360092	-3356.112948
[8_d-9_d-Z][‡]	-3338.270995	-3337.193234	-3337.356350	-3356.101304
9_d-Z	-3338.311511	-3337.229885	-3337.392117	-3356.132609
PhCOOH	-420.631045	-420.5059	-420.545949	-420.802196
1-hexyne	-234.466760	-234.314481	-234.354316	-234.563266
I	-655.167941	-654.886768	-654.946324	-655.415144
II	-655.167286	-654.885512	-654.946244	-655.414447
III	-655.166916	-654.885364	-654.946166	-655.414274

Table S2. Cartesian coordinates of the optimized structures of intermediates and transition states at system ONIOM{M06-2X/LANL2DZ(Ru)/6-31G*(H, C, O and P):HF/STO-3G} level of theory.

1_a	72			
	XYZ			
	Ru	-0.14145	-1.03780	1.32745
	C	-1.11258	-0.10028	3.06389
	C	0.05521	-3.21312	1.16553
	C	-2.02726	1.08496	2.90920
	H	-2.87316	0.85680	2.25368
	H	-2.43213	1.35144	3.89250
	H	-1.49913	1.95707	2.51346
	C	-1.01449	-4.15234	1.66192
	H	-0.74681	-5.17211	1.36097
	H	-1.10513	-4.14551	2.74968
	H	-1.98851	-3.91560	1.22416
	C	0.00450	-2.73682	-0.16432
	C	1.08883	-2.71326	2.01172
	C	0.26554	0.07151	3.25453
	C	-1.60109	-1.43050	2.88609
	P	-1.33839	0.23650	-0.34069
	P	1.48016	0.00066	-0.23814
	H	-2.66095	-1.55698	2.67222
	H	-1.17917	-2.21216	3.51261
	H	0.65432	1.08591	3.25829
	H	0.85044	-0.65881	3.80257
	H	1.06350	-3.01094	3.05962
	H	2.08916	-2.56785	1.61502
	H	-0.85073	-3.02307	-0.77363
	H	0.93002	-2.61233	-0.72160
	C	0.13911	0.33161	-1.49531
	H	0.22455	1.23815	-2.09398
	H	0.07534	-0.53278	-2.15945
	C	2.86282	-0.88162	-1.15786
	C	3.93118	-1.37324	-0.41188

C	2.88286	-1.03537	-2.53817
C	4.99275	-2.01064	-1.03281
H	3.93919	-1.25791	0.66507
C	3.94481	-1.67590	-3.16126
H	2.07384	-0.65809	-3.14913
C	5.00095	-2.16582	-2.41147
H	5.81511	-2.38870	-0.43848
H	3.94424	-1.78947	-4.23805
H	5.82866	-2.66576	-2.89829
C	2.36752	1.63835	-0.00921
C	2.82768	1.98962	1.25363
C	2.64304	2.48200	-1.08244
C	3.53356	3.16932	1.44656
H	2.63690	1.33920	2.09789
C	3.34402	3.66133	-0.89191
H	2.31701	2.22374	-2.08206
C	3.78943	4.00923	0.37528
H	3.88345	3.42988	2.43755
H	3.54733	4.30865	-1.73563
H	4.33840	4.93059	0.52402
C	-2.65663	-0.58939	-1.38097
C	-3.47635	-1.55385	-0.80980
C	-2.83731	-0.25646	-2.72070
C	-4.46047	-2.17908	-1.56349
H	-3.34444	-1.82587	0.23059
C	-3.81637	-0.88131	-3.47513
H	-2.21501	0.49789	-3.18615
C	-4.63076	-1.84487	-2.89697
H	-5.09233	-2.93000	-1.10617
H	-3.94578	-0.61509	-4.51653
H	-5.39624	-2.33314	-3.48700
C	-1.97334	2.01076	-0.33507
C	-1.08918	3.07627	-0.20158
C	-3.33499	2.28155	-0.41481
C	-1.55226	4.38224	-0.16971
H	-0.02525	2.89984	-0.11745

	C	-3.80091	3.58720	-0.38072
	H	-4.04788	1.47231	-0.50712
	C	-2.91069	4.64245	-0.26138
	H	-0.84787	5.19850	-0.06956
	H	-4.86462	3.77854	-0.44736
	H	-3.27355	5.66205	-0.23571
1_b	75			
	XYZ			
	Ru	0.04197	-1.15765	0.86220
	C	0.61741	-3.09581	-0.02058
	C	-0.01427	-0.83309	3.04981
	C	1.41595	-3.21973	-1.29176
	H	2.42385	-2.81687	-1.18652
	H	1.50929	-4.28070	-1.55048
	H	0.91712	-2.72037	-2.13035
	C	1.03206	-1.44437	3.94722
	H	0.87126	-1.08311	4.96997
	H	0.97422	-2.53430	3.97144
	H	2.03959	-1.15156	3.63757
	C	0.20684	0.43103	2.47948
	C	-1.19415	-1.53424	2.66321
	C	-0.78421	-3.02555	-0.07291
	C	1.21768	-2.96994	1.26938
	P	1.52764	0.06027	-0.54893
	P	-1.61919	-0.01085	-0.44500
	H	2.30182	-2.98564	1.33815
	H	0.71689	-3.45776	2.10196
	H	-1.26368	-3.02288	-1.05092
	H	-1.38314	-3.44003	0.72955
	H	-1.31564	-2.55465	3.02647
	H	-2.12473	-0.98143	2.57700
	H	1.15344	0.92331	2.68095
	H	-0.62198	1.09673	2.26687
	C	0.63895	0.36336	-2.18645
	C	-2.28011	1.74295	-0.22283
	C	-2.90441	2.04753	0.98474

C	-2.22557	2.72280	-1.20636
C	-3.44908	3.30174	1.20675
H	-2.97501	1.29736	1.76251
C	-2.76899	3.98095	-0.98598
H	-1.76125	2.52341	-2.16238
C	-3.38026	4.27524	0.22083
H	-3.92959	3.51921	2.15247
H	-2.71488	4.73128	-1.76481
H	-3.80435	5.25635	0.39247
C	-3.29635	-0.79814	-0.80334
C	-3.85332	-1.71818	0.07530
C	-4.02524	-0.42490	-1.93046
C	-5.10537	-2.26515	-0.17238
H	-3.30928	-2.01915	0.95980
C	-5.27241	-0.97194	-2.18104
H	-3.63063	0.30470	-2.62500
C	-5.81634	-1.89657	-1.30175
H	-5.52265	-2.98274	0.52267
H	-5.82276	-0.67222	-3.06378
H	-6.79195	-2.32384	-1.49651
C	1.95506	1.79475	0.07629
C	3.03747	1.94436	0.94252
C	1.22820	2.92461	-0.26951
C	3.38754	3.18913	1.43507
H	3.61863	1.08206	1.24087
C	1.57703	4.17542	0.22327
H	0.37283	2.85446	-0.92417
C	2.65817	4.31354	1.07444
H	4.23318	3.28204	2.10491
H	0.99460	5.04226	-0.06263
H	2.93121	5.28789	1.45889
C	3.27984	-0.36061	-1.11617
C	3.79714	0.11470	-2.31715
C	4.11274	-1.09488	-0.27731
C	5.10664	-0.15948	-2.68158
H	3.19037	0.71248	-2.98367

C	5.42373	-1.36721	-0.63836
H	3.73754	-1.46179	0.66903
C	5.92333	-0.90379	-1.84509
H	5.49031	0.21576	-3.62196
H	6.05475	-1.94345	0.02658
H	6.94579	-1.11680	-2.13033
C	-0.83808	-0.05787	-2.14811
H	-0.91638	-1.11963	-2.40496
H	-1.40702	0.49012	-2.90001
H	1.15430	-0.24217	-2.93591
H	0.74465	1.40309	-2.49879

1_c

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XYZ

Ru	-0.06490	-0.76155	0.98862
C	0.68342	-2.85621	0.88994
C	-0.36568	0.24932	2.92526
C	1.63441	-3.42418	-0.12709
H	2.63475	-3.00394	-0.03617
H	1.71324	-4.50307	0.05025
H	1.27792	-3.28655	-1.15263
C	0.60135	0.08726	4.07026
H	0.27474	0.73194	4.89497
H	0.63205	-0.93614	4.44875
H	1.61384	0.38803	3.78907
C	-0.20165	1.28446	1.99152
C	-1.44229	-0.66351	2.69708
C	-0.70018	-2.89732	0.65971
C	1.13559	-2.22861	2.09141
P	1.69990	0.07557	-0.49339
P	-1.83783	-0.10180	-0.57915
H	2.21009	-2.13566	2.23894
H	0.58009	-2.42291	3.00506
H	-1.04871	-3.26671	-0.30421
H	-1.38133	-3.05033	1.48716
H	-1.51959	-1.52204	3.36519
H	-2.40531	-0.26159	2.39569

H	0.66116	1.93459	2.08820
H	-1.06604	1.74543	1.52966
C	0.94718	0.52008	-2.13374
C	-2.49199	1.67700	-0.63553
C	-3.36772	2.07640	0.37481
C	-2.14962	2.60458	-1.61027
C	-3.88184	3.36089	0.40778
H	-3.65926	1.37553	1.14666
C	-2.66460	3.89433	-1.58067
H	-1.48303	2.34315	-2.41940
C	-3.53023	4.27816	-0.57262
H	-4.56021	3.64708	1.20175
H	-2.38468	4.59826	-2.35432
H	-3.93132	5.28331	-0.54937
C	-3.54297	-0.92344	-0.54428
C	-3.92904	-1.80748	0.45199
C	-4.45756	-0.61981	-1.55421
C	-5.19437	-2.38363	0.43886
H	-3.24732	-2.05502	1.25165
C	-5.71633	-1.19232	-1.57031
H	-4.19396	0.07719	-2.33910
C	-6.08935	-2.08078	-0.57079
H	-5.47499	-3.07174	1.22619
H	-6.41020	-0.94344	-2.36310
H	-7.07464	-2.52949	-0.58143
C	2.54874	1.68076	0.02522
C	3.10109	1.76831	1.30121
C	2.68980	2.76624	-0.83078
C	3.77645	2.90636	1.70954
H	2.99488	0.94297	1.99260
C	3.36152	3.91047	-0.42234
H	2.28142	2.74295	-1.83098
C	3.90857	3.98438	0.84680
H	4.19670	2.95271	2.70631
H	3.45748	4.74543	-1.10491
H	4.43336	4.87645	1.16423

C	3.29856	-0.79707	-1.04022
C	3.51403	-1.22590	-2.34430
C	4.30906	-1.00659	-0.10250
C	4.70829	-1.83534	-2.70560
H	2.75732	-1.10031	-3.10468
C	5.50121	-1.61236	-0.46087
H	4.17021	-0.70080	0.92523
C	5.70727	-2.02824	-1.76818
H	4.85259	-2.15998	-3.72844
H	6.27138	-1.76257	0.28527
H	6.63846	-2.50252	-2.05053
C	0.08171	-0.64375	-2.65174
H	0.41905	-1.58808	-2.20941
H	0.21333	-0.74616	-3.73443
H	1.70186	0.81284	-2.86363
H	0.32990	1.40201	-1.94568
C	-1.41356	-0.48770	-2.37166
H	-1.84525	0.27086	-3.02852
H	-1.92082	-1.42852	-2.60541

1_d

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XYZ

Ru	0.05939	-1.19835	0.51159
C	0.78667	-3.02061	-0.53230
C	-0.03481	-1.07454	2.69418
C	1.70592	-3.03641	-1.72633
H	2.62751	-2.47683	-1.54563
H	1.99310	-4.07605	-1.92268
H	1.22485	-2.65860	-2.63278
C	1.03308	-1.66473	3.57861
H	0.77336	-1.45868	4.62390
H	1.11767	-2.74753	3.46851
H	2.00957	-1.21288	3.38210
C	0.06743	0.25338	2.24741
C	-1.14756	-1.83590	2.21648
C	-0.60792	-3.03504	-0.66665
C	1.29478	-2.95743	0.80369

P	1.84414	0.17545	-0.62549
P	-2.02163	-0.05967	-0.52104
H	2.37374	-2.92859	0.92835
H	0.78805	-3.55905	1.55540
H	-1.04174	-2.98426	-1.66421
H	-1.20950	-3.54974	0.07245
H	-1.18567	-2.89153	2.48797
H	-2.12315	-1.35854	2.19034
H	0.95560	0.81538	2.51489
H	-0.81695	0.85749	2.08977
C	0.22126	0.88143	-2.80253
C	-2.45838	1.73830	-0.14568
C	-2.92195	2.02881	1.13835
C	-2.34977	2.78234	-1.05491
C	-3.24987	3.32264	1.50375
H	-3.04442	1.23327	1.86253
C	-2.67788	4.08223	-0.69112
H	-2.01995	2.60551	-2.06850
C	-3.12382	4.35851	0.58858
H	-3.60774	3.52312	2.50585
H	-2.58592	4.87895	-1.41855
H	-3.37914	5.37158	0.87193
C	-3.74841	-0.78884	-0.24459
C	-3.93291	-2.07456	0.24590
C	-4.87421	-0.05418	-0.61601
C	-5.20847	-2.60813	0.38042
H	-3.08112	-2.67323	0.53144
C	-6.14623	-0.58329	-0.48287
H	-4.76702	0.94629	-1.01402
C	-6.31831	-1.86478	0.01971
H	-5.32876	-3.61121	0.76958
H	-7.00599	0.00633	-0.77456
H	-7.31272	-2.27969	0.12543
C	2.13336	1.92921	0.05159
C	2.83177	2.09439	1.24695
C	1.68986	3.07226	-0.60394

C	3.07400	3.35338	1.76954
H	3.20303	1.23387	1.78461
C	1.92974	4.33629	-0.08215
H	1.15453	3.00834	-1.53845
C	2.62101	4.48386	1.10663
H	3.62030	3.45015	2.69931
H	1.57249	5.20807	-0.61562
H	2.80874	5.46934	1.51316
C	3.64476	-0.39654	-0.51352
C	4.54064	-0.26007	-1.56961
C	4.11381	-0.93236	0.68326
C	5.86328	-0.65614	-1.43568
H	4.22686	0.15626	-2.51580
C	5.43582	-1.32528	0.82088
H	3.44058	-1.05313	1.52050
C	6.31636	-1.19002	-0.24084
H	6.54140	-0.54304	-2.27206
H	5.77611	-1.74086	1.76095
H	7.34892	-1.49857	-0.13738
C	-0.65520	-0.35957	-2.99472
H	-0.17311	-1.20739	-2.50483
H	-0.72918	-0.60787	-4.06044
H	0.19061	1.51086	-3.69834
H	-0.20000	1.48726	-1.99601
C	-2.05331	-0.22272	-2.40113
H	-2.61276	0.60045	-2.85347
H	-2.62605	-1.13485	-2.59719
C	1.67527	0.53971	-2.45674
H	2.35058	1.34606	-2.74767
H	1.98369	-0.35935	-3.00074

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XYZ

Ru	-0.12302	-1.76453	-0.11682
C	0.42132	-2.42607	-2.12829
C	-0.13388	-3.09800	1.59029
C	1.28818	-1.61525	-3.05104

H	2.26192	-1.39874	-2.60306
H	1.47332	-2.19593	-3.96254
H	0.80257	-0.68213	-3.34696
C	0.90831	-4.16272	1.81014
H	0.65396	-4.71815	2.72081
H	0.95743	-4.88056	0.98938
H	1.89997	-3.72451	1.95554
C	0.00994	-1.82239	2.15668
C	-1.29239	-3.29362	0.76068
C	-0.97492	-2.30329	-2.13252
C	0.98636	-3.29072	-1.13773
P	2.06550	0.16705	-0.03784
P	-2.13808	0.02212	0.04059
H	2.07140	-3.35259	-1.08699
H	0.48942	-4.24167	-0.95483
H	-1.42727	-1.55982	-2.78520
H	-1.59487	-3.16398	-1.90565
H	-1.38095	-4.25300	0.24850
H	-2.24883	-2.90452	1.10488
H	0.93050	-1.58969	2.68504
H	-0.86207	-1.27374	2.49269
C	-2.11888	1.41830	1.30413
C	-2.32183	1.13909	2.65519
C	-1.84945	2.73120	0.93494
C	-2.27431	2.14676	3.60481
H	-2.53098	0.12719	2.97720
C	-1.79682	3.74135	1.88478
H	-1.68010	2.98259	-0.10367
C	-2.01161	3.45369	3.22212
H	-2.44287	1.90875	4.64754
H	-1.58878	4.75750	1.57415
H	-1.97384	4.24196	3.96318
C	-3.85668	-0.71845	0.28322
C	-4.19017	-1.86411	-0.43503
C	-4.82633	-0.14247	1.09713
C	-5.45095	-2.42918	-0.32706

H	-3.46005	-2.32500	-1.08516
C	-6.08759	-0.70897	1.20951
H	-4.61473	0.76094	1.65129
C	-6.40375	-1.85561	0.50069
H	-5.68749	-3.32188	-0.89200
H	-6.82572	-0.24543	1.85157
H	-7.38828	-2.29742	0.58849
C	2.45907	0.77912	1.70202
C	3.76493	0.90373	2.16616
C	1.42016	1.15058	2.54969
C	4.02371	1.37277	3.44514
H	4.59960	0.63483	1.53325
C	1.67489	1.62371	3.82751
H	0.39547	1.06930	2.21653
C	2.97957	1.73358	4.28118
H	5.04758	1.45802	3.78653
H	0.84937	1.90471	4.46880
H	3.18166	2.09958	5.27987
C	3.72768	-0.60506	-0.46668
C	4.69993	0.01212	-1.24474
C	4.00812	-1.85728	0.07608
C	5.91101	-0.61726	-1.49673
H	4.53130	0.99597	-1.65939
C	5.21773	-2.48532	-0.16982
H	3.27486	-2.34820	0.70214
C	6.17277	-1.86811	-0.96429
H	6.65355	-0.12086	-2.10858
H	5.41414	-3.45939	0.26009
H	7.11795	-2.35801	-1.16123
C	-2.45006	0.99129	-1.54434
C	-1.37913	1.30876	-2.37071
C	-3.72193	1.41728	-1.91675
C	-1.56729	2.02631	-3.54236
H	-0.38044	0.99522	-2.10060
C	-3.91575	2.13217	-3.08827
H	-4.57801	1.19227	-1.29460

C	-2.83881	2.43842	-3.90597
H	-0.71771	2.26175	-4.17052
H	-4.91328	2.45178	-3.36221
H	-2.99091	2.99610	-4.82144
C	2.08373	1.81033	-0.96853
C	2.25437	1.84150	-2.35161
C	1.86726	3.01636	-0.30988
C	2.22920	3.03849	-3.04916
H	2.41769	0.92639	-2.90231
C	1.83535	4.21587	-1.00586
H	1.72399	3.03580	0.76164
C	2.01918	4.23299	-2.37821
H	2.37363	3.03545	-4.12223
H	1.66804	5.14080	-0.46838
H	1.99778	5.16899	-2.92172

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XYZ

Ru	-0.11690	-0.49724	-0.19440
C	1.82893	-1.85030	-1.04269
C	-2.36256	-1.63663	-0.36076
P	0.92981	0.64485	1.47330
P	-0.85338	1.67426	-0.33121
C	-0.17960	2.15220	1.34958
H	0.26121	3.14210	1.46608
H	-0.97060	2.01811	2.09263
C	-2.65158	2.15622	-0.38580
C	-3.45665	1.56264	-1.35330
C	-3.21764	3.07210	0.49296
C	-4.80318	1.87940	-1.43971
H	-3.03257	0.84238	-2.04337
C	-4.56615	3.38648	0.41028
H	-2.61437	3.55077	1.25375
C	-5.36120	2.79171	-0.55627
H	-5.41881	1.40932	-2.19632
H	-4.99482	4.09983	1.10286
H	-6.41376	3.03722	-0.62067

C	-0.04322	2.85137	-1.53422
C	0.93158	2.37411	-2.40082
C	-0.39370	4.19835	-1.58198
C	1.54869	3.23338	-3.30094
H	1.21977	1.32846	-2.37318
C	0.22039	5.05449	-2.48015
H	-1.15585	4.58829	-0.91839
C	1.19475	4.57169	-3.34279
H	2.30782	2.85134	-3.97175
H	-0.06150	6.09932	-2.50887
H	1.67512	5.24009	-4.04648
C	0.78784	0.08849	3.24675
C	-0.12424	-0.91307	3.55606
C	1.54565	0.65622	4.26656
C	-0.27443	-1.34271	4.86735
H	-0.72567	-1.35896	2.77088
C	1.39816	0.22540	5.57489
H	2.26156	1.43834	4.04470
C	0.48681	-0.77612	5.87718
H	-0.98730	-2.12430	5.09790
H	1.99457	0.67231	6.36012
H	0.37147	-1.11353	6.89968
C	2.70637	1.17299	1.28184
C	3.07926	2.42460	0.81124
C	3.69831	0.23539	1.56062
C	4.41932	2.73950	0.63177
H	2.33410	3.17173	0.57310
C	5.03513	0.54948	1.38462
H	3.42744	-0.75047	1.91932
C	5.39974	1.80536	0.91956
H	4.69390	3.72043	0.26464
H	5.79492	-0.18902	1.60791
H	6.44465	2.05157	0.77962
C	-3.65147	-2.38215	-0.37406
C	-4.07541	-2.99843	-1.55194
C	-4.42827	-2.46165	0.78226

C	-5.27923	-3.69400	-1.57224
H	-3.44857	-2.92370	-2.43422
C	-5.63211	-3.15765	0.75839
H	-4.07449	-1.97665	1.68588
C	-6.05727	-3.77298	-0.41808
H	-5.61158	-4.17664	-2.48588
H	-6.23928	-3.22291	1.65583
H	-6.99682	-4.31711	-0.43501
C	2.94096	-2.64270	-1.63574
C	3.12289	-3.97012	-1.24622
C	3.79511	-2.05879	-2.57184
C	4.16265	-4.71345	-1.79396
H	2.44075	-4.39862	-0.51952
C	4.83406	-2.80507	-3.11757
H	3.62960	-1.02595	-2.85934
C	5.01783	-4.13112	-2.72845
H	4.30695	-5.74690	-1.49504
H	5.50048	-2.35546	-3.84697
H	5.82890	-4.71292	-3.15603
O	1.05895	-2.36452	-0.18425
O	1.65078	-0.63799	-1.39811
O	-1.96165	-1.08583	0.72110
O	-1.66423	-1.53967	-1.40573

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XYZ

Ru	-0.00131	-0.00962	0.22725
C	-2.04389	0.40688	1.65547
C	2.05432	-0.62059	1.56666
P	-1.11441	-0.98711	-1.47709
P	1.11199	1.17291	-1.34338
C	-0.27036	-0.53186	-3.08269
C	2.93132	0.79970	-1.55471
C	3.82196	1.30041	-0.60808
C	3.42203	0.00165	-2.57955
C	5.17448	1.01532	-0.69113
H	3.45873	1.91914	0.20374

C	4.77733	-0.28620	-2.66285
H	2.75776	-0.40801	-3.32834
C	5.65677	0.22003	-1.72097
H	5.85421	1.41330	0.05189
H	5.14386	-0.90919	-3.46902
H	6.71375	-0.00458	-1.78617
C	1.07328	3.03534	-1.19863
C	0.17862	3.63114	-0.31922
C	1.90710	3.84174	-1.96895
C	0.12193	5.01442	-0.20916
H	-0.48364	3.01540	0.28053
C	1.85171	5.22084	-1.85806
H	2.61180	3.39550	-2.66017
C	0.95739	5.81010	-0.97550
H	-0.57833	5.46905	0.48013
H	2.50654	5.83730	-2.46064
H	0.91367	6.88849	-0.88736
C	-1.10182	-2.85472	-1.53774
C	-1.95048	-3.56083	-2.38618
C	-0.21140	-3.55501	-0.73413
C	-1.91434	-4.94451	-2.42628
H	-2.65182	-3.03242	-3.02051
C	-0.17403	-4.94262	-0.77565
H	0.46267	-3.01709	-0.07557
C	-1.02457	-5.63862	-1.61865
H	-2.58073	-5.48260	-3.08833
H	0.52292	-5.47919	-0.14435
H	-0.99600	-6.72069	-1.64853
C	-2.92496	-0.56578	-1.67141
C	-3.39287	0.33103	-2.62253
C	-3.83351	-1.13935	-0.78493
C	-4.74302	0.64570	-2.69232
H	-2.71480	0.79788	-3.32391
C	-5.18083	-0.82765	-0.85472
H	-3.48835	-1.83714	-0.03141
C	-5.64014	0.06736	-1.81066

H	-5.09155	1.34612	-3.44087
H	-5.87460	-1.28316	-0.15923
H	-6.69309	0.31276	-1.86544
C	0.29928	0.88689	-3.00380
H	-0.50725	1.62524	-3.05371
H	0.98316	1.09597	-3.82983
H	-0.93691	-0.65500	-3.93963
H	0.53812	-1.26197	-3.19064
O	1.68332	-1.29318	0.54544
O	1.45049	0.44669	1.86273
O	-1.43143	-0.68799	1.79465
O	-1.68866	1.21527	0.73277
C	-3.17550	0.76151	2.55613
C	-3.86614	1.96063	2.37728
C	-3.53966	-0.11653	3.57751
C	-4.92394	2.27998	3.22201
H	-3.56155	2.62650	1.57684
C	-4.59723	0.20620	4.42070
H	-2.98194	-1.03963	3.69487
C	-5.28916	1.40332	4.24260
H	-5.46378	3.21204	3.08722
H	-4.88246	-0.47305	5.21785
H	-6.11450	1.65462	4.90203
C	3.19467	-1.10491	2.39284
C	3.58357	-0.38241	3.52135
C	3.86981	-2.27272	2.03589
C	4.65072	-0.82971	4.29282
H	3.03760	0.51962	3.77684
C	4.93692	-2.71683	2.80922
H	3.54604	-2.81659	1.15492
C	5.32716	-1.99558	3.93660
H	4.95530	-0.27195	5.17277
H	5.46465	-3.62513	2.53566
H	6.15978	-2.34400	4.54037

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XYZ

Ru	0.20494	-0.27954	0.03361
C	-1.33011	-1.45829	1.67595
C	2.53529	-1.28461	-0.11552
P	-1.32886	-0.02975	-1.60066
P	1.05369	1.79041	-0.32335
C	-0.53105	0.65097	-3.12770
C	2.72410	2.05224	0.48671
C	2.77425	2.13267	1.87648
C	3.90900	2.13322	-0.23214
C	3.98258	2.29922	2.53108
H	1.86258	2.06176	2.45714
C	5.12182	2.29732	0.42383
H	3.90842	2.06691	-1.31151
C	5.16227	2.38281	1.80461
H	4.00452	2.36091	3.61183
H	6.03702	2.35796	-0.15154
H	6.10816	2.51112	2.31524
C	0.09931	3.27158	0.31666
C	-0.78804	3.08846	1.37030
C	0.27753	4.55372	-0.19553
C	-1.49088	4.16388	1.89589
H	-0.93929	2.09824	1.78468
C	-0.42716	5.62728	0.32425
H	0.97194	4.73141	-1.00647
C	-1.31446	5.43426	1.37275
H	-2.17909	4.00544	2.71655
H	-0.28011	6.61768	-0.08754
H	-1.86416	6.27319	1.78073
C	-1.91108	-1.70618	-2.19630
C	-0.94626	-2.67519	-2.45906
C	-3.25167	-2.02506	-2.36317
C	-1.31915	-3.93786	-2.88986
H	0.10418	-2.44708	-2.31757
C	-3.62548	-3.29143	-2.79064
H	-4.01897	-1.28939	-2.15906
C	-2.66106	-4.24883	-3.05722

H	-0.55998	-4.68315	-3.09100
H	-4.67472	-3.52755	-2.91537
H	-2.95273	-5.23653	-3.39110
C	-2.88718	0.97689	-1.36661
C	-3.58152	1.55368	-2.42642
C	-3.37489	1.14036	-0.07484
C	-4.73504	2.28699	-2.19871
H	-3.23339	1.43648	-3.44433
C	-4.53250	1.87050	0.15324
H	-2.83351	0.69676	0.75597
C	-5.21374	2.44652	-0.90700
H	-5.26300	2.73180	-3.03258
H	-4.90178	1.99048	1.16392
H	-6.11607	3.01820	-0.72928
C	0.04429	2.06339	-2.95022
H	-0.71429	2.73463	-2.52660
H	0.27486	2.45926	-3.94494
H	-1.23553	0.62523	-3.96246
H	0.27712	-0.05222	-3.36027
C	1.33382	2.11971	-2.11741
H	2.01366	1.32588	-2.44495
H	1.83814	3.07749	-2.26194
C	3.84480	-1.97784	-0.26770
C	4.57881	-2.31315	0.87071
C	4.33505	-2.28433	-1.53755
C	5.80490	-2.95546	0.73673
H	4.17122	-2.06480	1.84494
C	5.56186	-2.92623	-1.66815
H	3.74377	-2.01695	-2.40688
C	6.29629	-3.26113	-0.53159
H	6.37807	-3.21962	1.61977
H	5.94613	-3.16780	-2.65419
H	7.25346	-3.76340	-0.63467
C	-2.14785	-2.10703	2.73825
C	-2.26703	-3.49711	2.75991
C	-2.78885	-1.32945	3.70323

C	-3.03130	-4.10879	3.74779
H	-1.75370	-4.07599	1.99920
C	-3.55152	-1.94425	4.69025
H	-2.67612	-0.25127	3.66749
C	-3.67336	-3.33291	4.71186
H	-3.12627	-5.18995	3.76867
H	-4.05036	-1.34318	5.44408
H	-4.26895	-3.81182	5.48336
O	-1.23871	-0.18159	1.63678
O	-0.73002	-2.15045	0.81304
O	2.08858	-0.99458	1.02383
O	1.85891	-0.97755	-1.16128

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XYZ			
Ru	0.22288	-0.21028	0.06753
C	2.49455	-1.34203	0.28267
C	-1.38488	-0.82345	1.92092
P	1.20363	1.71233	-0.63739
P	-1.38732	-0.27562	-1.51891
C	1.21188	1.69505	-3.53931
C	-3.14514	0.02481	-0.94895
C	-3.81524	-0.98503	-0.26289
C	-3.79108	1.23842	-1.14862
C	-5.10233	-0.78618	0.20841
H	-3.33017	-1.93861	-0.09350
C	-5.08053	1.43915	-0.67650
H	-3.29981	2.04575	-1.67459
C	-5.73996	0.42854	0.00240
H	-5.60874	-1.58244	0.73944
H	-5.56938	2.39083	-0.84270
H	-6.74591	0.58512	0.37041
C	-1.51373	-1.94999	-2.35502
C	-0.48822	-2.87546	-2.21516
C	-2.61626	-2.27792	-3.14105
C	-0.56674	-4.11119	-2.84521
H	0.38528	-2.63028	-1.62071

C	-2.69610	-3.50948	-3.76778
H	-3.42755	-1.57103	-3.26513
C	-1.66902	-4.43121	-3.61920
H	0.23941	-4.82428	-2.72780
H	-3.56021	-3.75171	-4.37321
H	-1.73032	-5.39535	-4.10824
C	0.18755	3.28860	-0.65949
C	-1.00349	3.33345	0.05508
C	0.61126	4.43321	-1.33027
C	-1.76375	4.49468	0.08709
H	-1.34116	2.45934	0.60093
C	-0.14885	5.59096	-1.30381
H	1.54480	4.43415	-1.87840
C	-1.34113	5.62354	-0.59517
H	-2.68886	4.51449	0.64935
H	0.19230	6.47147	-1.83343
H	-1.93477	6.52878	-0.57211
C	2.56230	2.18203	0.57016
C	3.90861	1.96511	0.30542
C	2.19843	2.71947	1.80220
C	4.87379	2.29109	1.24799
H	4.22645	1.53484	-0.63452
C	3.16126	3.04639	2.74226
H	1.15374	2.88486	2.03511
C	4.50431	2.83468	2.46651
H	5.91891	2.11619	1.02547
H	2.86167	3.46578	3.69448
H	5.25789	3.08899	3.20086
C	0.17593	0.57572	-3.70200
H	0.62345	-0.37280	-3.37659
H	-0.03297	0.45990	-4.76945
H	1.90958	1.64232	-4.38263
H	0.71209	2.66771	-3.62072
C	-1.16660	0.83604	-2.98038
H	-1.20830	1.86828	-2.61739
H	-2.01115	0.70195	-3.66144

C	2.07316	1.64396	-2.27094
H	2.82055	2.44062	-2.31180
H	2.60341	0.68549	-2.23323
C	-2.21668	-1.11539	3.12134
C	-2.42092	-2.43919	3.51189
C	-2.78658	-0.06966	3.84829
C	-3.19859	-2.71622	4.63101
H	-1.96111	-3.23128	2.93039
C	-3.56387	-0.35028	4.96689
H	-2.60890	0.95046	3.52499
C	-3.77011	-1.67258	5.35743
H	-3.35861	-3.74455	4.93951
H	-4.00831	0.46008	5.53619
H	-4.37645	-1.89023	6.23160
C	3.75836	-2.12438	0.37983
C	4.42763	-2.19638	1.60219
C	4.27052	-2.77424	-0.74370
C	5.61123	-2.92008	1.69891
H	4.00401	-1.68290	2.45894
C	5.45491	-3.49636	-0.64370
H	3.72913	-2.70611	-1.68136
C	6.12468	-3.56885	0.57682
H	6.13397	-2.98061	2.64823
H	5.85626	-4.00466	-1.51483
H	7.04863	-4.13410	0.65402
O	2.03193	-0.73933	1.28540
O	1.87559	-1.27750	-0.83808
O	-0.87091	-1.76254	1.24955
O	-1.18577	0.38550	1.56660

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XYZ

Ru	0.00004	0.64984	0.00001
C	1.92003	2.05733	0.83873
C	-1.91986	2.05746	-0.83871
P	1.51552	-0.85532	-0.94021
P	-1.51555	-0.85523	0.94022

C	-1.88673	-2.37684	-0.08030
C	-2.36901	-2.18635	-1.37358
C	-1.65952	-3.67262	0.36486
C	-2.64037	-3.26933	-2.19332
H	-2.52855	-1.18033	-1.74330
C	-1.92761	-4.75845	-0.45731
H	-1.26489	-3.85170	1.35600
C	-2.42308	-4.56070	-1.73510
H	-3.01922	-3.10451	-3.19406
H	-1.74622	-5.76210	-0.09410
H	-2.63400	-5.40822	-2.37493
C	-3.20928	-0.09253	1.26381
C	-3.27557	0.96809	2.16640
C	-4.38330	-0.54813	0.68225
C	-4.48773	1.56323	2.46913
H	-2.37249	1.33787	2.63621
C	-5.60028	0.05007	0.98363
H	-4.36899	-1.37785	-0.01077
C	-5.65636	1.10634	1.87503
H	-4.52089	2.38714	3.17064
H	-6.50600	-0.31791	0.51850
H	-6.60488	1.57231	2.10990
C	1.18205	-1.44190	-2.69005
C	2.05861	-2.31252	-3.33740
C	0.10265	-0.92990	-3.39648
C	1.84095	-2.68812	-4.65123
H	2.92719	-2.69775	-2.81772
C	-0.11381	-1.30320	-4.71756
H	-0.57108	-0.22390	-2.92460
C	0.74804	-2.18574	-5.34455
H	2.52812	-3.36799	-5.13850
H	-0.95946	-0.89545	-5.25674
H	0.57800	-2.47616	-6.37378
C	3.20924	-0.09263	-1.26395
C	4.38334	-0.54835	-0.68265
C	3.27541	0.96815	-2.16637

C	5.60029	0.04987	-0.98413
H	4.36913	-1.37818	0.01023
C	4.48754	1.56332	-2.46919
H	2.37227	1.33804	-2.63597
C	5.65625	1.10629	-1.87536
H	6.50607	-0.31821	-0.51920
H	4.52060	2.38734	-3.17056
H	6.60475	1.57228	-2.11030
C	-1.18221	-1.44178	2.69010
C	-0.10298	-0.92964	3.39669
C	-2.05876	-2.31250	3.33735
C	0.11335	-1.30291	4.71780
H	0.57071	-0.22352	2.92491
C	-1.84123	-2.68807	4.65120
H	-2.92722	-2.69783	2.81755
C	-0.74847	-2.18556	5.34467
H	0.95887	-0.89504	5.25710
H	-2.52838	-3.36802	5.13838
H	-0.57854	-2.47595	6.37392
C	1.88672	-2.37690	0.08034
C	2.36879	-2.18637	1.37369
C	1.65970	-3.67270	-0.36486
C	2.64015	-3.26933	2.19346
H	2.52816	-1.18034	1.74344
C	1.92779	-4.75851	0.45734
H	1.26523	-3.85181	-1.35606
C	2.42306	-4.56072	1.73520
H	3.01884	-3.10448	3.19426
H	1.74655	-5.76217	0.09409
H	2.63397	-5.40822	2.37506
O	-1.51162	1.04129	-1.49552
O	-1.42792	2.28654	0.30206
O	1.51171	1.04120	1.49554
O	1.42813	2.28644	-0.30205
C	2.96056	2.95108	1.41265
C	3.38951	4.06242	0.68598

C	3.50325	2.67562	2.66829
C	4.36495	4.89862	1.21793
H	2.94685	4.25361	-0.28585
C	4.47922	3.51349	3.19650
H	3.14941	1.80781	3.21439
C	4.90980	4.62368	2.47146
H	4.70082	5.76537	0.65760
H	4.90409	3.30391	4.17309
H	5.67129	5.27773	2.88554
C	-2.96033	2.95128	-1.41262
C	-3.38915	4.06268	-0.68595
C	-3.50309	2.67584	-2.66823
C	-4.36453	4.89896	-1.21790
H	-2.94643	4.25385	0.28585
C	-4.47900	3.51379	-3.19642
H	-3.14935	1.80798	-3.21431
C	-4.90945	4.62403	-2.47140
H	-4.70030	5.76575	-0.65757
H	-4.90392	3.30422	-4.17299
H	-5.67090	5.27814	-2.88546

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XYZ

Ru	-0.23482	0.21589	-0.67351
C	-1.81806	2.14350	-1.19168
C	2.49061	0.82419	0.34561
P	-0.64012	-0.20393	1.56098
P	-0.41782	-2.07325	-0.39741
C	-0.03615	-1.96798	1.42920
H	-0.44981	-2.71622	2.10388
H	1.05445	-1.92654	1.49979
C	0.75162	-3.30290	-1.16934
C	0.39061	-4.59746	-1.52052
C	2.04101	-2.85592	-1.43526
C	1.31340	-5.44004	-2.12267
H	-0.61180	-4.96070	-1.33500
C	2.96365	-3.70057	-2.03190

H	2.29965	-1.83731	-1.15682
C	2.60096	-4.99440	-2.37676
H	1.02386	-6.44721	-2.39417
H	3.96725	-3.34742	-2.23315
H	3.31990	-5.65390	-2.84668
C	-2.11263	-2.84289	-0.49979
C	-3.04004	-2.31636	-1.39082
C	-2.48326	-3.92998	0.28832
C	-4.31123	-2.86380	-1.49440
H	-2.78137	-1.45803	-1.99877
C	-3.75215	-4.47692	0.18885
H	-1.78122	-4.36183	0.99079
C	-4.66936	-3.94501	-0.70573
H	-5.02314	-2.43993	-2.19132
H	-4.02524	-5.32066	0.80986
H	-5.66148	-4.37178	-0.78450
C	0.28223	0.62545	2.94517
C	0.27475	2.01605	3.00260
C	0.96471	-0.08948	3.92169
C	0.93875	2.67844	4.02308
H	-0.23989	2.58845	2.23965
C	1.63336	0.57368	4.94015
H	0.98621	-1.17154	3.89753
C	1.61974	1.95800	4.99355
H	0.92892	3.76049	4.05630
H	2.16460	0.00548	5.69307
H	2.14172	2.47577	5.78843
C	-2.38343	-0.34253	2.21848
C	-2.63854	-0.81000	3.50533
C	-3.44803	0.03171	1.40919
C	-3.93752	-0.90473	3.97472
H	-1.82052	-1.09987	4.15372
C	-4.75109	-0.06370	1.88034
H	-3.25504	0.39692	0.40388
C	-4.99778	-0.53089	3.16048
H	-4.12431	-1.26882	4.97696

H	-5.57518	0.23028	1.24263
H	-6.01416	-0.60350	3.52712
C	3.93729	0.55781	0.69867
C	4.70687	1.63287	1.15158
C	4.52616	-0.70050	0.57293
C	6.05285	1.45737	1.45267
H	4.22396	2.59924	1.25252
C	5.87394	-0.87823	0.87723
H	3.92829	-1.53703	0.23404
C	6.64031	0.20084	1.31142
H	6.64610	2.29954	1.79551
H	6.32699	-1.85945	0.77252
H	7.69242	0.06265	1.54182
C	-2.76909	3.22698	-1.56687
C	-2.36342	4.55875	-1.47092
C	-4.05306	2.91173	-2.01264
C	-3.24521	5.57565	-1.82073
H	-1.35901	4.77371	-1.12109
C	-4.93224	3.93098	-2.36248
H	-4.34349	1.86866	-2.08007
C	-4.52856	5.26197	-2.26618
H	-2.93399	6.61294	-1.74676
H	-5.93187	3.69024	-2.71066
H	-5.21609	6.05688	-2.53942
O	-0.65033	2.41503	-0.81246
O	-2.19121	0.92067	-1.25173
O	1.82406	-0.18497	-0.13724
O	2.03371	1.95138	0.50292
C	-0.05188	0.03684	-3.10840
H	-0.77002	-0.65554	-3.48892
C	0.78350	0.89172	-2.87409
C	1.81516	1.91599	-2.67941
H	1.63963	2.39661	-1.71026
H	1.68175	2.68361	-3.45195
C	3.24028	1.34461	-2.73663
H	3.45970	0.99256	-3.75269

H	3.30096	0.47032	-2.07990
C	4.27095	2.38277	-2.29899
H	4.23575	3.24480	-2.97855
H	3.98733	2.75315	-1.30599
C	5.68374	1.80754	-2.25283
H	5.99892	1.46031	-3.24326
H	6.40739	2.55322	-1.91030
H	5.73108	0.95609	-1.56430

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XYZ			
Ru	0.28306	0.16645	0.45509
C	-2.40194	-1.01558	-0.08172
C	2.00276	-1.21150	1.75454
P	0.78200	-0.51879	-1.67809
P	0.16756	2.25433	-0.47016
C	0.51876	0.93334	-2.83802
C	1.76531	3.20463	-0.68228
C	2.86026	2.87576	0.10751
C	1.89763	4.23292	-1.61362
C	4.06141	3.55866	-0.02969
H	2.78857	2.06726	0.82573
C	3.09525	4.91422	-1.75352
H	1.06168	4.51480	-2.24131
C	4.18183	4.57848	-0.95882
H	4.90585	3.28809	0.59156
H	3.18064	5.70959	-2.48302
H	5.11895	5.11020	-1.06680
C	-1.04934	3.47019	0.25524
C	-2.30471	2.97572	0.59145
C	-0.75510	4.80538	0.49652
C	-3.25995	3.81110	1.14690
H	-2.50323	1.92185	0.41586
C	-1.71057	5.64031	1.05829
H	0.21960	5.20845	0.25463
C	-2.96445	5.14670	1.38021
H	-4.23604	3.41907	1.40392

H	-1.47219	6.67990	1.24387
H	-3.70891	5.80033	1.81726
C	2.51207	-1.03539	-2.17608
C	2.75248	-1.61421	-3.42056
C	3.58240	-0.80141	-1.32395
C	4.03800	-1.95779	-3.80227
H	1.93179	-1.80496	-4.10136
C	4.87247	-1.14541	-1.70663
H	3.40151	-0.36208	-0.34798
C	5.10302	-1.72273	-2.94371
H	4.21057	-2.40904	-4.77106
H	5.69899	-0.96215	-1.03170
H	6.10894	-1.99163	-3.24090
C	-0.25361	-1.92363	-2.33690
C	-1.33813	-1.72674	-3.18071
C	0.06362	-3.21931	-1.93556
C	-2.08835	-2.80652	-3.62608
H	-1.62048	-0.73158	-3.49689
C	-0.68356	-4.29631	-2.38107
H	0.89704	-3.39137	-1.26522
C	-1.76186	-4.09226	-3.23072
H	-2.93208	-2.63710	-4.28303
H	-0.42543	-5.29801	-2.06147
H	-2.34730	-4.93386	-3.57852
C	-0.42150	1.96427	-2.20893
H	-1.42931	1.55493	-2.09311
H	-0.47062	2.87909	-2.80287
H	0.16334	0.59774	-3.81414
H	1.50877	1.37659	-2.99246
O	2.26613	-0.04610	1.29023
O	0.89758	-1.74645	1.49089
O	-1.88700	-2.06023	0.30194
O	-1.79313	0.13238	-0.15447
C	-3.86059	-1.01481	-0.48345
C	-4.52641	0.13819	-0.90026
C	-4.56006	-2.22241	-0.41083

C	-5.88158	0.08963	-1.21888
H	-3.98170	1.07204	-0.97011
C	-5.91252	-2.27240	-0.72962
H	-4.01776	-3.10797	-0.09606
C	-6.57752	-1.11381	-1.12907
H	-6.39539	0.99222	-1.53585
H	-6.45082	-3.21299	-0.66372
H	-7.63510	-1.14956	-1.37275
C	3.00820	-1.91382	2.60032
C	2.72275	-3.19093	3.08504
C	4.22245	-1.29891	2.90733
C	3.65501	-3.85298	3.87666
H	1.77023	-3.64408	2.83033
C	5.15238	-1.96334	3.69971
H	4.42002	-0.30500	2.52029
C	4.86891	-3.23973	4.18364
H	3.43718	-4.84679	4.25511
H	6.09797	-1.48814	3.94153
H	5.59589	-3.75763	4.80213
C	0.07703	1.26739	2.67572
H	0.75589	2.09128	2.71243
C	-0.68862	0.33456	2.83396
C	-1.63000	-0.75398	3.11342
H	-1.40606	-1.58170	2.43176
H	-1.44124	-1.10802	4.13471
C	-3.09653	-0.32233	2.96296
H	-3.34988	0.40771	3.74238
H	-3.22255	0.18932	2.00312
C	-4.04327	-1.51793	3.02483
H	-3.73342	-2.24086	2.26031
H	-3.93985	-2.02019	3.99599
C	-5.49619	-1.10930	2.79720
H	-5.60928	-0.61097	1.82748
H	-6.16154	-1.97786	2.80413
H	-5.83588	-0.41673	3.57555

XYZ

Ru	-0.05219	-0.03718	0.42687
C	-1.61965	-1.61914	1.67044
C	2.56686	-1.07335	-0.74864
P	-1.03653	-0.38451	-1.61583
P	0.13264	2.20450	-0.07192
C	-0.00474	0.35198	-2.96712
C	1.34976	3.16814	0.98212
C	1.04389	4.38469	1.57709
C	2.61675	2.62514	1.16518
C	1.99141	5.04933	2.34310
H	0.06456	4.82771	1.45117
C	3.56505	3.28980	1.92500
H	2.84466	1.66899	0.70955
C	3.25341	4.50554	2.51682
H	1.74037	5.99676	2.80305
H	4.54851	2.85703	2.05900
H	3.99214	5.02576	3.11338
C	-1.42126	3.24175	0.01879
C	-1.67631	4.30919	-0.83654
C	-2.34894	2.94978	1.01368
C	-2.83493	5.05992	-0.70799
H	-0.97209	4.57289	-1.61441
C	-3.50431	3.70420	1.15027
H	-2.17963	2.11598	1.68429
C	-3.75136	4.76078	0.28783
H	-3.01845	5.88440	-1.38531
H	-4.21462	3.46237	1.93078
H	-4.65462	5.34889	0.39081
C	-1.28467	-2.16534	-2.16059
C	-0.28623	-3.09783	-1.90470
C	-2.44227	-2.57337	-2.81617
C	-0.44889	-4.41689	-2.30552
H	0.62511	-2.80256	-1.38175
C	-2.60267	-3.89168	-3.21030
H	-3.23511	-1.86789	-3.02367

C	-1.60349	-4.81825	-2.95695
H	0.33506	-5.13509	-2.10139
H	-3.51023	-4.19364	-3.71687
H	-1.72736	-5.84893	-3.26494
C	-2.74174	0.35615	-1.87297
C	-3.18756	0.80276	-3.11532
C	-3.61561	0.40864	-0.79312
C	-4.46844	1.30757	-3.26975
H	-2.54310	0.75504	-3.98290
C	-4.90141	0.90723	-0.94856
H	-3.27634	0.06514	0.17986
C	-5.33037	1.36087	-2.18488
H	-4.79608	1.65320	-4.24190
H	-5.56974	0.94155	-0.09748
H	-6.33288	1.75173	-2.30572
C	0.06610	1.88705	-2.92449
H	-0.94378	2.31077	-2.94666
H	0.55310	2.21865	-3.84814
H	-0.37865	0.02140	-3.93945
H	0.99575	-0.07260	-2.83429
C	0.85859	2.48411	-1.75525
H	1.83916	2.00405	-1.69505
H	1.01594	3.55416	-1.91283
C	3.95804	-0.89376	-1.31694
C	4.66448	-2.03664	-1.70021
C	4.55761	0.35929	-1.44693
C	5.95968	-1.92896	-2.19463
H	4.17572	-2.99930	-1.59312
C	5.85604	0.46839	-1.93941
H	4.00970	1.24564	-1.14873
C	6.55938	-0.67553	-2.31083
H	6.50486	-2.82171	-2.48539
H	6.32026	1.44577	-2.03027
H	7.57320	-0.59029	-2.69065
C	-2.52300	-2.48658	2.47490
C	-2.22295	-3.84205	2.61743

C	-3.65856	-1.94769	3.08081
C	-3.06218	-4.65869	3.36767
H	-1.33379	-4.23317	2.13377
C	-4.49491	-2.76709	3.83119
H	-3.86921	-0.89095	2.95574
C	-4.19695	-4.12155	3.97399
H	-2.83343	-5.71375	3.48041
H	-5.37888	-2.35209	4.30522
H	-4.85106	-4.76034	4.55992
O	-1.89887	-0.37980	1.51094
O	-0.57685	-2.08720	1.14413
O	2.14004	-2.22179	-0.59689
O	1.93919	0.00831	-0.44213
C	0.56297	0.50977	2.79822
H	-0.07170	1.30885	3.11352
C	1.30621	-0.43570	2.61635
C	2.22564	-1.56811	2.47259
H	2.14908	-2.18152	3.37913
H	1.88155	-2.18378	1.63428
C	3.68110	-1.13135	2.24859
H	3.71234	-0.38946	1.44399
H	4.06174	-0.63257	3.14907
C	4.57506	-2.31127	1.87541
H	4.56891	-3.04971	2.68824
H	4.14419	-2.80474	0.99577
C	6.00587	-1.87002	1.57813
H	6.46677	-1.41095	2.46002
H	6.62978	-2.71531	1.27265
H	6.02176	-1.13362	0.76629

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XYZ

Ru	-0.51013	0.29152	0.23703
C	-2.88650	-0.40897	0.93258
C	1.77938	-1.53975	0.61397
P	-0.77836	-0.70142	-1.80397
P	0.33895	2.24885	-0.58154

C	-1.47785	1.33285	-3.77974
C	2.09708	2.62950	-0.05259
C	2.35327	2.90723	1.28853
C	3.16199	2.62600	-0.94493
C	3.63823	3.18388	1.72330
H	1.54379	2.91160	2.00657
C	4.45167	2.90072	-0.51021
H	3.00647	2.40915	-1.99256
C	4.69396	3.18302	0.82290
H	3.81638	3.40055	2.76906
H	5.26804	2.89394	-1.22141
H	5.69926	3.39917	1.16126
C	-0.58745	3.80680	-0.06441
C	-1.94298	3.73895	0.23939
C	0.04411	5.04708	-0.03488
C	-2.64798	4.88681	0.57485
H	-2.45507	2.78256	0.22392
C	-0.65786	6.19270	0.30330
H	1.09722	5.12870	-0.27345
C	-2.00836	6.11497	0.60953
H	-3.70244	4.81805	0.81107
H	-0.14976	7.14851	0.32573
H	-2.55860	7.00932	0.87357
C	0.67008	-1.03846	-2.94537
C	1.96120	-0.70704	-2.55761
C	0.47355	-1.62644	-4.19400
C	3.03668	-0.95243	-3.40160
H	2.12789	-0.27420	-1.57744
C	1.54376	-1.86922	-5.03783
H	-0.52253	-1.90493	-4.51565
C	2.83057	-1.53017	-4.64268
H	4.03850	-0.69387	-3.08246
H	1.37528	-2.32607	-6.00474
H	3.66864	-1.72173	-5.30103
C	-1.57632	-2.39420	-1.67527
C	-2.95972	-2.53413	-1.63809

C	-0.78567	-3.53630	-1.59975
C	-3.54090	-3.78836	-1.53286
H	-3.60376	-1.66658	-1.68803
C	-1.36672	-4.79056	-1.49419
H	0.29337	-3.45294	-1.61155
C	-2.74619	-4.92079	-1.46220
H	-4.61942	-3.87782	-1.50560
H	-0.73628	-5.66870	-1.43598
H	-3.19975	-5.90034	-1.38053
C	-1.03075	2.60968	-3.06602
H	-1.79446	2.90240	-2.33534
H	-1.00854	3.41198	-3.81036
H	-2.30238	1.60007	-4.45064
H	-0.66747	0.97434	-4.42622
C	0.36435	2.54824	-2.41413
H	0.96389	1.75914	-2.87782
H	0.89524	3.49072	-2.57360
C	-1.99323	0.19216	-2.89723
H	-2.46480	-0.55708	-3.53945
H	-2.75804	0.56505	-2.20659
C	3.23352	-1.87807	0.85482
C	3.59660	-3.21897	0.99236
C	4.20820	-0.88440	0.95231
C	4.92290	-3.56428	1.23114
H	2.81845	-3.97131	0.91229
C	5.53653	-1.22981	1.18890
H	3.90797	0.15235	0.84814
C	5.89494	-2.56938	1.32963
H	5.20066	-4.60805	1.34200
H	6.29231	-0.45409	1.26780
H	6.93016	-2.83795	1.51811
C	-4.26407	-0.68062	1.43300
C	-4.51842	-1.86326	2.12896
C	-5.28977	0.23810	1.20744
C	-5.80060	-2.12490	2.59977
H	-3.70181	-2.56023	2.28672

C	-6.57101	-0.02665	1.67924
H	-5.06736	1.15044	0.66434
C	-6.82597	-1.20736	2.37515
H	-6.00248	-3.04351	3.14157
H	-7.37149	0.68588	1.50642
H	-7.82654	-1.41279	2.74361
O	-1.95522	-1.22722	1.13728
O	-2.64848	0.67253	0.28863
O	0.94327	-2.44151	0.57508
O	1.52678	-0.27937	0.46341
C	-0.71886	1.48487	2.46649
H	-1.12000	2.46007	2.30164
C	-0.32841	0.39320	2.83334
C	0.13285	-0.90327	3.33358
H	-0.01275	-1.64605	2.54059
H	-0.52006	-1.19478	4.16603
C	1.60012	-0.88778	3.78293
H	1.71581	-0.24079	4.66178
H	2.21099	-0.45261	2.98424
C	2.08861	-2.30053	4.09437
H	1.90690	-2.93113	3.21500
H	1.48911	-2.72185	4.91267
C	3.56995	-2.33280	4.45727
H	3.76705	-1.73625	5.35522
H	3.91221	-3.35421	4.64862
H	4.17475	-1.92495	3.63995

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XYZ

Ru	-0.28444	-0.10712	-0.48686
C	-2.73651	-0.82951	-0.55405
C	0.95096	2.66320	-0.92573
P	-0.25506	-0.22548	1.86611
P	1.78279	-1.14043	-1.10888
C	2.79330	-0.07272	-2.26878
C	2.75260	-0.25712	-3.64569
C	3.55559	0.97519	-1.75804

C	3.47270	0.57243	-4.49262
H	2.15942	-1.05282	-4.07573
C	4.28126	1.79987	-2.60222
H	3.58379	1.16221	-0.69255
C	4.24350	1.59921	-3.97370
H	3.42916	0.41190	-5.56242
H	4.87091	2.60681	-2.18587
H	4.80767	2.24517	-4.63448
C	1.57392	-2.76878	-2.04325
C	0.36189	-3.44555	-2.03910
C	2.66798	-3.35810	-2.67733
C	0.24061	-4.67728	-2.67185
H	-0.50276	-3.01850	-1.54454
C	2.54708	-4.58244	-3.30989
H	3.62928	-2.85964	-2.67920
C	1.32780	-5.24671	-3.31005
H	-0.71250	-5.19079	-2.66154
H	3.40596	-5.02226	-3.80070
H	1.23127	-6.20580	-3.80328
C	1.08159	0.63991	2.85751
C	0.80704	1.17254	4.11601
C	2.36792	0.77119	2.35190
C	1.79364	1.81313	4.84764
H	-0.18805	1.09445	4.53498
C	3.36007	1.41010	3.08201
H	2.60576	0.37985	1.37471
C	3.07574	1.93219	4.33269
H	1.55957	2.22072	5.82286
H	4.35583	1.50236	2.66748
H	3.84760	2.43338	4.90310
C	-1.76388	0.72050	2.45588
C	-2.75767	0.15599	3.24098
C	-1.87304	2.05715	2.07567
C	-3.84878	0.91531	3.64508
H	-2.69407	-0.88000	3.54762
C	-2.95770	2.81366	2.48232

H	-1.10431	2.49185	1.44625
C	-3.94958	2.24307	3.27007
H	-4.61844	0.46319	4.25766
H	-3.03322	3.85137	2.18287
H	-4.79882	2.83481	3.58746
C	3.03937	-1.83468	0.11598
C	2.57002	-2.70074	1.09943
C	4.40652	-1.59975	0.03684
C	3.43927	-3.29750	1.99691
H	1.51351	-2.92281	1.16536
C	5.27994	-2.19393	0.93724
H	4.81065	-0.95373	-0.73000
C	4.80031	-3.04074	1.92203
H	3.05199	-3.96627	2.75527
H	6.34159	-1.99475	0.86173
H	5.48251	-3.50423	2.62330
C	-0.43014	-1.89905	2.69649
C	-1.13918	-2.89625	2.03236
C	0.11746	-2.18390	3.94301
C	-1.30058	-4.14778	2.60664
H	-1.55725	-2.69039	1.05149
C	-0.03980	-3.43710	4.51536
H	0.67880	-1.43084	4.47999
C	-0.75204	-4.42202	3.84986
H	-1.85513	-4.91317	2.07852
H	0.39500	-3.64235	5.48535
H	-0.87635	-5.40018	4.29720
O	0.56275	1.78969	-0.05134
O	0.99086	2.50075	-2.14137
O	-1.81029	-1.70032	-0.65489
O	-2.42335	0.37206	-0.31670
C	-4.16352	-1.21123	-0.72314
C	-5.15781	-0.24393	-0.55897
C	-4.50309	-2.52383	-1.05197
C	-6.49345	-0.59202	-0.72997
H	-4.86574	0.76928	-0.29854

C	-5.83987	-2.86804	-1.22148
H	-3.71232	-3.25638	-1.17325
C	-6.83340	-1.90306	-1.06191
H	-7.26929	0.15666	-0.60383
H	-6.10899	-3.88726	-1.47975
H	-7.87628	-2.17368	-1.19636
C	1.37487	3.99618	-0.34613
C	1.72765	5.01689	-1.23074
C	1.42684	4.22971	1.02800
C	2.12255	6.25980	-0.74784
H	1.68528	4.80771	-2.29431
C	1.82518	5.47250	1.51280
H	1.16054	3.42952	1.70842
C	2.17170	6.48970	0.62614
H	2.39353	7.05043	-1.44106
H	1.86576	5.64795	2.58373
H	2.48079	7.45944	1.00491
C	-0.66953	-0.30273	-2.94415
H	-0.38248	-1.27173	-3.28716
C	-1.10447	0.81625	-2.74344
C	-1.79535	2.10098	-2.60446
H	-1.26689	2.84951	-3.20192
H	-1.72779	2.41795	-1.55875
C	-3.26860	1.97032	-3.01554
H	-3.69744	1.08914	-2.52560
H	-3.33504	1.79649	-4.09689
C	-4.08152	3.20294	-2.63124
H	-3.64418	4.09611	-3.09541
H	-4.00666	3.34846	-1.54564
C	-5.54741	3.06769	-3.03522
H	-6.13190	3.94097	-2.73182
H	-5.64552	2.95688	-4.12025
H	-5.99472	2.18097	-2.57165

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XYZ			
Ru	0.16142	-0.07175	-0.59040

C	1.75786	-1.87990	-1.37012
C	-2.59567	-0.01170	-1.80239
P	-0.73622	-0.98121	1.30193
P	0.06297	1.61139	1.02425
C	-1.22034	0.67199	2.02160
H	-1.20864	0.78672	3.10512
H	-2.19768	0.92475	1.60600
C	-0.62909	3.30716	0.67829
C	-0.08367	4.48320	1.17516
C	-1.72532	3.36549	-0.17667
C	-0.64238	5.70738	0.83649
H	0.78145	4.46075	1.82478
C	-2.28447	4.58852	-0.50890
H	-2.10847	2.42956	-0.58148
C	-1.74552	5.76188	0.00002
H	-0.21210	6.62023	1.22828
H	-3.13933	4.62817	-1.17238
H	-2.18050	6.71839	-0.26161
C	1.45757	1.82607	2.24280
C	2.72528	1.35658	1.92606
C	1.25322	2.41781	3.48832
C	3.77238	1.48313	2.82955
H	2.90077	0.87069	0.97423
C	2.29526	2.54577	4.39090
H	0.27186	2.78457	3.76381
C	3.56045	2.07977	4.06097
H	4.75459	1.11004	2.56832
H	2.12085	3.00861	5.35394
H	4.37631	2.17866	4.76615
C	-2.26223	-2.02854	1.14938
C	-2.30531	-2.97602	0.13209
C	-3.35433	-1.89421	1.99982
C	-3.42306	-3.78180	-0.02689
H	-1.46819	-3.07775	-0.54989
C	-4.47256	-2.69726	1.83840
H	-3.34639	-1.15630	2.79226

C	-4.50736	-3.64426	0.82620
H	-3.44801	-4.51410	-0.82397
H	-5.31862	-2.58196	2.50393
H	-5.38148	-4.27061	0.69951
C	0.30221	-1.81722	2.60861
C	-0.22523	-2.19180	3.84175
C	1.64045	-2.07401	2.33945
C	0.57186	-2.81068	4.79003
H	-1.26739	-2.00597	4.07060
C	2.44024	-2.69429	3.29009
H	2.06038	-1.78442	1.38086
C	1.90852	-3.06318	4.51465
H	0.15038	-3.09794	5.74494
H	3.48210	-2.89021	3.07021
H	2.53231	-3.54803	5.25525
C	-4.08928	0.20444	-1.72961
C	-4.87303	-0.24515	-2.79368
C	-4.70191	0.81786	-0.63686
C	-6.25328	-0.07781	-2.76817
H	-4.37441	-0.72558	-3.62858
C	-6.08363	0.98367	-0.60832
H	-4.09036	1.16600	0.18811
C	-6.86095	0.53727	-1.67485
H	-6.85728	-0.42753	-3.59980
H	-6.55494	1.46161	0.24529
H	-7.93882	0.66779	-1.65348
C	2.74348	-2.87535	-1.87453
C	2.32512	-3.86618	-2.76375
C	4.07487	-2.81477	-1.46146
C	3.24169	-4.79838	-3.23793
H	1.28460	-3.88623	-3.07069
C	4.98867	-3.74880	-1.93724
H	4.37503	-2.03385	-0.77075
C	4.57195	-4.74016	-2.82461
H	2.92106	-5.57022	-3.93049
H	6.02540	-3.70581	-1.61823

H	5.28637	-5.46886	-3.19584
O	0.55070	-1.93311	-1.72407
O	2.13562	-0.95830	-0.56627
O	-1.91116	0.51375	-0.82724
O	-2.12265	-0.64251	-2.74158
C	0.44158	0.79960	-2.85200
H	-0.39095	0.29709	-3.31496
C	1.38189	1.34430	-2.30435
C	2.58961	2.03170	-1.83555
H	3.23725	1.28888	-1.35662
H	2.31969	2.77004	-1.06859
C	3.33549	2.72751	-2.98221
H	2.66515	3.44905	-3.46432
H	3.59555	1.98161	-3.74255
C	4.59739	3.43491	-2.49406
H	4.32579	4.17145	-1.72664
H	5.25426	2.70484	-2.00434
C	5.34853	4.12606	-3.62903
H	4.71643	4.87687	-4.11433
H	6.24923	4.62855	-3.26569
H	5.65138	3.40268	-4.39301

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XYZ

Ru	-0.29763	-0.14961	-0.22637
C	-2.63390	-0.97792	-1.13788
C	1.55343	1.12435	-1.96981
P	-1.37127	1.50784	0.92025
P	0.36735	-0.86050	1.80692
C	-1.34783	1.06396	2.74035
C	1.80840	-0.11360	2.73351
C	2.64912	0.76420	2.06252
C	2.03792	-0.37669	4.08271
C	3.70968	1.36463	2.72908
H	2.45794	0.98006	1.01379
C	3.09567	0.22115	4.74629
H	1.39195	-1.05353	4.62826

C	3.93573	1.09376	4.06811
H	4.35940	2.04947	2.19875
H	3.26520	0.00790	5.79398
H	4.76264	1.56257	4.58701
C	0.51589	-2.71790	1.97691
C	-0.52387	-3.50038	1.48103
C	1.62232	-3.34264	2.53799
C	-0.46093	-4.88211	1.56160
H	-1.37749	-3.02131	1.01242
C	1.68631	-4.72673	2.61433
H	2.44887	-2.75721	2.91871
C	0.64349	-5.49936	2.13091
H	-1.27558	-5.48050	1.17337
H	2.55515	-5.19999	3.05401
H	0.69276	-6.57922	2.19166
C	-0.73317	3.26176	0.93961
C	-1.48192	4.29541	1.49820
C	0.52317	3.53537	0.41857
C	-0.98196	5.58562	1.52897
H	-2.46464	4.09919	1.90978
C	1.02417	4.83070	0.45057
H	1.09950	2.72096	-0.01562
C	0.27469	5.85518	1.00354
H	-1.57169	6.38291	1.96293
H	2.00406	5.03783	0.03920
H	0.66560	6.86483	1.02668
C	-3.16649	1.72040	0.45160
C	-4.19653	1.09773	1.14418
C	-3.47616	2.49438	-0.66409
C	-5.51457	1.25520	0.73872
H	-3.98715	0.47619	2.00446
C	-4.79117	2.65216	-1.06879
H	-2.68591	2.97658	-1.22690
C	-5.81550	2.03410	-0.36573
H	-6.30661	0.76384	1.28950
H	-5.01651	3.25791	-1.93743

H	-6.84364	2.15643	-0.68187
C	-1.08042	-0.43475	2.90031
H	-1.91915	-1.02409	2.51833
H	-0.90141	-0.70354	3.94407
H	-2.26890	1.37367	3.23813
H	-0.52967	1.64058	3.18598
O	1.48572	0.94115	-0.67634
O	0.58233	1.11810	-2.71339
O	-2.04947	-0.17100	-1.89097
O	-2.11020	-1.30585	-0.01012
C	-3.93382	-1.59783	-1.53437
C	-4.57431	-2.50658	-0.69108
C	-4.50210	-1.25910	-2.76333
C	-5.78305	-3.07591	-1.07723
H	-4.11408	-2.75673	0.25871
C	-5.71058	-1.83046	-3.14724
H	-3.98170	-0.54939	-3.39809
C	-6.35077	-2.73818	-2.30484
H	-6.28304	-3.78407	-0.42380
H	-6.15450	-1.56960	-4.10278
H	-7.29388	-3.18423	-2.60593
C	2.94373	1.27512	-2.53723
C	3.08687	1.28670	-3.92609
C	4.07939	1.32640	-1.72728
C	4.35328	1.33502	-4.50030
H	2.18784	1.24430	-4.53190
C	5.34731	1.37894	-2.30097
H	3.96362	1.31996	-0.64959
C	5.48616	1.37873	-3.68829
H	4.45925	1.33600	-5.58091
H	6.22851	1.41509	-1.66651
H	6.47572	1.41335	-4.13497
C	0.32728	-1.88458	-1.90675
H	-0.54196	-1.84754	-2.53000
C	1.38182	-1.90307	-1.30342
C	2.74318	-1.94039	-0.75763

H	2.93924	-0.97418	-0.28125
H	2.82076	-2.72173	0.00816
C	3.78627	-2.17669	-1.86169
H	3.59505	-3.14108	-2.34776
H	3.67217	-1.40058	-2.62787
C	5.20693	-2.14092	-1.30522
H	5.35539	-1.19043	-0.77640
H	5.33155	-2.93875	-0.56102
C	6.25540	-2.27982	-2.40490
H	6.16020	-1.45999	-3.12474
H	7.27012	-2.25834	-1.99669
H	6.13108	-3.22219	-2.94901

3'

100			
XYZ			
Ru	-0.14204	-0.00741	-0.34657
C	1.47050	-1.55035	-1.60067
C	-2.97625	0.28093	-1.33434
P	-0.78355	-1.55798	1.20080
P	-0.06562	1.62807	1.26779
C	-2.15505	-0.91935	2.26623
C	-0.23117	3.37833	0.61344
C	0.64517	4.40366	0.94165
C	-1.29647	3.64344	-0.24213
C	0.45977	5.67806	0.42346
H	1.48116	4.22117	1.60443
C	-1.48399	4.91596	-0.75571
H	-1.97010	2.83445	-0.50557
C	-0.60488	5.93730	-0.42337
H	1.15026	6.46956	0.68602
H	-2.31669	5.11170	-1.41965
H	-0.74958	6.93197	-0.82575
C	1.42126	1.68030	2.40368
C	1.39359	2.30557	3.64838
C	2.60431	1.08157	1.98751
C	2.51708	2.32546	4.45852
H	0.49242	2.78990	4.00107

C	3.73301	1.10369	2.79504
H	2.64878	0.58062	1.02826
C	3.69216	1.72418	4.03252
H	2.47577	2.81439	5.42355
H	4.64549	0.63087	2.45455
H	4.57138	1.74012	4.66437
C	-1.52068	-3.12871	0.48111
C	-2.16997	-3.08722	-0.74840
C	-1.44813	-4.33895	1.16452
C	-2.73451	-4.23988	-1.27796
H	-2.23955	-2.16319	-1.31584
C	-2.00872	-5.48836	0.63229
H	-0.94568	-4.39864	2.12065
C	-2.65589	-5.44095	-0.59259
H	-3.23616	-4.19322	-2.23618
H	-1.93971	-6.42155	1.17636
H	-3.09510	-6.33800	-1.01074
C	0.49848	-2.18986	2.41557
C	0.17629	-2.60324	3.70631
C	1.82284	-2.27446	2.00055
C	1.15453	-3.08276	4.56273
H	-0.84430	-2.55907	4.06214
C	2.80222	-2.75978	2.85514
H	2.08955	-1.93658	1.00407
C	2.47165	-3.16475	4.13801
H	0.88537	-3.39707	5.56308
H	3.82876	-2.81873	2.51611
H	3.23595	-3.54189	4.80585
C	-1.73927	0.26522	3.15140
H	-0.84034	0.01526	3.72852
H	-2.53451	0.42645	3.88746
H	-2.55496	-1.73245	2.87699
H	-2.93765	-0.60734	1.56639
C	-1.53306	1.58486	2.40060
H	-2.38010	1.76843	1.73610
H	-1.47355	2.41810	3.10454

C	-4.42170	0.70265	-1.21540
C	-5.30234	0.34077	-2.23613
C	-4.89746	1.42130	-0.11868
C	-6.64456	0.69676	-2.16198
H	-4.90797	-0.22176	-3.07557
C	-6.24133	1.77612	-0.04154
H	-4.20906	1.70157	0.67121
C	-7.11608	1.41479	-1.06387
H	-7.32535	0.41399	-2.95904
H	-6.60663	2.33562	0.81442
H	-8.16436	1.69229	-1.00480
C	2.47525	-2.31751	-2.38793
C	2.04671	-3.12161	-3.44491
C	3.83221	-2.22746	-2.07526
C	2.97896	-3.83711	-4.18866
H	0.98538	-3.16987	-3.66563
C	4.76182	-2.94386	-2.82149
H	4.14033	-1.59644	-1.24815
C	4.33509	-3.74830	-3.87724
H	2.65019	-4.46368	-5.01176
H	5.81847	-2.87700	-2.58174
H	5.06188	-4.30730	-4.45911
O	1.85798	-0.80768	-0.62840
O	0.24905	-1.60807	-1.88068
O	-2.62362	-0.41032	-2.29230
O	-2.19772	0.68220	-0.38412
C	-0.07334	1.20340	-2.50225
H	-0.97420	0.78925	-2.92015
C	0.97731	1.61714	-2.05063
C	2.29822	2.14463	-1.69039
H	2.20594	2.82279	-0.83275
H	2.92295	1.30221	-1.37448
C	2.95347	2.88509	-2.86446
H	3.03434	2.20060	-3.71719
H	2.30399	3.70986	-3.18132
C	4.33441	3.42217	-2.49619

H	4.24248	4.09838	-1.63635
H	4.96989	2.58940	-2.16917
C	4.99935	4.15380	-3.65920
H	4.39057	5.00382	-3.98434
H	5.98650	4.53366	-3.38160
H	5.12452	3.48686	-4.51836

3'a

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XYZ

Ru	-0.13624	0.06914	-0.03876
C	-2.33552	1.35165	-0.19583
C	1.95055	0.49470	-2.14811
P	0.70065	1.47283	1.52580
P	0.51624	-1.84229	1.03022
C	0.61516	0.27476	4.16439
C	1.65755	-2.92056	0.00920
C	1.16335	-3.49325	-1.16082
C	2.98054	-3.15894	0.35958
C	1.96907	-4.29068	-1.95541
H	0.13696	-3.31956	-1.45764
C	3.78976	-3.95874	-0.43646
H	3.40394	-2.72507	1.25481
C	3.28748	-4.52803	-1.59380
H	1.56664	-4.72879	-2.86010
H	4.81808	-4.13439	-0.14653
H	3.91895	-5.15153	-2.21380
C	-0.85858	-3.03605	1.50606
C	-2.10509	-2.53751	1.86562
C	-0.64269	-4.40959	1.57775
C	-3.11671	-3.39333	2.27944
H	-2.29691	-1.47244	1.81292
C	-1.65280	-5.26621	1.98426
H	0.32161	-4.82461	1.31292
C	-2.89441	-4.75900	2.33788
H	-4.08227	-2.98866	2.55548
H	-1.46866	-6.33218	2.02951
H	-3.68389	-5.42702	2.65845

C	2.53795	1.62353	1.86299
C	3.43545	0.93764	1.05779
C	3.02339	2.43545	2.88687
C	4.80199	1.04776	1.28336
H	3.03889	0.34418	0.23304
C	4.38456	2.54163	3.11315
H	2.34117	2.99608	3.51400
C	5.27784	1.84288	2.31181
H	5.49605	0.51344	0.64679
H	4.75127	3.17287	3.91244
H	6.34300	1.92774	2.48757
C	0.27776	3.23706	1.05417
C	-0.83386	3.89778	1.56272
C	1.08455	3.89347	0.12879
C	-1.12682	5.19393	1.16404
H	-1.49088	3.41012	2.27030
C	0.79224	5.18764	-0.26930
H	1.94950	3.39363	-0.28960
C	-0.31426	5.84333	0.24989
H	-1.99619	5.69524	1.57045
H	1.43050	5.68456	-0.98906
H	-0.54338	6.85472	-0.06053
C	0.49261	-1.21300	3.83273
H	-0.56060	-1.46198	3.66178
H	0.78350	-1.76605	4.73175
H	0.15174	0.42933	5.14551
H	1.67392	0.52993	4.28866
C	1.37275	-1.72944	2.67783
H	2.25496	-1.09257	2.55282
H	1.73213	-2.73458	2.91418
C	-0.05410	1.27005	3.20868
H	-0.06261	2.25325	3.68724
H	-1.09499	0.98628	3.01715
C	3.32883	0.35899	-2.74984
C	3.65101	1.16199	-3.84544
C	4.26788	-0.54818	-2.25986

C	4.90648	1.06983	-4.43649
H	2.89788	1.84922	-4.21598
C	5.52126	-0.64763	-2.85741
H	4.00176	-1.18022	-1.42097
C	5.84406	0.16415	-3.94279
H	5.15440	1.70087	-5.28461
H	6.24720	-1.36047	-2.47764
H	6.82346	0.08831	-4.40606
C	-3.73374	1.76662	-0.50557
C	-3.96890	2.59062	-1.60739
C	-4.80133	1.26745	0.24269
C	-5.27543	2.90970	-1.96339
H	-3.11835	2.95173	-2.17626
C	-6.10690	1.58810	-0.11612
H	-4.59342	0.62346	1.09158
C	-6.34327	2.40717	-1.22029
H	-5.46341	3.54426	-2.82358
H	-6.94080	1.19647	0.45868
H	-7.36289	2.65197	-1.50291
O	-1.37341	1.77989	-0.87536
O	-2.13076	0.47604	0.72069
O	1.09897	1.15483	-2.74033
O	1.76322	-0.12627	-1.02319
C	-1.03804	-0.83251	-2.26907
H	-0.26135	-0.32246	-2.81424
C	-2.01916	-1.29851	-1.72584
C	-3.30665	-1.77402	-1.21103
H	-3.46454	-1.33121	-0.22278
H	-3.28920	-2.86328	-1.08654
C	-4.46513	-1.36358	-2.13496
H	-4.31620	-1.80142	-3.12929
H	-4.45036	-0.27392	-2.26028
C	-5.81490	-1.79466	-1.56757
H	-5.91815	-1.38973	-0.55218
H	-5.84269	-2.88822	-1.47345
C	-6.97866	-1.31256	-2.42859

	H	-6.90192	-1.70615	-3.44765
	H	-7.94146	-1.62940	-2.01709
	H	-6.97778	-0.21897	-2.49051
3'e	113			
	XYZ			
	Ru	-0.26348	0.05564	-0.44794
	C	-2.50703	1.25834	-0.66649
	C	1.80572	0.45062	-2.54096
	P	0.65385	1.71554	0.90516
	P	0.42057	-1.87393	0.71045
	C	0.39664	-3.34977	-0.45053
	C	-0.22145	-4.55465	-0.14282
	C	1.02536	-3.20702	-1.68464
	C	-0.20514	-5.60414	-1.05087
	H	-0.72554	-4.69004	0.80467
	C	1.04736	-4.25693	-2.58798
	H	1.47882	-2.24902	-1.92383
	C	0.43242	-5.45987	-2.27194
	H	-0.69208	-6.53772	-0.79928
	H	1.54133	-4.13478	-3.54374
	H	0.44617	-6.28057	-2.97814
	C	-0.62236	-2.42358	2.17026
	C	-1.86323	-1.84540	2.39993
	C	-0.17660	-3.41875	3.04038
	C	-2.64417	-2.25304	3.47435
	H	-2.22667	-1.06150	1.74694
	C	-0.95240	-3.82447	4.11218
	H	0.78869	-3.88457	2.88559
	C	-2.19282	-3.24138	4.33132
	H	-3.60887	-1.79060	3.64030
	H	-0.58983	-4.59766	4.77747
	H	-2.80156	-3.55739	5.16926
	C	2.50305	2.02463	0.97232
	C	3.00863	3.17433	1.57992
	C	3.38752	1.13654	0.37947
	C	4.37047	3.41584	1.61155

H	2.33626	3.89443	2.02944
C	4.75540	1.37970	0.40725
H	2.99548	0.27253	-0.14484
C	5.24951	2.51345	1.02756
H	4.74794	4.31135	2.08828
H	5.43303	0.68043	-0.06580
H	6.31541	2.70309	1.04926
C	0.10583	3.41120	0.30638
C	-0.46597	4.35635	1.14652
C	0.33287	3.73822	-1.02985
C	-0.81504	5.61022	0.66362
H	-0.64711	4.12745	2.18832
C	-0.01264	4.99156	-1.50782
H	0.75478	3.00418	-1.71091
C	-0.58717	5.93110	-0.66294
H	-1.26255	6.33580	1.33070
H	0.16412	5.23388	-2.54800
H	-0.85762	6.90920	-1.04027
C	2.14261	-1.96865	1.46016
C	2.37666	-1.35581	2.68801
C	3.19546	-2.61950	0.83004
C	3.63199	-1.39119	3.27146
H	1.57126	-0.85159	3.20532
C	4.45510	-2.65394	1.41178
H	3.04422	-3.11328	-0.11990
C	4.67816	-2.04016	2.63284
H	3.79306	-0.91115	4.22849
H	5.26334	-3.16709	0.90599
H	5.66049	-2.06874	3.08691
C	0.10995	1.67609	2.70083
C	-1.25038	1.54935	2.97198
C	0.99710	1.75615	3.76799
C	-1.71117	1.51564	4.27821
H	-1.95006	1.45405	2.14940
C	0.53719	1.71576	5.07649
H	2.06015	1.84777	3.59168

C	-0.81823	1.60067	5.33584
H	-2.77213	1.41910	4.47089
H	1.24375	1.77775	5.89441
H	-1.17739	1.57288	6.35682
O	1.58455	-0.28558	-1.49468
O	1.02937	1.30693	-2.96453
O	-2.25468	0.46801	0.31226
O	-1.56526	1.63661	-1.40234
C	-3.92043	1.61407	-0.96798
C	-4.21061	2.36522	-2.10739
C	-4.95071	1.11664	-0.16708
C	-5.53637	2.61689	-2.44634
H	-3.38857	2.72723	-2.71632
C	-6.27493	1.36752	-0.51069
H	-4.69853	0.52885	0.70985
C	-6.56682	2.11606	-1.65146
H	-5.76819	3.19729	-3.33361
H	-7.07977	0.97727	0.10499
H	-7.60090	2.30814	-1.92163
C	3.10067	0.19078	-3.27018
C	3.37029	0.94108	-4.41612
C	4.02134	-0.76387	-2.83749
C	4.54969	0.73834	-5.12451
H	2.63833	1.67745	-4.73029
C	5.20190	-0.96705	-3.54646
H	3.80762	-1.34038	-1.94524
C	5.46737	-0.21693	-4.69029
H	4.75505	1.32436	-6.01522
H	5.91605	-1.71131	-3.20692
H	6.38886	-0.37648	-5.24260
C	-1.12779	-0.88673	-2.58363
H	-0.48800	-0.30823	-3.22387
C	-1.94688	-1.46996	-1.90001
C	-3.09139	-2.10826	-1.23751
H	-3.20771	-1.66244	-0.24519
H	-2.90619	-3.18087	-1.10631

C	-4.38056	-1.87857	-2.04575
H	-4.30450	-2.39638	-3.00941
H	-4.47329	-0.80821	-2.26608
C	-5.62063	-2.34721	-1.29032
H	-5.66389	-1.82763	-0.32382
H	-5.53648	-3.41868	-1.06646
C	-6.90162	-2.07268	-2.07310
H	-7.78687	-2.40650	-1.52419
H	-7.00612	-0.99974	-2.26775
H	-6.88936	-2.58901	-3.03869

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XYZ			
Ru	-0.53273	0.10141	-0.17683
C	2.28782	-0.42372	-1.50262
C	-2.22945	1.75786	-1.09884
P	-1.67510	-2.02382	-0.68945
P	-0.31355	-1.29317	1.61958
C	-0.65144	-2.85121	0.65563
H	0.29286	-3.13617	0.18499
H	-1.09235	-3.70147	1.17666
C	-1.58946	-1.25550	2.98432
C	-1.68986	-2.28579	3.91615
C	-2.44444	-0.16666	3.08697
C	-2.63218	-2.23111	4.92885
H	-1.02616	-3.14027	3.85873
C	-3.38957	-0.10980	4.10339
H	-2.38188	0.64038	2.36525
C	-3.48509	-1.13995	5.02387
H	-2.70119	-3.03847	5.64676
H	-4.05193	0.74375	4.17325
H	-4.22175	-1.09529	5.81630
C	1.26388	-1.55924	2.58453
C	1.80951	-0.47205	3.26195
C	1.90917	-2.78713	2.65870
C	2.97779	-0.60941	3.99347
H	1.31862	0.49277	3.22002

C	3.08207	-2.92562	3.38769
H	1.50540	-3.65304	2.15052
C	3.61922	-1.83812	4.05606
H	3.38986	0.24525	4.51520
H	3.57436	-3.88889	3.43404
H	4.53369	-1.94638	4.62531
C	-3.42532	-2.32218	-0.12916
C	-4.24049	-1.22856	0.13407
C	-3.92818	-3.60725	0.06300
C	-5.54466	-1.41757	0.57301
H	-3.84279	-0.22375	0.01838
C	-5.22835	-3.79515	0.49971
H	-3.30570	-4.47281	-0.12927
C	-6.04066	-2.69809	0.75255
H	-6.17216	-0.55927	0.77733
H	-5.60943	-4.79804	0.64408
H	-7.05785	-2.84496	1.09397
C	-1.42311	-3.07322	-2.20982
C	-2.47812	-3.60522	-2.94005
C	-0.12179	-3.26227	-2.66696
C	-2.23604	-4.33857	-4.09298
H	-3.50023	-3.45132	-2.61957
C	0.12011	-3.99720	-3.81569
H	0.70658	-2.81485	-2.13046
C	-0.93756	-4.54172	-4.52991
H	-3.06778	-4.74992	-4.65084
H	1.13734	-4.13874	-4.15867
H	-0.74935	-5.11442	-5.42921
C	-3.18429	2.81160	-1.54936
C	-3.04148	3.36821	-2.82155
C	-4.17514	3.27715	-0.68446
C	-3.88590	4.39816	-3.22384
H	-2.26050	2.98728	-3.47216
C	-5.01621	4.30933	-1.08828
H	-4.25956	2.83286	0.30226
C	-4.86942	4.87176	-2.35568

H	-3.77527	4.83651	-4.21072
H	-5.78047	4.68212	-0.41323
H	-5.52286	5.68093	-2.66763
C	3.41883	-1.37636	-1.80763
C	4.32599	-1.06162	-2.82200
C	3.59272	-2.54379	-1.06428
C	5.39485	-1.91069	-3.09343
H	4.17211	-0.15188	-3.39381
C	4.67181	-3.38372	-1.32258
H	2.88765	-2.77122	-0.27152
C	5.57222	-3.06972	-2.33883
H	6.08920	-1.66977	-3.89253
H	4.81234	-4.28336	-0.73148
H	6.41031	-3.72870	-2.54425
O	2.42842	0.75964	-1.90581
O	1.30452	-0.91002	-0.86991
O	-2.35581	1.24769	0.06614
O	-1.27783	1.40509	-1.84140
C	0.84071	1.57809	0.36420
H	1.78016	1.08985	0.61539
C	0.89663	2.75392	-0.17091
C	0.16522	3.95990	-0.61484
H	-0.31809	3.75320	-1.57931
H	0.89014	4.76262	-0.77468
C	-0.86503	4.40793	0.43198
H	-0.32995	4.64811	1.35953
H	-1.54113	3.57709	0.66619
C	-1.66604	5.61984	-0.03920
H	-0.97545	6.43780	-0.28426
H	-2.19752	5.36989	-0.96654
C	-2.66556	6.08919	1.01423
H	-2.15242	6.40695	1.92832
H	-3.26481	6.92959	0.65098
H	-3.35237	5.27873	1.28052
O	3.21008	4.34007	0.88725
C	3.49113	3.39755	0.19938

O	2.57111	2.98003	-0.73838
C	4.76310	2.63058	0.29593
C	5.11146	1.59686	-0.57745
C	5.62038	2.98087	1.34534
C	6.30332	0.90392	-0.38528
H	4.46959	1.31897	-1.40565
C	6.81103	2.29128	1.52679
H	5.32890	3.78977	2.00657
C	7.15063	1.24841	0.66399
H	6.55713	0.08994	-1.05782
H	7.47339	2.56126	2.34277
H	8.07854	0.70456	0.81207
H	2.63999	2.04075	-1.19747

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XYZ			
Ru	-0.53153	-0.20527	0.14886
C	2.20064	-1.08152	-1.27980
C	-1.92780	1.75045	-0.73960
P	-1.93822	-1.71825	-1.04307
P	-0.63344	-1.29166	2.11987
C	-1.24913	-4.39942	-0.11501
C	-1.71108	-0.34274	3.31900
C	-1.36881	0.97915	3.59590
C	-2.84555	-0.87776	3.91604
C	-2.14071	1.74458	4.45384
H	-0.49325	1.41616	3.13130
C	-3.62306	-0.11001	4.77221
H	-3.14313	-1.89955	3.72350
C	-3.27241	1.20102	5.04487
H	-1.85983	2.76970	4.65984
H	-4.50468	-0.54273	5.22784
H	-3.87803	1.79902	5.71394
C	0.92649	-1.61534	3.11945
C	2.11488	-1.90626	2.45913
C	0.91727	-1.61228	4.51033
C	3.27077	-2.18509	3.17301

H	2.13564	-1.90978	1.37646
C	2.07249	-1.88617	5.22622
H	0.00470	-1.39161	5.04968
C	3.25280	-2.17412	4.55877
H	4.18856	-2.40940	2.64412
H	2.04943	-1.87607	6.30863
H	4.15520	-2.38860	5.11718
C	-3.70571	-1.97285	-0.48233
C	-4.29535	-0.99771	0.31494
C	-4.45542	-3.08696	-0.85043
C	-5.60565	-1.14193	0.74874
H	-3.72417	-0.11285	0.58338
C	-5.76218	-3.23307	-0.41369
H	-4.02949	-3.85146	-1.48729
C	-6.33951	-2.26115	0.39013
H	-6.05357	-0.37532	1.36841
H	-6.33237	-4.10604	-0.70485
H	-7.36112	-2.37523	0.73049
C	-2.13257	-1.17685	-2.82913
C	-1.01399	-1.17277	-3.65890
C	-3.34885	-0.74778	-3.34374
C	-1.11490	-0.76123	-4.97731
H	-0.05043	-1.48591	-3.27789
C	-3.45032	-0.33220	-4.66402
H	-4.23242	-0.73312	-2.71913
C	-2.33558	-0.34039	-5.48492
H	-0.23595	-0.76560	-5.60955
H	-4.40671	-0.00166	-5.04924
H	-2.41462	-0.01725	-6.51504
C	-0.50623	-3.92654	1.14027
H	0.42026	-3.43112	0.82637
H	-0.20416	-4.80625	1.71602
H	-0.77372	-5.32129	-0.47127
H	-2.27723	-4.67196	0.15128
C	-1.33609	-3.00519	2.06432
H	-2.36347	-2.91462	1.69491

H	-1.39247	-3.41536	3.07602
C	-1.24245	-3.42600	-1.29966
H	-1.74301	-3.88675	-2.15566
H	-0.20610	-3.22812	-1.59399
C	-2.70993	2.96077	-1.12734
C	-2.43913	3.58860	-2.34439
C	-3.66772	3.48829	-0.26041
C	-3.13038	4.74324	-2.69510
H	-1.68491	3.15817	-2.99544
C	-4.35741	4.64357	-0.61462
H	-3.85198	2.98717	0.68405
C	-4.08865	5.27062	-1.83029
H	-2.92230	5.23459	-3.64038
H	-5.10196	5.05833	0.05762
H	-4.62588	6.17385	-2.10361
C	2.93331	-2.22665	-1.93842
C	3.92733	-1.95925	-2.88125
C	2.63819	-3.55036	-1.60762
C	4.60949	-3.00385	-3.49612
H	4.14593	-0.92578	-3.12633
C	3.32629	-4.59579	-2.21546
H	1.87614	-3.74996	-0.86128
C	4.31061	-4.32377	-3.16337
H	5.37538	-2.79010	-4.23534
H	3.09691	-5.62294	-1.94894
H	4.84535	-5.13931	-3.64071
O	2.66466	0.06777	-1.51311
O	1.20150	-1.39470	-0.57186
O	-1.01705	1.31295	-1.48922
O	-2.15451	1.19003	0.38676
C	1.05660	1.05792	0.84132
H	1.91783	0.45469	1.10696
C	1.23502	2.19693	0.27384
C	0.66695	3.44863	-0.24474
H	-0.37064	3.44818	0.11084
H	0.64002	3.42544	-1.34079

C	1.35127	4.72460	0.25430
H	2.38109	4.75729	-0.11872
H	1.42033	4.70120	1.34784
C	0.58785	5.96540	-0.20584
H	-0.44215	5.91920	0.17168
H	0.51047	5.95730	-1.30101
C	1.25352	7.25850	0.25684
H	2.27290	7.33420	-0.13584
H	0.69703	8.13876	-0.07769
H	1.31673	7.29432	1.34936
O	2.94180	2.22756	-0.38325
C	3.98493	2.40760	0.47691
C	5.25988	1.73349	0.09581
C	6.26628	1.68097	1.06426
C	5.47586	1.18965	-1.17249
C	7.47733	1.06701	0.77263
H	6.07550	2.12462	2.03579
C	6.69267	0.57905	-1.46016
H	4.70103	1.24048	-1.92852
C	7.68945	0.51349	-0.48980
H	8.25636	1.01896	1.52653
H	6.86138	0.15295	-2.44401
H	8.63563	0.03248	-0.71791
O	3.85051	3.08555	1.46133
H	2.83738	1.25242	-0.85955

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XYZ

Ru	-0.36626	-0.08107	-0.04345
C	2.00197	0.30438	-1.83434
C	-2.46237	0.99121	-1.01093
P	-1.20934	-2.52404	-0.35970
P	0.05278	-1.23723	1.86675
C	-1.02389	-2.72089	1.50295
H	-0.68288	-3.69054	1.86717
H	-1.99411	-2.49751	1.95571
C	-0.55882	-0.63527	3.52376

C	-0.40463	-1.40320	4.67579
C	-1.20183	0.59151	3.60792
C	-0.88446	-0.94947	5.89208
H	0.09687	-2.36246	4.62952
C	-1.68324	1.04809	4.82872
H	-1.32331	1.19905	2.71812
C	-1.52568	0.27969	5.96982
H	-0.75828	-1.55336	6.78160
H	-2.17966	2.00870	4.88372
H	-1.89969	0.63601	6.92156
C	1.77175	-1.85652	2.26424
C	2.64770	-0.99104	2.91601
C	2.23063	-3.11141	1.88681
C	3.94907	-1.37705	3.18992
H	2.31366	-0.00558	3.21767
C	3.53509	-3.49942	2.15969
H	1.58037	-3.80638	1.37324
C	4.39726	-2.63501	2.81221
H	4.61575	-0.69307	3.70015
H	3.87484	-4.48290	1.86018
H	5.41424	-2.93789	3.02630
C	-2.95503	-3.05217	-0.74532
C	-3.53158	-2.59021	-1.92488
C	-3.70265	-3.87452	0.09033
C	-4.82767	-2.94502	-2.26468
H	-2.96770	-1.94289	-2.58619
C	-5.00098	-4.22769	-0.24641
H	-3.28247	-4.24915	1.01479
C	-5.56592	-3.76483	-1.42430
H	-5.26296	-2.57666	-3.18514
H	-5.57156	-4.86758	0.41490
H	-6.57982	-4.04052	-1.68592
C	-0.17848	-3.92103	-1.05610
C	-0.63948	-5.23284	-1.10682
C	1.09468	-3.63802	-1.53791
C	0.15718	-6.24050	-1.62724

H	-1.62928	-5.47947	-0.74423
C	1.89502	-4.64540	-2.05654
H	1.47134	-2.62283	-1.50350
C	1.42696	-5.94895	-2.10315
H	-0.21530	-7.25658	-1.66157
H	2.88499	-4.40959	-2.42623
H	2.04874	-6.73650	-2.51025
C	-3.67718	1.69128	-1.50831
C	-3.69379	2.21748	-2.80104
C	-4.77148	1.86894	-0.66000
C	-4.80394	2.92980	-3.24215
H	-2.82781	2.07049	-3.43786
C	-5.87973	2.58211	-1.10443
H	-4.72873	1.45780	0.34358
C	-5.89393	3.11575	-2.39257
H	-4.81844	3.34652	-4.24418
H	-6.72824	2.73262	-0.44437
H	-6.75652	3.67927	-2.73482
C	3.38206	0.20292	-2.36295
C	3.68818	0.65268	-3.64954
C	4.37324	-0.34511	-1.54868
C	4.99049	0.54418	-4.12259
H	2.90527	1.08152	-4.26550
C	5.67809	-0.43522	-2.02075
H	4.11091	-0.67781	-0.54976
C	5.98533	0.00522	-3.30683
H	5.23235	0.88260	-5.12490
H	6.45554	-0.84867	-1.38657
H	7.00352	-0.07194	-3.67596
O	1.21926	1.11442	-2.51152
O	1.64512	-0.35254	-0.85232
O	-2.42566	0.55222	0.17325
O	-1.44590	0.87013	-1.77257
C	0.39605	1.65622	0.70387
H	1.23575	1.47411	1.38342
C	0.13290	2.95813	0.55122

C	-0.93992	3.67602	-0.21715
H	-1.25493	3.07838	-1.07446
H	-0.50954	4.60480	-0.61645
C	-2.14962	4.03506	0.65726
H	-1.79385	4.54472	1.56206
H	-2.63116	3.10440	0.98564
C	-3.16339	4.91928	-0.06576
H	-2.67481	5.85484	-0.36897
H	-3.48927	4.42495	-0.99050
C	-4.37903	5.23231	0.80238
H	-4.08573	5.77966	1.70478
H	-5.11534	5.83623	0.26293
H	-4.87275	4.30726	1.12001
O	2.58869	3.83631	2.68937
C	2.17483	3.71145	1.56536
O	0.86552	3.92301	1.28743
C	3.09033	3.43905	0.40771
C	2.73333	3.72177	-0.91241
C	4.38016	2.99196	0.69802
C	3.66625	3.56201	-1.93131
H	1.73247	4.07488	-1.13841
C	5.30720	2.81979	-0.32476
H	4.63976	2.79998	1.73393
C	4.95310	3.11235	-1.63963
H	3.38617	3.78128	-2.95720
H	6.30725	2.46314	-0.09766
H	5.67356	2.97394	-2.44028
H	0.29737	1.13123	-2.15276

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XYZ

Ru	-0.47674	-0.32325	0.03589
C	0.03602	-2.84596	-1.60668
C	-1.20964	1.76387	-1.22278
P	-2.89059	-0.74622	0.52272
P	0.20310	-0.58245	2.18772
C	-2.93362	-2.94142	2.44621

C	0.54292	1.07591	2.98511
C	1.55440	1.87099	2.45087
C	-0.19462	1.56044	4.05921
C	1.82001	3.12134	2.98704
H	2.15356	1.52376	1.61535
C	0.06910	2.81409	4.59098
H	-0.98655	0.97094	4.49969
C	1.07760	3.59808	4.05695
H	2.61258	3.72433	2.56232
H	-0.51616	3.17492	5.42707
H	1.28502	4.57592	4.47277
C	1.72153	-1.59747	2.63855
C	2.04017	-2.73016	1.89747
C	2.52010	-1.26959	3.72922
C	3.13186	-3.51576	2.23475
H	1.43455	-3.00347	1.04369
C	3.61500	-2.05044	4.06691
H	2.29552	-0.39372	4.32484
C	3.92363	-3.17673	3.32042
H	3.36608	-4.39320	1.64536
H	4.22795	-1.77761	4.91669
H	4.77855	-3.78685	3.58295
C	-3.80480	0.36675	1.71498
C	-3.28361	1.63350	1.95770
C	-4.98773	-0.01054	2.34408
C	-3.92919	2.50360	2.82480
H	-2.37080	1.94113	1.45365
C	-5.62918	0.85688	3.21357
H	-5.42485	-0.98330	2.15957
C	-5.09963	2.11562	3.45727
H	-3.51452	3.48731	3.00573
H	-6.54692	0.55051	3.69927
H	-5.60233	2.79313	4.13616
C	-3.92004	-0.60617	-1.04124
C	-3.76894	-1.55648	-2.04793
C	-4.80328	0.44624	-1.24560

C	-4.49495	-1.46423	-3.22353
H	-3.07763	-2.37966	-1.92396
C	-5.52931	0.54201	-2.42440
H	-4.93490	1.20466	-0.48495
C	-5.37996	-0.41349	-3.41531
H	-4.36651	-2.21368	-3.99437
H	-6.21390	1.36900	-2.56553
H	-5.94666	-0.33955	-4.33465
C	-1.44436	-2.80214	2.78816
H	-0.86028	-3.08404	1.90316
H	-1.19167	-3.52849	3.56606
H	-3.21818	-3.99725	2.52800
H	-3.53148	-2.40692	3.19389
C	-1.05199	-1.39344	3.28884
H	-1.92790	-0.73636	3.29095
H	-0.68037	-1.43192	4.31630
C	-3.32183	-2.49181	1.03232
H	-4.38733	-2.67015	0.86604
H	-2.77416	-3.10646	0.30862
C	-1.56093	3.03720	-1.91270
C	-1.89076	3.01705	-3.26876
C	-1.50940	4.24644	-1.21770
C	-2.15998	4.21002	-3.93177
H	-1.91855	2.06238	-3.78417
C	-1.78029	5.43742	-1.88357
H	-1.23924	4.23551	-0.16652
C	-2.10087	5.41969	-3.24038
H	-2.40985	4.19956	-4.98805
H	-1.73035	6.38107	-1.34912
H	-2.30398	6.35098	-3.76042
C	-0.16924	-4.24246	-2.06288
C	0.19741	-4.63225	-3.35305
C	-0.73999	-5.16370	-1.18145
C	-0.01461	-5.94492	-3.75953
H	0.64199	-3.90543	-4.02356
C	-0.94635	-6.47474	-1.59186

H	-1.00722	-4.84129	-0.18000
C	-0.58526	-6.86422	-2.88117
H	0.26650	-6.25185	-4.76146
H	-1.38682	-7.19379	-0.90899
H	-0.74791	-7.88859	-3.20161
O	0.61196	-2.05875	-2.47879
O	-0.32801	-2.47917	-0.48345
O	-1.21484	0.66978	-1.85464
O	-0.86509	1.79087	0.00378
C	1.51694	-0.10547	-0.53722
H	2.19590	-0.81626	-0.05338
C	2.19508	0.68342	-1.37998
C	1.77718	1.81353	-2.27581
H	0.74794	1.66739	-2.60708
H	2.40823	1.78034	-3.17374
C	1.93252	3.18553	-1.60379
H	2.93879	3.27155	-1.17250
H	1.23006	3.24116	-0.76222
C	1.68931	4.34158	-2.57195
H	0.69755	4.23407	-3.03047
H	2.41811	4.28583	-3.39180
C	1.79120	5.70051	-1.88491
H	2.79315	5.85641	-1.47024
H	1.57895	6.52011	-2.57864
H	1.07538	5.76700	-1.05835
O	3.60390	0.47991	-1.51418
C	4.41327	0.84038	-0.50582
C	5.84737	0.54916	-0.81392
C	6.79814	0.88913	0.14964
C	6.24475	-0.04084	-2.01491
C	8.14499	0.63972	-0.08634
H	6.45800	1.34642	1.07284
C	7.59387	-0.28948	-2.24747
H	5.49580	-0.29842	-2.75513
C	8.54303	0.05007	-1.28529
H	8.88514	0.90446	0.66211

H	7.90581	-0.74788	-3.18059
H	9.59514	-0.14473	-1.47038
O	4.04702	1.34670	0.52803
H	0.82185	-1.17846	-2.05460

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XYZ			
Ru	0.27146	0.46641	-0.27156
C	2.32943	1.45476	-1.47214
C	-2.15446	-1.24059	-0.73522
P	1.09734	-1.74283	0.18281
P	-0.31877	-0.09244	1.86196
C	0.40543	-1.83170	1.94186
H	1.18375	-1.95604	2.71435
H	-0.37485	-2.59725	2.03660
C	-2.07864	-0.12116	2.54008
C	-2.56029	-1.14906	3.34425
C	-2.92135	0.94015	2.23056
C	-3.86031	-1.11677	3.82518
H	-1.92840	-1.98953	3.60021
C	-4.22052	0.97510	2.71384
H	-2.56632	1.74631	1.60192
C	-4.69357	-0.05408	3.51223
H	-4.22259	-1.92537	4.44745
H	-4.86585	1.80754	2.46333
H	-5.70853	-0.02956	3.88794
C	0.58566	0.81680	3.27304
C	1.62336	1.69032	2.97450
C	0.24187	0.61823	4.60766
C	2.30204	2.35360	3.98798
H	1.91707	1.85411	1.94444
C	0.91633	1.28042	5.62040
H	-0.56367	-0.05583	4.86960
C	1.95027	2.15212	5.31209
H	3.10973	3.03031	3.73895
H	0.63470	1.11558	6.65274
H	2.47871	2.67050	6.10216

C	0.55850	-3.25521	-0.78782
C	0.53414	-3.15441	-2.17472
C	0.19407	-4.45604	-0.18857
C	0.15505	-4.23925	-2.95086
H	0.80482	-2.22141	-2.65536
C	-0.18851	-5.53918	-0.96497
H	0.19968	-4.55754	0.88913
C	-0.20701	-5.43352	-2.34715
H	0.13837	-4.14871	-4.02962
H	-0.47279	-6.46839	-0.48766
H	-0.50639	-6.27987	-2.95233
C	2.94461	-2.07148	0.46389
C	3.45719	-3.36171	0.55761
C	3.80574	-0.99142	0.61659
C	4.80606	-3.56901	0.79822
H	2.80797	-4.21949	0.43869
C	5.15600	-1.19927	0.85987
H	3.41826	0.01908	0.52518
C	5.65923	-2.48677	0.95212
H	5.19142	-4.57842	0.86637
H	5.81782	-0.35003	0.97421
H	6.71320	-2.64822	1.14015
C	-3.35560	-1.59679	-1.57640
C	-4.19101	-2.65259	-1.15831
C	-3.65700	-0.90534	-2.76811
C	-5.31501	-3.00890	-1.91689
H	-3.93498	-3.17873	-0.23296
C	-4.77934	-1.26589	-3.52772
H	-2.99741	-0.09226	-3.08610
C	-5.61185	-2.31653	-3.10370
H	-5.96117	-3.82998	-1.58424
H	-5.00601	-0.72753	-4.45580
H	-6.48922	-2.59669	-3.69876
C	3.51802	2.06112	-2.13275
C	3.62684	2.02871	-3.53918
C	4.53341	2.66942	-1.36501

C	4.74152	2.59842	-4.16900
H	2.82941	1.55197	-4.11817
C	5.64570	3.23904	-1.99944
H	4.43636	2.68641	-0.27489
C	5.75194	3.20439	-3.40123
H	4.82470	2.57010	-5.26157
H	6.43365	3.71044	-1.40070
H	6.62346	3.64937	-3.89564
O	1.39153	0.91650	-2.15306
O	2.22505	1.46364	-0.17144
O	-1.47856	-0.20896	-1.16261
O	-1.86978	-1.91734	0.28444
C	-0.58063	2.29454	-0.33869
H	0.23982	3.07258	-0.00125
C	-1.17932	3.40950	-0.46949
C	-1.88070	4.68326	-0.62834
H	-1.30112	5.36917	-1.27758
H	-2.02231	5.18572	0.34936
C	-3.27549	4.42540	-1.28101
H	-3.84874	3.72443	-0.64637
H	-3.12865	3.92634	-2.25642
C	-4.06204	5.73709	-1.46566
H	-4.18697	6.23143	-0.48178
H	-3.47030	6.43410	-2.09170
C	-5.44003	5.50629	-2.10804
H	-6.06429	4.83762	-1.48769
H	-5.98549	6.45877	-2.22988
H	-5.34364	5.04329	-3.10700

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103			
XYZ			
Ru	-0.02714	0.05085	0.24269
C	-1.34059	-0.69860	2.34182
C	2.72051	-0.85303	-0.94452
P	-1.64998	-0.87033	-1.27088
P	0.26340	1.95138	-0.98635
C	0.02683	-0.41207	-3.64684

C	1.37095	3.30475	-0.23363
C	0.86711	4.53141	0.17838
C	2.73336	3.05201	-0.09753
C	1.70968	5.49740	0.71060
H	-0.18815	4.75138	0.08827
C	3.57308	4.01987	0.42988
H	3.12683	2.07664	-0.37568
C	3.06554	5.24644	0.83277
H	1.30184	6.44918	1.02631
H	4.63151	3.81448	0.52896
H	3.72393	6.00114	1.24386
C	-1.31734	2.94273	-1.32535
C	-2.31285	2.94880	-0.35499
C	-1.50372	3.70546	-2.47456
C	-3.47625	3.68271	-0.53573
H	-2.18119	2.37763	0.55591
C	-2.66837	4.43358	-2.66135
H	-0.73822	3.74983	-3.23710
C	-3.66001	4.42241	-1.69262
H	-4.24071	3.67478	0.23086
H	-2.79805	5.01693	-3.56417
H	-4.56871	4.99293	-1.83706
C	-1.65713	-2.75804	-1.10610
C	-2.79923	-3.52859	-1.28944
C	-0.45871	-3.38370	-0.78207
C	-2.74409	-4.90715	-1.15226
H	-3.74525	-3.06475	-1.53395
C	-0.40474	-4.76341	-0.64941
H	0.42934	-2.77273	-0.64281
C	-1.54658	-5.52750	-0.83294
H	-3.64051	-5.49691	-1.29481
H	0.53332	-5.24238	-0.39887
H	-1.50502	-6.60417	-0.72591
C	-3.48862	-0.43698	-1.08894
C	-3.95509	0.04942	0.12663
C	-4.39886	-0.60968	-2.13008

C	-5.29808	0.35263	0.30005
H	-3.25414	0.21346	0.93803
C	-5.73936	-0.30318	-1.95914
H	-4.07703	-0.98903	-3.09021
C	-6.19439	0.17688	-0.74087
H	-5.64304	0.73105	1.25401
H	-6.43057	-0.44381	-2.78033
H	-7.24218	0.41421	-0.60642
C	0.44013	1.06862	-3.83325
H	-0.43928	1.64260	-4.18435
H	1.16960	1.11352	-4.66594
H	0.08766	-0.89528	-4.64060
H	0.75427	-0.93088	-3.00032
C	1.12175	1.80251	-2.65714
H	2.06848	1.29839	-2.39485
H	1.39324	2.82634	-2.97702
C	-1.41899	-0.62543	-3.13354
H	-1.87086	-1.50375	-3.62802
H	-2.04249	0.24512	-3.41112
C	3.52255	-1.93630	-1.64828
C	4.92629	-1.79409	-1.68055
C	2.93735	-3.04725	-2.28900
C	5.72826	-2.74592	-2.32447
H	5.36275	-0.91621	-1.19413
C	3.73923	-3.99736	-2.94071
H	1.85173	-3.16389	-2.28271
C	5.13640	-3.85292	-2.95731
H	6.81790	-2.62309	-2.33725
H	3.26956	-4.85492	-3.43731
H	5.76140	-4.59772	-3.46452
C	-2.06154	-1.06692	3.59147
C	-1.91237	-2.36394	4.12650
C	-2.88840	-0.12874	4.24469
C	-2.58617	-2.71724	5.30346
H	-1.26724	-3.07809	3.60453
C	-3.55866	-0.48646	5.42230

H	-2.99377	0.87372	3.81782
C	-3.40930	-1.78017	5.95301
H	-2.47070	-3.72596	5.71645
H	-4.20031	0.24392	5.92858
H	-3.93546	-2.05840	6.87375
O	-0.55694	-1.52222	1.75743
O	-1.49978	0.48596	1.81808
O	3.32533	0.16435	-0.53384
O	1.43106	-1.08643	-0.85246
C	1.39225	0.59968	1.57425
H	0.86260	1.13174	2.48899
C	2.35967	0.77651	2.37499
C	3.51513	1.01301	3.23504
H	3.28930	0.74051	4.28449
H	3.80817	2.08163	3.21637
C	4.69981	0.13425	2.71682
H	4.82029	0.29997	1.63133
H	4.43193	-0.93069	2.84568
C	6.00410	0.45386	3.47052
H	5.84844	0.30876	4.55848
H	6.25450	1.52448	3.33201
C	7.17930	-0.41684	2.99506
H	7.37547	-0.26774	1.91778
H	8.10524	-0.17005	3.54443
H	6.97064	-1.49096	3.15143

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XYZ

Ru	-0.37220	0.51945	0.75857
C	-2.53471	0.49616	2.06216
C	2.23266	-0.88861	0.33802
P	-1.00443	-1.56882	-0.88581
P	0.14787	1.03267	-1.46968
C	-0.36732	-0.53607	-2.32566
H	-1.13324	-0.36285	-3.08259
H	0.50032	-1.01847	-2.76680
C	1.80671	1.58859	-2.11509

C	2.36436	1.09014	-3.28731
C	2.48494	2.57712	-1.41089
C	3.58602	1.56429	-3.73989
H	1.85720	0.32467	-3.85932
C	3.70503	3.05341	-1.86572
H	2.06350	2.97873	-0.49811
C	4.25945	2.54658	-3.03056
H	4.01130	1.16471	-4.65183
H	4.22355	3.82156	-1.30597
H	5.21331	2.91606	-3.38528
C	-0.96118	2.33952	-2.23910
C	-1.69207	3.20545	-1.43842
C	-1.04471	2.47294	-3.62367
C	-2.49987	4.18173	-2.00799
H	-1.64411	3.11996	-0.36007
C	-1.84950	3.44395	-4.19394
H	-0.47514	1.81739	-4.27095
C	-2.58121	4.30221	-3.38459
H	-3.06603	4.84806	-1.36950
H	-1.90495	3.53408	-5.27140
H	-3.21085	5.06281	-3.82901
C	-0.13223	-3.20595	-0.97074
C	0.09336	-3.88885	0.22014
C	0.29864	-3.77380	-2.16572
C	0.73788	-5.11663	0.21805
H	-0.22980	-3.45947	1.16119
C	0.94575	-4.99972	-2.16827
H	0.13459	-3.26592	-3.10751
C	1.16624	-5.67379	-0.97681
H	0.90881	-5.63578	1.15267
H	1.27760	-5.42953	-3.10491
H	1.67253	-6.63095	-0.98008
C	-2.76261	-1.93281	-1.41016
C	-3.12335	-3.09585	-2.08080
C	-3.74119	-0.98502	-1.12557
C	-4.43820	-3.30607	-2.46770

H	-2.38247	-3.85217	-2.30499
C	-5.05481	-1.19387	-1.51666
H	-3.47779	-0.08539	-0.57761
C	-5.40629	-2.35392	-2.18984
H	-4.70549	-4.21692	-2.98836
H	-5.80769	-0.44969	-1.28937
H	-6.43285	-2.51819	-2.49256
C	3.55723	-1.37025	0.86504
C	4.55291	-1.75427	-0.03378
C	3.80150	-1.41945	2.23886
C	5.79254	-2.17421	0.43919
H	4.33494	-1.71280	-1.09587
C	5.03716	-1.85213	2.71075
H	3.01304	-1.11624	2.92013
C	6.03478	-2.22472	1.81128
H	6.57025	-2.46444	-0.26044
H	5.22539	-1.89217	3.77951
H	7.00161	-2.55438	2.17942
C	-3.83314	0.48325	2.78674
C	-3.91735	-0.13778	4.03375
C	-4.95568	1.09189	2.22366
C	-5.12887	-0.15237	4.71590
H	-3.02767	-0.59983	4.44858
C	-6.16503	1.07675	2.90977
H	-4.86294	1.57308	1.25596
C	-6.25155	0.45420	4.15417
H	-5.19975	-0.63526	5.68534
H	-7.04054	1.55028	2.47687
H	-7.19675	0.44279	4.68851
O	-1.50041	-0.00350	2.58163
O	-2.46173	1.01625	0.89393
O	1.47161	-0.35250	1.22143
O	1.95552	-1.01062	-0.86265
C	0.28269	2.01224	1.51443
H	0.77649	3.95889	2.08462
C	0.97452	2.89469	2.18269

C	2.11642	2.38731	3.06179
H	1.85238	1.39842	3.45103
H	2.21509	3.05993	3.92177
C	3.43939	2.27868	2.30012
H	3.68151	3.23889	1.82503
H	3.30153	1.54708	1.49430
C	4.60203	1.83651	3.18601
H	4.79474	2.59853	3.95271
H	4.31738	0.92124	3.72051
C	5.86693	1.57438	2.37238
H	6.19789	2.48515	1.86111
H	6.68802	1.22503	3.00573
H	5.68079	0.80747	1.61193

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	103		
	XYZ		
Ru	-0.29755	0.42543	0.28798
C	-2.56799	0.22446	1.41696
C	2.13895	-1.16175	-0.61102
P	-1.47381	-1.22256	-1.55275
P	0.82368	2.05527	-1.00888
C	-0.23257	-0.17387	-3.84984
C	2.55339	2.49938	-0.43363
C	2.72525	3.45778	0.56147
C	3.67604	1.88061	-0.96954
C	3.99343	3.80053	1.00057
H	1.86632	3.94966	0.99943
C	4.94657	2.22378	-0.52944
H	3.56331	1.10631	-1.71736
C	5.10963	3.18654	0.45265
H	4.10916	4.55017	1.77298
H	5.81114	1.73179	-0.95682
H	6.10132	3.45473	0.79437
C	-0.02231	3.74176	-0.95288
C	-1.28025	3.91018	-0.39238
C	0.61325	4.85144	-1.51189
C	-1.89063	5.15959	-0.39191

H	-1.80115	3.07136	0.05297
C	0.00802	6.09488	-1.51046
H	1.59948	4.75279	-1.94814
C	-1.25207	6.25236	-0.94898
H	-2.87253	5.27271	0.04991
H	0.51919	6.94363	-1.94660
H	-1.72881	7.22453	-0.94648
C	-0.70382	-2.89866	-1.26844
C	-0.74884	-3.42105	0.02373
C	-0.05907	-3.62164	-2.26300
C	-0.17842	-4.65059	0.30554
H	-1.22763	-2.85646	0.81573
C	0.51909	-4.85142	-1.97787
H	0.01158	-3.23923	-3.27197
C	0.45665	-5.37097	-0.69659
H	-0.22431	-5.04571	1.31243
H	1.02023	-5.40154	-2.76411
H	0.90686	-6.33051	-0.47565
C	-3.31051	-1.51607	-1.31375
C	-4.16739	-0.42112	-1.39458
C	-3.85698	-2.77688	-1.11048
C	-5.53760	-0.58277	-1.27198
H	-3.76526	0.57295	-1.54700
C	-5.22908	-2.94026	-0.98213
H	-3.21723	-3.64748	-1.05149
C	-6.07301	-1.84512	-1.06326
H	-6.18867	0.27989	-1.33625
H	-5.63758	-3.93020	-0.82236
H	-7.14349	-1.97320	-0.96463
C	-0.31570	1.32235	-3.47966
H	-1.16359	1.48602	-2.79852
H	-0.55252	1.90520	-4.37537
H	-0.12330	-0.27487	-4.93517
H	0.65931	-0.61647	-3.39739
C	0.97710	1.86962	-2.85005
H	1.80936	1.19588	-3.04275

H	1.22866	2.85501	-3.24877
C	-1.47203	-0.94800	-3.39943
H	-1.57591	-1.90272	-3.91872
H	-2.37756	-0.37269	-3.62079
C	3.21361	-2.16289	-0.26418
C	4.28578	-2.34435	-1.13865
C	3.15594	-2.89348	0.92395
C	5.30039	-3.24246	-0.82191
H	4.30412	-1.77058	-2.05916
C	4.16530	-3.80024	1.23499
H	2.31407	-2.73781	1.59091
C	5.24055	-3.97166	0.36499
H	6.13778	-3.37648	-1.49979
H	4.11781	-4.36793	2.15968
H	6.03206	-4.67295	0.61155
C	-3.87626	0.18782	2.12482
C	-4.19426	-0.91109	2.92404
C	-4.77309	1.24916	1.99460
C	-5.41405	-0.94894	3.59059
H	-3.47644	-1.71980	3.01103
C	-5.99107	1.20852	2.66416
H	-4.50054	2.09331	1.37032
C	-6.31145	0.10988	3.46052
H	-5.66599	-1.80191	4.21268
H	-6.69130	2.03217	2.56739
H	-7.26304	0.07967	3.98263
O	-1.72705	-0.70740	1.56743
O	-2.28092	1.20549	0.65322
O	2.13378	-0.62019	-1.72271
O	1.30114	-0.94113	0.33381
C	0.47065	1.11592	1.77009
H	1.09418	2.27334	3.37975
C	1.13431	1.31045	2.87607
C	2.01989	0.18782	3.40928
H	1.55261	-0.77422	3.17452
H	2.06114	0.27225	4.50145

C	3.42601	0.21688	2.80685
H	3.86784	1.21455	2.92827
H	3.32907	0.04067	1.72839
C	4.35233	-0.83454	3.41459
H	3.85067	-1.81033	3.39710
H	4.53623	-0.59822	4.47100
C	5.67437	-0.93341	2.65788
H	6.21321	0.02011	2.68777
H	6.32539	-1.70348	3.08286
H	5.49509	-1.18833	1.60723

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XYZ

Ru	0.14004	-0.00382	0.27550
C	-2.15855	0.71648	-0.61910
C	2.44925	0.34009	-1.37289
P	0.35108	2.26747	1.24743
P	1.02300	-1.78802	1.37819
C	2.50320	1.28319	2.80565
C	1.88366	-3.11487	0.38185
C	1.27639	-4.34861	0.16833
C	3.13869	-2.87976	-0.16496
C	1.91727	-5.32988	-0.57042
H	0.29318	-4.55069	0.57260
C	3.78028	-3.86212	-0.90502
H	3.61906	-1.92091	-0.03045
C	3.17310	-5.09035	-1.10742
H	1.43165	-6.28448	-0.72797
H	4.75739	-3.66163	-1.32588
H	3.67356	-5.85738	-1.68487
C	-0.20536	-2.72220	2.43415
C	-1.56130	-2.42998	2.36901
C	0.22900	-3.72517	3.29904
C	-2.46493	-3.12292	3.16534
H	-1.92556	-1.66163	1.69671
C	-0.67152	-4.41392	4.09270
H	1.27852	-3.98530	3.35524

C	-2.02439	-4.11136	4.02842
H	-3.51943	-2.88532	3.10586
H	-0.31803	-5.18952	4.75990
H	-2.73101	-4.64933	4.64810
C	0.92573	3.66324	0.14616
C	1.13578	3.46146	-1.21100
C	1.12548	4.93764	0.67787
C	1.55611	4.51246	-2.01837
H	0.97706	2.48561	-1.65667
C	1.54308	5.98269	-0.12600
H	0.94544	5.12817	1.72851
C	1.76322	5.77017	-1.48038
H	1.71958	4.33867	-3.07439
H	1.69372	6.96522	0.30251
H	2.09071	6.58690	-2.11159
C	-1.32332	2.84885	1.84471
C	-1.87430	2.31425	3.00558
C	-2.06264	3.77072	1.11366
C	-3.12978	2.70978	3.43730
H	-1.33151	1.57569	3.58116
C	-3.32127	4.16508	1.54399
H	-1.66286	4.18827	0.19855
C	-3.85652	3.63932	2.70837
H	-3.54330	2.28657	4.34399
H	-3.88389	4.88546	0.96361
H	-4.83839	3.94748	3.04465
C	2.00165	-0.04124	3.42841
H	0.92080	0.00399	3.61792
H	2.45619	-0.16432	4.41660
H	3.35573	1.64303	3.39109
H	2.87428	1.09467	1.79393
C	2.33958	-1.28122	2.58641
H	3.23748	-1.09460	1.99399
H	2.54380	-2.14829	3.22059
C	1.45592	2.40580	2.74992
H	1.95141	3.37764	2.71982

H	0.83192	2.39918	3.64838
C	3.89491	0.46477	-1.77765
C	4.19421	0.57676	-3.13597
C	4.92505	0.49091	-0.83692
C	5.51539	0.70265	-3.55125
H	3.37266	0.56321	-3.84443
C	6.24695	0.62426	-1.25193
H	4.68207	0.41472	0.21828
C	6.54316	0.72683	-2.60958
H	5.74595	0.78431	-4.60898
H	7.04667	0.64901	-0.51782
H	7.57468	0.82802	-2.93355
C	-3.50609	0.75964	-1.25165
C	-3.66173	1.40275	-2.48013
C	-4.58403	0.10294	-0.65702
C	-4.89906	1.38568	-3.11571
H	-2.80068	1.89107	-2.92446
C	-5.82047	0.08960	-1.29397
H	-4.43211	-0.40176	0.29114
C	-5.97695	0.72829	-2.52364
H	-5.02353	1.87872	-4.07475
H	-6.66132	-0.42392	-0.83800
H	-6.94043	0.70863	-3.02437
O	-1.17096	1.27394	-1.15743
O	-1.99250	0.05040	0.45972
O	1.55069	0.49516	-2.18933
O	2.24288	0.09294	-0.11040
C	-0.37194	-1.62433	-0.82260
C	-0.93551	-2.37426	-1.59579
C	-1.70585	-3.17081	-2.55391
H	-1.83265	-4.19670	-2.18376
H	-1.15673	-3.24819	-3.50106
C	-3.08420	-2.54036	-2.80734
H	-2.94360	-1.50873	-3.15420
H	-3.62243	-2.46814	-1.85381
C	-3.92266	-3.31577	-3.81880

H	-4.06109	-4.34704	-3.46768
H	-3.37679	-3.38371	-4.76891
C	-5.28216	-2.66022	-4.05021
H	-5.15914	-1.63337	-4.41115
H	-5.87935	-3.21193	-4.78248
H	-5.85131	-2.60773	-3.11561
H	-0.06742	0.03553	1.81372

[3'a-6'a][‡]

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XYZ			
Ru	0.16856	-0.06667	-0.57758
C	1.74682	-1.91910	-1.27106
C	-2.56553	0.07183	-1.93172
P	-0.78909	-0.92152	1.31399
P	0.04013	1.65881	0.98597
C	-1.27512	0.75568	1.97605
H	-1.28926	0.90006	3.05613
H	-2.23990	1.00848	1.53175
C	-0.63573	3.35090	0.59224
C	-0.06007	4.53228	1.04021
C	-1.74761	3.40492	-0.24257
C	-0.60282	5.75578	0.67411
H	0.81694	4.51370	1.67384
C	-2.29099	4.62698	-0.60303
H	-2.15928	2.47067	-0.61642
C	-1.72116	5.80546	-0.14202
H	-0.14796	6.67193	1.02874
H	-3.15762	4.66115	-1.25135
H	-2.14390	6.76119	-0.42545
C	1.40894	1.89746	2.22798
C	2.67910	1.41002	1.95107
C	1.18290	2.52672	3.45111
C	3.70796	1.55471	2.87271
H	2.87059	0.89737	1.01640
C	2.20669	2.67259	4.37157
H	0.19914	2.90972	3.69416
C	3.47472	2.18764	4.08195

H	4.69262	1.16770	2.64289
H	2.01605	3.16452	5.31696
H	4.27635	2.30076	4.80119
C	-2.32068	-1.96020	1.15591
C	-2.35251	-2.92773	0.15726
C	-3.42649	-1.80285	1.98441
C	-3.47210	-3.73011	-0.00522
H	-1.50340	-3.04937	-0.50639
C	-4.54670	-2.60260	1.81974
H	-3.42774	-1.04939	2.76214
C	-4.57007	-3.56937	0.82612
H	-3.48767	-4.47858	-0.78741
H	-5.40321	-2.46937	2.46836
H	-5.44556	-4.19332	0.69702
C	0.20985	-1.72695	2.66932
C	-0.34918	-2.05393	3.90213
C	1.55031	-2.00822	2.43840
C	0.41916	-2.65031	4.88773
H	-1.39351	-1.84806	4.10183
C	2.32116	-2.60601	3.42668
H	1.99402	-1.75491	1.48000
C	1.75826	-2.92766	4.65057
H	-0.02659	-2.90051	5.84203
H	3.36509	-2.82131	3.23671
H	2.35959	-3.39488	5.42052
C	-4.06670	0.20152	-1.84504
C	-4.83065	-0.16753	-2.95326
C	-4.70388	0.66719	-0.69505
C	-6.21711	-0.06935	-2.91266
H	-4.31281	-0.52990	-3.83479
C	-6.09131	0.76496	-0.65239
H	-4.10603	0.95247	0.16369
C	-6.84964	0.39718	-1.76165
H	-6.80587	-0.35668	-3.77849
H	-6.58201	1.12750	0.24600
H	-7.93241	0.47372	-1.72862

C	2.72963	-2.93622	-1.73417
C	2.32854	-3.91452	-2.64468
C	4.04192	-2.90760	-1.26125
C	3.24337	-4.86696	-3.08019
H	1.30286	-3.90797	-2.99885
C	4.95362	-3.86251	-1.69760
H	4.32925	-2.13509	-0.55561
C	4.55420	-4.84132	-2.60640
H	2.93668	-5.62880	-3.79005
H	5.97581	-3.84582	-1.33214
H	5.26767	-5.58545	-2.94808
O	0.55009	-1.95307	-1.66271
O	2.11571	-0.99622	-0.46409
O	-1.90752	0.50221	-0.90344
O	-2.07177	-0.41189	-2.95351
C	0.53482	0.80157	-2.82804
C	1.53161	1.27026	-2.30555
C	2.79956	1.85587	-1.85787
H	3.39117	1.06562	-1.38150
H	2.60484	2.61890	-1.09227
C	3.58510	2.47956	-3.01925
H	2.97533	3.25996	-3.49038
H	3.75979	1.71270	-3.78333
C	4.91695	3.06644	-2.55802
H	4.73159	3.82205	-1.78329
H	5.51417	2.27695	-2.08398
C	5.70391	3.68926	-3.70796
H	5.13571	4.50025	-4.17540
H	6.65751	4.10055	-3.36511
H	5.91733	2.94478	-4.48203
H	-0.55864	0.23818	-3.24863

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XYZ

Ru	-0.21309	0.05091	-0.29928
C	2.03823	-0.84375	-1.08373
C	-2.88981	0.73101	-1.56150

P	-0.56936	-1.81854	1.03890
P	-0.80629	1.62217	1.26411
C	-2.89476	-0.88568	2.32606
C	-0.54773	3.39500	0.69604
C	0.72504	3.95365	0.77441
C	-1.58080	4.15682	0.16434
C	0.95592	5.24929	0.34325
H	1.54876	3.37528	1.17338
C	-1.34978	5.45493	-0.26870
H	-2.57789	3.74893	0.06999
C	-0.08303	6.00605	-0.17812
H	1.95149	5.66889	0.41376
H	-2.16665	6.03424	-0.68015
H	0.09644	7.01886	-0.51551
C	0.19590	1.64448	2.85461
C	1.43371	1.01340	2.88886
C	-0.24054	2.32655	3.98836
C	2.21083	1.04773	4.03925
H	1.80414	0.49989	2.00815
C	0.53135	2.35668	5.13782
H	-1.18851	2.84885	3.98421
C	1.76039	1.71361	5.16672
H	3.17358	0.55244	4.04997
H	0.17555	2.88790	6.01148
H	2.36576	1.73870	6.06410
C	-1.58939	-3.13512	0.17384
C	-1.51224	-3.24513	-1.21079
C	-2.40617	-4.02042	0.87081
C	-2.24346	-4.21345	-1.88384
H	-0.86889	-2.57585	-1.76923
C	-3.14015	-4.98524	0.19914
H	-2.48089	-3.97109	1.94881
C	-3.06174	-5.08333	-1.18139
H	-2.17179	-4.28606	-2.96169
H	-3.77260	-5.66389	0.75714
H	-3.63440	-5.83752	-1.70638

C	0.93560	-2.79673	1.58004
C	1.47508	-2.67187	2.85474
C	1.55724	-3.64848	0.67131
C	2.60871	-3.38560	3.21572
H	1.02109	-2.01624	3.58519
C	2.68911	-4.36190	1.03088
H	1.15888	-3.75875	-0.32941
C	3.21878	-4.23304	2.30610
H	3.01422	-3.27700	4.21376
H	3.15942	-5.02014	0.31117
H	4.10315	-4.79009	2.58793
C	-3.05473	0.56280	2.80301
H	-2.56050	0.68329	3.77412
H	-4.11924	0.75566	2.97811
H	-3.63688	-1.50167	2.84203
H	-3.14441	-0.93302	1.25840
C	-2.57992	1.64897	1.82900
H	-3.16815	1.57604	0.90777
H	-2.78684	2.63230	2.25983
C	-1.49590	-1.48577	2.60141
H	-1.56076	-2.38516	3.21692
H	-0.88452	-0.77090	3.16138
C	-4.33791	0.52527	-1.85907
C	-5.06106	1.51618	-2.52555
C	-4.96605	-0.65569	-1.45836
C	-6.41398	1.32624	-2.78509
H	-4.55030	2.42212	-2.83294
C	-6.31826	-0.84266	-1.72247
H	-4.38042	-1.41879	-0.95585
C	-7.04218	0.14866	-2.38338
H	-6.97887	2.09458	-3.30303
H	-6.80817	-1.76160	-1.41676
H	-8.09807	0.00141	-2.58885
C	3.39901	-1.16000	-1.61052
C	3.53106	-1.73168	-2.87666
C	4.53260	-0.86517	-0.85082

C	4.79827	-2.00206	-3.38486
H	2.63300	-1.94976	-3.44555
C	5.79777	-1.14998	-1.35536
H	4.40390	-0.41168	0.12719
C	5.93061	-1.71498	-2.62348
H	4.90438	-2.43835	-4.37313
H	6.68078	-0.92457	-0.76511
H	6.91856	-1.92946	-3.01981
O	1.00690	-1.28060	-1.66463
O	1.92302	-0.09662	-0.05967
O	-2.36303	1.82365	-1.96077
O	-2.27875	-0.15157	-0.91421
C	0.20632	1.61315	-1.81780
C	1.22424	1.89227	-2.43767
C	2.51604	2.08629	-3.09426
H	2.45886	2.90104	-3.82690
H	2.76136	1.17549	-3.65904
C	3.63728	2.36341	-2.07840
H	3.50145	1.69665	-1.21896
H	3.53805	3.38832	-1.69953
C	5.02080	2.14622	-2.68342
H	5.14268	2.78471	-3.56884
H	5.09172	1.10715	-3.03312
C	6.13898	2.42587	-1.68383
H	6.02180	1.79743	-0.79407
H	7.12454	2.22085	-2.11296
H	6.12275	3.47128	-1.35711
H	-1.18733	1.76539	-1.85334

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XYZ

Ru	0.08575	-0.40152	0.36532
C	1.58861	-1.77645	1.86520
C	-2.72450	0.75406	1.09241
P	1.55324	1.66237	0.00263
P	0.02134	0.15759	-1.83152
C	0.73406	1.87828	-1.67908

H	1.36994	2.22055	-2.49664
H	-0.09708	2.57466	-1.55023
C	-1.59075	0.29920	-2.77021
C	-1.98307	-0.72670	-3.62457
C	-2.45933	1.36526	-2.56562
C	-3.20727	-0.67865	-4.27285
H	-1.33162	-1.57597	-3.78854
C	-3.68309	1.41661	-3.21560
H	-2.19502	2.17008	-1.89261
C	-4.06035	0.39581	-4.07308
H	-3.49543	-1.48514	-4.93546
H	-4.34457	2.25721	-3.04764
H	-5.01625	0.43480	-4.57958
C	1.14210	-0.73394	-3.02478
C	1.70520	-1.94604	-2.64988
C	1.42260	-0.21560	-4.28733
C	2.54150	-2.62947	-3.52429
H	1.49934	-2.35616	-1.66695
C	2.25650	-0.89521	-5.15799
H	0.98542	0.72470	-4.60147
C	2.81814	-2.10627	-4.77599
H	2.97633	-3.57378	-3.22212
H	2.46803	-0.48284	-6.13627
H	3.47012	-2.63932	-5.45679
C	1.47373	3.33928	0.81288
C	1.56082	3.39885	2.20090
C	1.32292	4.52329	0.09950
C	1.50341	4.61588	2.86183
H	1.67087	2.48642	2.77543
C	1.26120	5.74188	0.75925
H	1.25099	4.50977	-0.98045
C	1.35266	5.79122	2.14113
H	1.57305	4.64581	3.94196
H	1.14312	6.65525	0.18990
H	1.30507	6.74277	2.65553
C	3.36068	1.44838	-0.41558

C	4.15510	2.51505	-0.82632
C	3.91730	0.17818	-0.32390
C	5.48820	2.31508	-1.14287
H	3.74028	3.51262	-0.89819
C	5.25383	-0.02015	-0.64457
H	3.29877	-0.65792	-0.00008
C	6.03985	1.04479	-1.05312
H	6.09821	3.15124	-1.45997
H	5.68127	-1.01226	-0.57175
H	7.08251	0.88858	-1.30058
C	-3.63679	1.85492	1.49648
C	-4.96352	1.58942	1.84204
C	-3.14739	3.16237	1.52521
C	-5.79961	2.63670	2.21273
H	-5.32571	0.56778	1.81705
C	-3.98665	4.20493	1.89850
H	-2.11041	3.34211	1.26118
C	-5.31236	3.94205	2.24073
H	-6.83134	2.43513	2.48121
H	-3.60850	5.22162	1.92602
H	-5.96720	4.75722	2.53251
C	2.47981	-2.64199	2.68820
C	2.33037	-2.65799	4.07533
C	3.45568	-3.42934	2.07655
C	3.16083	-3.46006	4.85075
H	1.55989	-2.03889	4.52284
C	4.28409	-4.23133	2.85441
H	3.54744	-3.40471	0.99607
C	4.13764	-4.24586	4.24075
H	3.04737	-3.47490	5.93033
H	5.04308	-4.84701	2.38171
H	4.78496	-4.87263	4.84705
O	0.68353	-1.09039	2.40354
O	1.75644	-1.72398	0.59642
O	-1.57412	0.99913	0.71159
O	-3.23710	-0.44191	1.17617

C	-1.09166	-2.00478	0.17297
C	-1.84991	-2.96226	0.09628
C	-2.78081	-4.09652	0.03701
H	-2.39017	-4.92861	0.63694
H	-2.85553	-4.46713	-0.99386
C	-4.18404	-3.72903	0.54100
H	-4.57281	-2.89472	-0.05745
H	-4.10802	-3.36168	1.57251
C	-5.15394	-4.90620	0.48055
H	-5.21632	-5.27076	-0.55302
H	-4.75232	-5.73588	1.07640
C	-6.54808	-4.53922	0.98255
H	-6.97681	-3.72913	0.38302
H	-7.23166	-5.39174	0.93381
H	-6.50952	-4.19759	2.02224
H	-2.58406	-1.14536	0.85810

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XYZ

Ru	-0.16553	-0.46437	0.28334
C	-1.24586	-2.57866	-0.63374
C	0.13312	1.72147	-1.75300
P	-2.46478	0.56720	1.20628
P	1.36930	-0.21006	1.96370
C	-1.29983	0.91905	3.71044
C	2.28235	1.42494	1.92475
C	3.04707	1.69922	0.79096
C	2.20276	2.38720	2.92193
C	3.72213	2.90107	0.66704
H	3.11180	0.96149	-0.00087
C	2.87532	3.59607	2.79631
H	1.61876	2.21403	3.81542
C	3.63799	3.85562	1.67180
H	4.31582	3.09570	-0.21729
H	2.80218	4.33359	3.58555
H	4.16500	4.79624	1.57552
C	2.75632	-1.47584	1.93680

C	2.45030	-2.79018	1.59273
C	4.05274	-1.16581	2.32557
C	3.42907	-3.77006	1.62812
H	1.44311	-3.04448	1.28242
C	5.03424	-2.14670	2.35656
H	4.31348	-0.15394	2.60767
C	4.72471	-3.45018	2.00831
H	3.18044	-4.78752	1.35438
H	6.04156	-1.88859	2.65750
H	5.48940	-4.21612	2.03298
C	-2.63640	2.29679	0.48167
C	-3.15672	2.45403	-0.80040
C	-2.22783	3.43117	1.17393
C	-3.28159	3.71157	-1.36778
H	-3.47692	1.58876	-1.36662
C	-2.35209	4.69166	0.60750
H	-1.80739	3.35115	2.16686
C	-2.88216	4.83734	-0.66346
H	-3.69388	3.81196	-2.36402
H	-2.03226	5.56260	1.16575
H	-2.98101	5.82083	-1.10462
C	-4.12743	-0.14173	0.70904
C	-5.28879	0.13271	1.42680
C	-4.21372	-0.92680	-0.43478
C	-6.50842	-0.38086	1.01732
H	-5.25905	0.75386	2.31194
C	-5.43646	-1.43854	-0.84630
H	-3.31175	-1.14488	-1.00050
C	-6.58530	-1.16981	-0.12081
H	-7.40214	-0.16096	1.58729
H	-5.48854	-2.05163	-1.73726
H	-7.53904	-1.57082	-0.44025
C	-0.71000	-0.48678	3.86789
H	-1.13639	-1.15695	3.11032
H	-1.00108	-0.89798	4.84173
H	-1.37293	1.40630	4.68917

H	-0.62363	1.54120	3.11002
C	0.80700	-0.52447	3.73011
H	1.29482	0.16945	4.42042
H	1.17687	-1.52363	3.97674
C	-2.67399	0.87241	3.04004
H	-3.25031	1.78230	3.21591
H	-3.24980	0.03594	3.44897
C	0.41823	3.05094	-2.34690
C	0.34983	3.24745	-3.72824
C	0.76246	4.10530	-1.49874
C	0.62479	4.50316	-4.25749
H	0.08507	2.41740	-4.37307
C	1.03804	5.35780	-2.03421
H	0.81237	3.92463	-0.43041
C	0.96821	5.55656	-3.41213
H	0.57324	4.66036	-5.32974
H	1.30799	6.17912	-1.37861
H	1.18389	6.53550	-3.82898
C	-1.72856	-3.87853	-1.17605
C	-2.31237	-3.92944	-2.44230
C	-1.59296	-5.04145	-0.41636
C	-2.76285	-5.14442	-2.94722
H	-2.40117	-3.01261	-3.01516
C	-2.04564	-6.25456	-0.92336
H	-1.13113	-4.97600	0.56300
C	-2.63069	-6.30604	-2.18784
H	-3.21575	-5.18773	-3.93280
H	-1.94174	-7.16104	-0.33521
H	-2.98274	-7.25427	-2.58321
O	-1.40316	-1.50653	-1.30986
O	-0.69827	-2.53519	0.50515
O	-0.18718	0.79716	-2.63169
O	0.18524	1.53901	-0.53464
C	1.38041	-1.03598	-0.83030
C	2.23617	-1.33524	-1.64761
C	3.28786	-1.71072	-2.59998

H	3.14532	-1.17209	-3.54704
H	3.20338	-2.77860	-2.84248
C	4.70225	-1.42988	-2.07516
H	4.84116	-1.96133	-1.12561
H	4.79387	-0.36004	-1.84950
C	5.78674	-1.84318	-3.06689
H	5.63084	-1.31375	-4.01605
H	5.68283	-2.91277	-3.29104
C	7.19363	-1.56128	-2.54561
H	7.37738	-2.10200	-1.61116
H	7.95974	-1.86360	-3.26568
H	7.32631	-0.49352	-2.34129
H	-0.26015	-0.09452	-2.21333

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XYZ

Ru	0.16952	-0.38096	-0.44675
C	2.36956	-1.18694	0.47620
C	-2.09270	-2.29679	0.14353
P	-0.57579	1.18556	1.58067
P	-0.68068	1.63741	-1.24652
C	-1.60665	2.08685	0.29717
H	-1.80179	3.14459	0.46836
H	-2.55903	1.55176	0.22474
C	-1.89259	1.77731	-2.65336
C	-2.03270	2.95672	-3.37548
C	-2.67763	0.67845	-2.98142
C	-2.94846	3.03516	-4.41405
H	-1.42572	3.82166	-3.13905
C	-3.59557	0.75801	-4.01711
H	-2.57481	-0.24658	-2.42833
C	-3.73205	1.93677	-4.73571
H	-3.04895	3.95739	-4.97291
H	-4.20283	-0.10337	-4.26592
H	-4.44686	1.99859	-5.54743
C	0.62777	2.91884	-1.55317
C	1.77416	2.53598	-2.24045

C	0.49055	4.23977	-1.13937
C	2.77341	3.46043	-2.50575
H	1.89698	1.51152	-2.57067
C	1.49149	5.16245	-1.40061
H	-0.39508	4.56554	-0.60919
C	2.63441	4.77448	-2.08467
H	3.66225	3.15150	-3.04165
H	1.37597	6.18760	-1.07134
H	3.41543	5.49666	-2.28993
C	-1.73245	0.76332	2.96995
C	-1.36434	-0.25303	3.84624
C	-2.93930	1.42459	3.16546
C	-2.18923	-0.60204	4.90382
H	-0.42682	-0.77863	3.70834
C	-3.76718	1.07245	4.22139
H	-3.24868	2.22034	2.50011
C	-3.39393	0.06023	5.09245
H	-1.89134	-1.39316	5.58084
H	-4.70547	1.59413	4.36429
H	-4.04065	-0.21226	5.91765
C	0.56605	2.48483	2.26484
C	0.10316	3.46217	3.14067
C	1.90417	2.47867	1.89031
C	0.96929	4.42468	3.63290
H	-0.93492	3.47659	3.44927
C	2.77035	3.44475	2.38277
H	2.27845	1.72080	1.21079
C	2.30487	4.41747	3.25375
H	0.60181	5.18117	4.31510
H	3.81170	3.43399	2.08601
H	2.98187	5.16975	3.64034
C	-3.46811	-2.82058	0.21097
C	-3.71383	-4.09878	0.72470
C	-4.52405	-2.02120	-0.23860
C	-5.01814	-4.57291	0.78290
H	-2.88749	-4.70832	1.07181

C	-5.82481	-2.50170	-0.17581
H	-4.31573	-1.03304	-0.63377
C	-6.07048	-3.77648	0.33392
H	-5.21523	-5.56317	1.17838
H	-6.64760	-1.88680	-0.52371
H	-7.08782	-4.15088	0.38129
C	3.66924	-1.71123	0.92967
C	3.71802	-2.87879	1.69500
C	4.84459	-1.05211	0.55701
C	4.94950	-3.39018	2.08629
H	2.79306	-3.37528	1.96904
C	6.07277	-1.57045	0.94855
H	4.77984	-0.14828	-0.03957
C	6.12358	-2.73850	1.71020
H	4.99714	-4.29691	2.67973
H	6.99045	-1.06866	0.66106
H	7.08426	-3.14223	2.01318
O	1.28378	-1.82981	0.71305
O	2.28202	-0.10475	-0.18233
O	-1.84866	-1.16467	-0.31276
O	-1.16905	-3.10872	0.59711
C	0.41816	-1.10948	-2.09489
C	0.60948	-1.62568	-3.27492
C	1.63523	-2.71522	-3.53619
H	2.24108	-2.40444	-4.39552
H	1.10359	-3.62482	-3.84117
C	2.54054	-3.00508	-2.33918
H	1.92792	-3.30752	-1.47659
H	3.05742	-2.07942	-2.04846
C	3.57053	-4.09181	-2.64034
H	3.05154	-5.00332	-2.96249
H	4.19080	-3.77209	-3.48698
C	4.45732	-4.40185	-1.43731
H	3.85973	-4.77212	-0.59773
H	5.20255	-5.16356	-1.68086
H	4.98763	-3.50567	-1.09524

	H	-0.26403	-2.71780	0.59036
	H	0.00896	-1.24467	-4.10155
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	XYZ			
	Ru	0.28180	-0.81766	0.02628
	C	2.58509	-1.60502	0.73326
	C	-0.80024	1.38746	1.77140
	P	1.56583	1.26306	-1.46486
	P	-1.17276	-1.61624	-1.65050
	C	0.79143	-0.06515	-3.83218
	C	-2.41520	-0.50505	-2.49899
	C	-2.65278	0.77971	-2.03334
	C	-3.14611	-0.97389	-3.58987
	C	-3.59680	1.59044	-2.64996
	H	-2.10557	1.15496	-1.17943
	C	-4.08494	-0.16601	-4.20790
	H	-2.99573	-1.97991	-3.96154
	C	-4.31176	1.12162	-3.73893
	H	-3.77165	2.59104	-2.27514
	H	-4.64508	-0.54269	-5.05480
	H	-5.04804	1.75328	-4.22095
	C	-2.26158	-3.04010	-1.09566
	C	-1.76765	-4.33685	-1.00727
	C	-3.57843	-2.79435	-0.72316
	C	-2.58253	-5.37168	-0.57418
	H	-0.74117	-4.55953	-1.26650
	C	-4.39269	-3.82845	-0.28755
	H	-3.98340	-1.79190	-0.77388
	C	-3.89829	-5.12160	-0.21565
	H	-2.18476	-6.37730	-0.51587
	H	-5.41758	-3.62130	-0.00553
	H	-4.53439	-5.93074	0.12127
	C	0.58084	2.85863	-1.41658
	C	0.66987	3.66403	-0.28379
	C	-0.23768	3.26536	-2.46228
	C	-0.03746	4.85144	-0.20108

H	1.31037	3.37567	0.54037
C	-0.94772	4.45572	-2.38097
H	-0.33388	2.66646	-3.35755
C	-0.85027	5.25207	-1.25218
H	0.04989	5.46891	0.68439
H	-1.57646	4.76030	-3.20856
H	-1.40127	6.18230	-1.19125
C	3.24217	1.91869	-0.94593
C	3.97104	2.74060	-1.80360
C	3.75677	1.63646	0.31207
C	5.19540	3.25590	-1.41306
H	3.58932	2.99259	-2.78432
C	4.98335	2.15451	0.70531
H	3.20708	0.99880	0.99237
C	5.70615	2.96288	-0.15576
H	5.75135	3.89155	-2.09102
H	5.37290	1.92285	1.68872
H	6.66369	3.36681	0.14957
C	1.08728	-1.49715	-3.36055
H	1.73555	-1.47748	-2.47860
H	1.65521	-2.02545	-4.13381
H	0.79197	-0.02232	-4.92562
H	-0.21547	0.24584	-3.52863
C	-0.14750	-2.33548	-3.02469
H	-0.78578	-2.48084	-3.90042
H	0.17570	-3.32351	-2.69126
C	1.81903	0.92887	-3.28616
H	1.80235	1.86944	-3.83811
H	2.82650	0.51322	-3.39083
C	-1.77189	2.34350	2.32826
C	-1.46197	3.07948	3.47704
C	-3.01938	2.48040	1.71033
C	-2.40679	3.94936	4.00672
H	-0.49255	2.96179	3.94807
C	-3.95809	3.35219	2.24610
H	-3.24475	1.89528	0.82613

C	-3.65212	4.08317	3.39423
H	-2.17451	4.52138	4.89830
H	-4.92887	3.45993	1.77476
H	-4.38847	4.76103	3.81356
C	3.91173	-2.12666	1.10943
C	4.53740	-1.66063	2.26892
C	4.53005	-3.08723	0.30385
C	5.78596	-2.15765	2.62066
H	4.03718	-0.91962	2.88292
C	5.78021	-3.57775	0.65954
H	4.02417	-3.43747	-0.58964
C	6.40593	-3.11312	1.81597
H	6.27702	-1.80343	3.52057
H	6.26779	-4.32196	0.03906
H	7.38177	-3.49905	2.09271
O	2.01709	-0.68155	1.41047
O	1.96963	-2.06400	-0.28535
O	0.29223	1.23331	2.48496
O	-1.02371	0.76910	0.71637
C	-0.44238	-2.01575	1.18048
C	-0.84897	-2.87457	2.06964
C	-1.81363	-2.62786	3.21025
H	-1.36960	-3.04438	4.12171
H	-2.72385	-3.20874	3.01582
C	-2.16731	-1.15899	3.43405
H	-2.57404	-0.72928	2.50612
H	-1.25131	-0.60052	3.67328
C	-3.17887	-0.98967	4.56736
H	-2.79859	-1.49847	5.46214
H	-4.11104	-1.49955	4.29462
C	-3.46364	0.47288	4.89654
H	-3.85013	1.00940	4.02288
H	-4.20149	0.55981	5.69831
H	-2.55147	0.98306	5.22304
H	0.91182	0.56073	2.11726
H	-0.43795	-3.87911	1.93701

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XYZ

Ru	-0.63913	0.13958	0.04008
C	2.15252	-0.83703	-0.66469
C	-2.92698	0.96060	-0.82194
P	-1.98278	-2.13999	0.39737
P	0.23599	0.23122	2.16914
C	-2.99783	-1.17328	2.87720
C	1.41628	1.62765	2.58392
C	2.75974	1.39053	2.84925
C	0.93971	2.93378	2.64048
C	3.60939	2.43930	3.16923
H	3.15498	0.38450	2.80063
C	1.78894	3.98138	2.95941
H	-0.10074	3.14714	2.43389
C	3.12699	3.73665	3.22638
H	4.65307	2.23859	3.37549
H	1.40261	4.99194	2.99871
H	3.79077	4.55465	3.47625
C	1.02327	-1.24470	3.01080
C	1.30485	-2.40503	2.30339
C	1.33583	-1.19943	4.36891
C	1.88187	-3.49957	2.93383
H	1.08034	-2.46465	1.24752
C	1.91046	-2.28872	5.00134
H	1.13577	-0.30443	4.94481
C	2.18484	-3.44444	4.28352
H	2.09468	-4.39515	2.36386
H	2.14641	-2.23570	6.05663
H	2.63516	-4.29678	4.77668
C	-3.62082	-2.22303	-0.50624
C	-3.59057	-2.27089	-1.89896
C	-4.85013	-2.25312	0.13773
C	-4.76421	-2.34828	-2.62864
H	-2.64188	-2.24387	-2.42145
C	-6.02823	-2.32694	-0.59393

H	-4.91286	-2.22045	1.21629
C	-5.98926	-2.37563	-1.97635
H	-4.72314	-2.38544	-3.70992
H	-6.97856	-2.34808	-0.07567
H	-6.90820	-2.43409	-2.54578
C	-1.24263	-3.76517	-0.15576
C	-1.83135	-4.98404	0.17156
C	-0.10558	-3.75071	-0.95291
C	-1.28163	-6.17123	-0.28146
H	-2.72782	-5.01864	0.77778
C	0.44340	-4.94234	-1.40852
H	0.35438	-2.79747	-1.20353
C	-0.14136	-6.15203	-1.07299
H	-1.74553	-7.11379	-0.02014
H	1.33164	-4.92155	-2.02753
H	0.28681	-7.08122	-1.42798
C	-2.07038	-0.45658	3.87018
H	-1.46483	-1.19396	4.41089
H	-2.70199	0.02197	4.62748
H	-3.87990	-1.50484	3.43356
H	-3.35392	-0.44368	2.14052
C	-1.17826	0.66197	3.31405
H	-1.79667	1.36301	2.74204
H	-0.75051	1.21422	4.15664
C	-2.39104	-2.41639	2.18549
H	-3.04835	-3.28008	2.29660
H	-1.44138	-2.68998	2.65868
C	-4.22175	1.55661	-1.25450
C	-4.56127	1.55134	-2.60818
C	-5.07391	2.14034	-0.31554
C	-5.75840	2.12590	-3.02077
H	-3.87524	1.09810	-3.31591
C	-6.27001	2.71490	-0.73226
H	-4.78320	2.13925	0.72988
C	-6.61184	2.70665	-2.08368
H	-6.02638	2.12495	-4.07243

H	-6.93541	3.17106	-0.00616
H	-7.54508	3.15686	-2.40798
C	3.04152	-1.41893	-1.72728
C	2.56902	-1.59545	-3.02898
C	4.35676	-1.75848	-1.40924
C	3.41476	-2.10325	-4.01020
H	1.54475	-1.32169	-3.25820
C	5.19463	-2.28277	-2.38716
H	4.70576	-1.59882	-0.39455
C	4.72543	-2.45126	-3.68897
H	3.05167	-2.22904	-5.02557
H	6.21773	-2.54739	-2.13779
H	5.38328	-2.85174	-4.45482
O	0.89800	-0.92265	-0.90641
O	2.66038	-0.32723	0.35220
O	-2.12975	0.46884	-1.65895
O	-2.61146	0.98619	0.42181
C	-0.05277	1.82826	-0.36228
H	0.98558	3.41964	-1.18530
C	0.02535	3.04068	-0.83324
C	-1.22437	3.89821	-0.94112
H	-2.06423	3.40129	-0.44356
H	-1.48787	3.98808	-2.00304
C	-1.02843	5.29070	-0.34050
H	-0.17304	5.78051	-0.82405
H	-0.77119	5.19443	0.72195
C	-2.27461	6.16129	-0.49240
H	-3.12923	5.65276	-0.02706
H	-2.51865	6.25760	-1.55794
C	-2.09685	7.54686	0.12328
H	-1.26280	8.07800	-0.34714
H	-2.99550	8.15866	0.00306
H	-1.88068	7.47326	1.19435
O	2.86201	2.22589	-0.34744
C	3.54719	2.43946	-1.47611
O	3.16042	3.25055	-2.28531

C	4.82150	1.67058	-1.64608
C	5.55074	1.22163	-0.54393
C	5.31245	1.47583	-2.93795
C	6.77674	0.59089	-0.73553
H	5.17093	1.38166	0.46043
C	6.52383	0.82263	-3.12715
H	4.73155	1.84618	-3.77621
C	7.26125	0.38953	-2.02526
H	7.35289	0.25719	0.12187
H	6.89842	0.65568	-4.13204
H	8.21519	-0.10793	-2.17380
H	3.01851	1.32411	0.02501

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XYZ

Ru	-0.50575	0.08057	0.00765
C	2.51152	-0.21697	-0.60692
C	-2.90907	0.10987	-0.89607
P	-1.12636	-2.38873	0.63121
P	0.26653	0.65356	2.10501
C	-2.44083	-1.50265	3.01719
C	1.01123	2.36479	2.33873
C	2.38164	2.54037	2.49598
C	0.18801	3.48685	2.35653
C	2.91631	3.80850	2.66867
H	3.04482	1.68565	2.47408
C	0.72152	4.75426	2.52973
H	-0.88162	3.38458	2.23247
C	2.08850	4.91918	2.68745
H	3.98564	3.92590	2.79022
H	0.06513	5.61507	2.54091
H	2.50591	5.90881	2.82325
C	1.43881	-0.40744	3.11546
C	2.04678	-1.52403	2.55932
C	1.71877	-0.09093	4.44428
C	2.91190	-2.31158	3.30765
H	1.85303	-1.79087	1.52960

C	2.57959	-0.87342	5.19477
H	1.26645	0.77907	4.90395
C	3.17939	-1.98888	4.62686
H	3.37638	-3.17785	2.85365
H	2.78476	-0.61216	6.22523
H	3.85364	-2.60117	5.21237
C	-2.65299	-3.03533	-0.24317
C	-2.57559	-3.22998	-1.62139
C	-3.83963	-3.34151	0.40866
C	-3.65990	-3.71996	-2.32836
H	-1.66079	-2.99256	-2.15093
C	-4.92948	-3.82973	-0.30042
H	-3.93701	-3.20605	1.47656
C	-4.84323	-4.02113	-1.66807
H	-3.58248	-3.86531	-3.39844
H	-5.84778	-4.06157	0.22410
H	-5.69303	-4.40235	-2.21990
C	0.03015	-3.81873	0.28701
C	-0.21466	-5.09925	0.77721
C	1.13826	-3.60438	-0.52043
C	0.64494	-6.14197	0.47614
H	-1.08234	-5.29802	1.39329
C	1.99968	-4.65037	-0.82443
H	1.32509	-2.60678	-0.90531
C	1.75622	-5.91870	-0.32522
H	0.44587	-7.13283	0.86416
H	2.86244	-4.46937	-1.45311
H	2.42715	-6.73536	-0.56075
C	-1.77405	-0.44996	3.91370
H	-0.99410	-0.92151	4.52412
H	-2.52930	-0.08941	4.62180
H	-3.19025	-2.02127	3.62329
H	-2.98785	-0.98970	2.21863
C	-1.22343	0.80478	3.22387
H	-2.00510	1.23663	2.58820
H	-0.97758	1.54280	3.99333

C	-1.48791	-2.57526	2.44267
H	-1.87295	-3.57590	2.64387
H	-0.51085	-2.51842	2.93562
C	-4.30914	0.28443	-1.37558
C	-4.60265	0.08889	-2.72577
C	-5.30960	0.68198	-0.48711
C	-5.90045	0.28681	-3.18488
H	-3.80227	-0.20871	-3.39501
C	-6.60592	0.88095	-0.95009
H	-5.05425	0.83632	0.55644
C	-6.90081	0.68269	-2.29816
H	-6.13287	0.13756	-4.23446
H	-7.38618	1.19274	-0.26295
H	-7.91258	0.84022	-2.65931
C	3.61639	-0.87253	-1.38663
C	3.34215	-1.55522	-2.57447
C	4.93260	-0.74817	-0.94300
C	4.38107	-2.11721	-3.30787
H	2.31564	-1.61894	-2.91942
C	5.96942	-1.32671	-1.66953
H	5.12336	-0.18810	-0.03346
C	5.69496	-2.00906	-2.85248
H	4.16807	-2.63882	-4.23598
H	6.99314	-1.23526	-1.31885
H	6.50511	-2.45342	-3.42334
O	1.32402	-0.55765	-0.90356
O	2.81168	0.65007	0.25159
O	-1.98429	-0.18890	-1.69102
O	-2.64348	0.31247	0.34271
C	-0.45347	1.93003	-0.52949
H	-0.47920	3.85061	-1.33669
C	-1.05248	3.04854	-0.88453
C	-2.54746	3.24443	-0.75115
H	-2.95434	2.56440	0.00156
H	-3.02441	2.98047	-1.70599
C	-2.91459	4.68508	-0.39381

H	-2.51799	5.36693	-1.15851
H	-2.43154	4.96531	0.55169
C	-4.42559	4.87470	-0.27412
H	-4.81318	4.19248	0.49394
H	-4.90141	4.57291	-1.21597
C	-4.81161	6.31177	0.06620
H	-4.45848	7.00332	-0.70599
H	-5.89591	6.42838	0.15046
H	-4.36518	6.62142	1.01719
O	1.43065	2.47211	-0.92511
C	1.84907	2.46288	-2.22863
O	1.06810	2.62725	-3.12568
C	3.31765	2.28283	-2.42319
C	4.24621	2.67183	-1.45562
C	3.74734	1.73139	-3.63137
C	5.60459	2.51018	-1.70293
H	3.90816	3.09973	-0.51756
C	5.10436	1.53917	-3.85969
H	3.00383	1.44398	-4.36783
C	6.03198	1.93373	-2.89720
H	6.32964	2.82039	-0.95732
H	5.43904	1.07910	-4.78360
H	7.09259	1.78501	-3.07648
H	2.00600	1.87225	-0.33612

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XYZ			
Ru	0.42219	-0.07122	0.02579
C	-2.72046	0.10543	-0.61592
C	2.69156	-0.06568	-1.11043
P	1.02923	2.37545	0.66385
P	-0.07982	-0.71745	2.16663
C	2.66365	1.40410	2.81509
C	-0.87554	-2.40461	2.46015
C	-2.23332	-2.52185	2.73624
C	-0.10939	-3.56432	2.38795
C	-2.81299	-3.76578	2.93706

H	-2.85689	-1.64004	2.80246
C	-0.68662	-4.80824	2.58924
H	0.94791	-3.50847	2.16854
C	-2.04144	-4.91344	2.86459
H	-3.87174	-3.83439	3.15257
H	-0.07383	-5.69877	2.52836
H	-2.49230	-5.88506	3.02142
C	-1.14337	0.32037	3.32706
C	-1.90907	1.36303	2.82565
C	-1.21052	0.05042	4.69355
C	-2.71396	2.12856	3.65896
H	-1.88240	1.59210	1.76888
C	-2.00911	0.81072	5.53084
H	-0.63944	-0.76703	5.11595
C	-2.76385	1.85554	5.01477
H	-3.30106	2.93840	3.24435
H	-2.04614	0.58678	6.58961
H	-3.38917	2.45006	5.66876
C	2.42936	3.10188	-0.35154
C	2.19876	3.31853	-1.70913
C	3.66491	3.44621	0.17899
C	3.18102	3.86829	-2.51450
H	1.24497	3.04891	-2.14606
C	4.65271	3.99417	-0.62905
H	3.88101	3.29318	1.22690
C	4.41419	4.20780	-1.97515
H	2.98545	4.02888	-3.56716
H	5.61158	4.25427	-0.19887
H	5.18479	4.63484	-2.60431
C	-0.14913	3.83603	0.56985
C	0.17139	5.07738	1.11445
C	-1.35715	3.69684	-0.09987
C	-0.70455	6.14496	1.00592
H	1.11440	5.22832	1.62382
C	-2.23661	4.76455	-0.21330
H	-1.61235	2.74396	-0.54350

C	-1.91376	5.99061	0.34317
H	-0.44055	7.10266	1.43654
H	-3.17436	4.63606	-0.73908
H	-2.59732	6.82591	0.25758
C	2.15620	0.30700	3.76093
H	1.47851	0.74408	4.50411
H	3.01534	-0.07304	4.32618
H	3.48242	1.92067	3.32581
H	3.09816	0.93217	1.92769
C	1.51308	-0.92745	3.11511
H	2.20766	-1.34697	2.37909
H	1.34595	-1.68322	3.88780
C	1.61293	2.47013	2.42762
H	1.98823	3.46985	2.64843
H	0.70559	2.34517	3.02932
C	4.03852	-0.20117	-1.73346
C	4.20078	0.08929	-3.08824
C	5.12304	-0.63969	-0.97151
C	5.45260	-0.05087	-3.67820
H	3.33563	0.41264	-3.65746
C	6.37266	-0.78114	-1.56524
H	4.96649	-0.87521	0.07658
C	6.53740	-0.48452	-2.91769
H	5.58310	0.17222	-4.73241
H	7.21763	-1.12543	-0.97709
H	7.51299	-0.59665	-3.38111
C	-3.88636	0.68203	-1.32330
C	-3.66260	1.62398	-2.33164
C	-5.17953	0.23627	-1.04415
C	-4.73784	2.13111	-3.04847
H	-2.64521	1.92367	-2.55843
C	-6.25321	0.75567	-1.76021
H	-5.33242	-0.51985	-0.28218
C	-6.03313	1.70053	-2.75935
H	-4.56812	2.85656	-3.83731
H	-7.26044	0.41311	-1.54622

H	-6.87260	2.09819	-3.32157
O	-1.57353	0.50590	-0.79802
O	-3.00587	-0.88680	0.21147
O	1.69330	0.27927	-1.78762
O	2.55214	-0.31915	0.13911
C	0.24210	-1.99832	-0.62854
H	0.64822	-3.89927	-1.32253
C	1.06510	-3.04007	-0.79104
C	2.50665	-3.18825	-0.38469
H	2.72468	-2.59795	0.51000
H	3.15810	-2.77988	-1.17178
C	2.90574	-4.64703	-0.15705
H	2.71696	-5.22351	-1.07353
H	2.27011	-5.09320	0.62019
C	4.37390	-4.79246	0.23731
H	4.55467	-4.23012	1.16332
H	4.99893	-4.32075	-0.53241
C	4.79484	-6.24733	0.42796
H	4.65166	-6.81766	-0.49595
H	5.84763	-6.33042	0.71386
H	4.19560	-6.72792	1.20891
O	-1.08633	-2.28635	-1.12580
C	-1.34935	-1.95592	-2.40987
O	-0.53769	-1.52254	-3.18490
C	-2.79569	-2.14837	-2.74751
C	-3.64839	-2.93758	-1.97343
C	-3.28969	-1.47207	-3.86455
C	-4.99302	-3.04214	-2.31536
H	-3.25432	-3.46157	-1.10913
C	-4.63800	-1.56002	-4.19109
H	-2.60168	-0.87019	-4.44971
C	-5.48956	-2.34602	-3.41625
H	-5.65571	-3.66157	-1.71897
H	-5.02656	-1.01386	-5.04477
H	-6.54307	-2.41574	-3.67070
H	-2.18571	-1.41613	0.31290

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XYZ

Ru	-0.53322	0.20423	-0.23915
C	1.75365	0.68033	-1.29837
C	-0.68519	-2.08756	1.58476
P	0.55424	1.54488	1.89004
P	-2.56890	1.30498	-0.16759
C	-1.79441	0.91700	3.36093
C	-3.98206	0.53426	-1.13206
C	-4.65605	1.20722	-2.14182
C	-4.39126	-0.74911	-0.78423
C	-5.72248	0.60670	-2.79632
H	-4.35961	2.20729	-2.42886
C	-5.46034	-1.34587	-1.43223
H	-3.86384	-1.29033	-0.00876
C	-6.12908	-0.66854	-2.44170
H	-6.23806	1.14273	-3.58313
H	-5.77048	-2.34423	-1.15051
H	-6.96323	-1.13535	-2.95011
C	-2.45250	3.03592	-0.86903
C	-1.80320	3.20413	-2.08986
C	-2.99402	4.15252	-0.24290
C	-1.69780	4.45820	-2.66948
H	-1.36920	2.35036	-2.59537
C	-2.88326	5.41014	-0.81857
H	-3.51087	4.06256	0.70252
C	-2.23735	5.56646	-2.03370
H	-1.19190	4.56902	-3.62025
H	-3.30837	6.26879	-0.31443
H	-2.15437	6.54752	-2.48425
C	2.32673	1.16811	2.36588
C	3.28461	2.16136	2.52457
C	2.67333	-0.15663	2.61565
C	4.56910	1.83994	2.93846
H	3.04050	3.19729	2.33096
C	3.95239	-0.47270	3.04451

H	1.94328	-0.94528	2.45185
C	4.90353	0.52353	3.20818
H	5.30577	2.62422	3.05725
H	4.20776	-1.50370	3.25195
H	5.90302	0.27339	3.54099
C	0.57216	3.40958	1.70690
C	0.77937	3.92843	0.43216
C	0.43534	4.29090	2.77558
C	0.84424	5.29916	0.23100
H	0.88537	3.24871	-0.40887
C	0.49229	5.66093	2.57308
H	0.28556	3.92446	3.78207
C	0.69845	6.16904	1.29993
H	1.00766	5.68789	-0.76613
H	0.38079	6.33238	3.41492
H	0.74663	7.23938	1.14317
C	-2.58137	2.02305	2.62608
H	-1.90533	2.80345	2.25687
H	-3.24976	2.53167	3.32754
H	-2.21901	0.76927	4.35996
H	-1.92735	-0.02557	2.82638
C	-3.43030	1.47382	1.46982
H	-3.77409	0.46322	1.71272
H	-4.32712	2.07586	1.29870
C	-0.29084	1.16354	3.51193
H	0.18682	0.24480	3.86608
H	-0.07730	1.93384	4.25549
C	-1.36854	-3.21792	2.30357
C	-0.58787	-4.24135	2.84355
C	-2.75953	-3.28402	2.39430
C	-1.19531	-5.32822	3.46325
H	0.49074	-4.17102	2.75432
C	-3.36679	-4.36852	3.01921
H	-3.35352	-2.48728	1.96120
C	-2.58536	-5.39332	3.54957
H	-0.58721	-6.12805	3.87413

H	-4.44921	-4.42102	3.08442
H	-3.05977	-6.24461	4.02840
C	3.05319	1.05820	-1.91447
C	4.18235	0.27427	-1.67457
C	3.13867	2.19127	-2.72635
C	5.39862	0.62612	-2.25066
H	4.09657	-0.59746	-1.03398
C	4.35547	2.53621	-3.30309
H	2.24688	2.78430	-2.89842
C	5.48527	1.75394	-3.06456
H	6.27607	0.01479	-2.06337
H	4.42554	3.41312	-3.93894
H	6.43517	2.02526	-3.51556
O	1.60865	-0.40810	-0.68598
O	0.76020	1.48925	-1.37728
O	0.55614	-2.04636	1.54100
O	-1.46537	-1.22877	1.03441
C	-1.07632	-0.71145	-1.71568
H	-1.33063	-0.76420	-3.71332
C	-1.36842	-1.36791	-2.80314
C	-1.62813	-2.85776	-2.91993
H	-0.67863	-3.32104	-3.21363
H	-2.33958	-3.02239	-3.73766
C	-2.13594	-3.51905	-1.63676
H	-3.19368	-3.27330	-1.48301
H	-1.58978	-3.12005	-0.77613
C	-1.95206	-5.03361	-1.67839
H	-0.89011	-5.24542	-1.85330
H	-2.49953	-5.44597	-2.53725
C	-2.41265	-5.71218	-0.39067
H	-3.46439	-5.48726	-0.17892
H	-2.30703	-6.79978	-0.45042
H	-1.82343	-5.36204	0.46404
O	0.80317	-3.10438	-0.96972
C	1.77353	-3.37035	-1.84436
O	1.50962	-3.82518	-2.93504

C	3.18991	-3.14747	-1.40868
C	4.17124	-3.14313	-2.40120
C	3.54828	-3.00335	-0.06709
C	5.50805	-2.97553	-2.05994
H	3.86153	-3.27220	-3.43260
C	4.89088	-2.85490	0.27214
H	2.79137	-3.00996	0.71270
C	5.86902	-2.83381	-0.72066
H	6.26808	-2.95968	-2.83497
H	5.17652	-2.75509	1.31338
H	6.91344	-2.71271	-0.44859
H	1.07661	-2.51649	-0.23132

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XYZ

Ru	-0.24669	0.38559	-0.05513
C	1.92464	-0.45610	-1.09371
C	-1.78241	-1.42334	1.83553
P	1.45489	1.35822	1.77230
P	-1.58478	2.29155	-0.19815
C	-0.73328	2.18848	3.30164
C	-3.32527	2.10216	-0.87605
C	-3.85062	2.93834	-1.85079
C	-4.13110	1.10828	-0.32731
C	-5.16272	2.78181	-2.27731
H	-3.24302	3.71962	-2.28928
C	-5.44137	0.95574	-0.74840
H	-3.72086	0.44588	0.42660
C	-5.96029	1.79317	-1.72656
H	-5.56041	3.43855	-3.04070
H	-6.05948	0.17953	-0.31499
H	-6.98390	1.67272	-2.05809
C	-0.80527	3.59984	-1.28646
C	-0.29833	3.20010	-2.52086
C	-0.69378	4.93689	-0.92302
C	0.30016	4.11525	-3.37178
H	-0.35982	2.16179	-2.82294

C	-0.08871	5.85359	-1.77083
H	-1.07367	5.28714	0.02678
C	0.40730	5.44659	-2.99812
H	0.68651	3.78550	-4.32793
H	-0.00831	6.89012	-1.46872
H	0.87729	6.16267	-3.66039
C	2.76250	0.10666	2.25383
C	4.12258	0.36919	2.16829
C	2.34560	-1.14056	2.71531
C	5.05215	-0.59190	2.54287
H	4.47411	1.32700	1.80787
C	3.27156	-2.09808	3.09238
H	1.28970	-1.37637	2.77177
C	4.63001	-1.82508	3.00800
H	6.10950	-0.37086	2.46992
H	2.93191	-3.06258	3.44807
H	5.35461	-2.57433	3.30060
C	2.45446	2.85469	1.25256
C	2.70169	3.02761	-0.10615
C	2.97655	3.77990	2.15222
C	3.44573	4.10896	-0.55479
H	2.31211	2.30150	-0.81557
C	3.71548	4.86296	1.70318
H	2.82029	3.66953	3.21674
C	3.95082	5.03149	0.34741
H	3.62990	4.22993	-1.61481
H	4.11173	5.57446	2.41636
H	4.52935	5.87728	-0.00260
C	-0.95245	3.40819	2.38406
H	-0.02582	3.67194	1.85742
H	-1.20164	4.28859	2.98491
H	-1.14877	2.39335	4.29504
H	-1.28307	1.33407	2.89968
C	-2.07815	3.16844	1.37112
H	-2.84473	2.52623	1.81809
H	-2.58150	4.09508	1.08253

C	0.72464	1.75724	3.44736
H	0.77560	0.83121	4.02773
H	1.31968	2.49909	3.98255
C	-2.64467	-1.65922	3.04712
C	-2.69788	-2.93526	3.61011
C	-3.38897	-0.62275	3.61293
C	-3.48111	-3.17048	4.73510
H	-2.11809	-3.72884	3.15189
C	-4.17632	-0.85902	4.73528
H	-3.35010	0.36240	3.16056
C	-4.22096	-2.13269	5.29899
H	-3.51736	-4.16356	5.17195
H	-4.75713	-0.05128	5.16985
H	-4.83446	-2.31697	6.17572
C	3.17892	-0.94092	-1.72512
C	3.83618	-2.04508	-1.18101
C	3.69208	-0.29604	-2.85146
C	5.00983	-2.50647	-1.76933
H	3.41385	-2.53251	-0.30763
C	4.86254	-0.76255	-3.43807
H	3.15807	0.55720	-3.25568
C	5.52114	-1.86690	-2.89669
H	5.52075	-3.36812	-1.35062
H	5.26198	-0.26997	-4.31892
H	6.43545	-2.22953	-3.35708
O	1.35569	-1.14474	-0.19584
O	1.41302	0.65991	-1.43495
O	-1.20133	-2.40931	1.33076
O	-1.70066	-0.22223	1.42631
C	-1.25924	-0.45455	-1.46024
H	-2.37096	0.46446	-2.80214
C	-2.04123	-0.53575	-2.51109
C	-2.58048	-1.70459	-3.29184
H	-1.76742	-2.40872	-3.48138
H	-2.92569	-1.34288	-4.26699
C	-3.73696	-2.40430	-2.56990

H	-4.54515	-1.68413	-2.38479
H	-3.38324	-2.74120	-1.58821
C	-4.28035	-3.59188	-3.36170
H	-3.46641	-4.30565	-3.54139
H	-4.61409	-3.24937	-4.35002
C	-5.43126	-4.29207	-2.64353
H	-6.26584	-3.60203	-2.47928
H	-5.80729	-5.14334	-3.21848
H	-5.11011	-4.66213	-1.66431
O	-0.85154	-2.42473	-1.16164
C	0.22205	-2.92624	-1.82025
O	0.49814	-2.50651	-2.91761
C	0.97120	-4.05209	-1.18164
C	2.04685	-4.56797	-1.91040
C	0.64871	-4.59328	0.06428
C	2.80627	-5.60977	-1.39260
H	2.27846	-4.12457	-2.87295
C	1.41446	-5.63624	0.57871
H	-0.18346	-4.20844	0.64209
C	2.49164	-6.14365	-0.14406
H	3.64410	-6.00229	-1.96052
H	1.16645	-6.05392	1.54928
H	3.08387	-6.95707	0.26446
H	-0.84463	-2.45247	-0.12803

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XYZ			
Ru	-0.56353	0.19051	-0.16008
C	-1.46850	-0.53943	2.10914
C	1.57399	-1.72911	-1.10082
P	-2.47046	-1.18877	-1.35183
P	-0.49313	2.07052	-1.44731
C	-1.44933	-0.49749	-3.88298
C	0.99771	3.20335	-1.29038
C	0.89185	4.53188	-0.90204
C	2.25446	2.69653	-1.61078
C	2.01717	5.34295	-0.84438

H	-0.07137	4.95053	-0.64136
C	3.37716	3.50529	-1.55822
H	2.36235	1.65854	-1.89881
C	3.26094	4.83434	-1.17706
H	1.91684	6.37726	-0.54031
H	4.34703	3.09756	-1.81371
H	4.13807	5.46735	-1.13533
C	-1.94919	3.23607	-1.22549
C	-2.61381	3.24176	-0.00422
C	-2.38478	4.10433	-2.22369
C	-3.69146	4.08911	0.21258
H	-2.29507	2.57473	0.78797
C	-3.46362	4.94727	-2.01137
H	-1.88592	4.13739	-3.18288
C	-4.12095	4.94215	-0.79051
H	-4.19595	4.07988	1.17046
H	-3.78916	5.61262	-2.80084
H	-4.96301	5.60191	-0.62321
C	-2.15188	-2.99067	-0.92996
C	-2.76588	-3.58276	0.16915
C	-1.25005	-3.74309	-1.67497
C	-2.49559	-4.89989	0.50606
H	-3.46488	-3.01755	0.77246
C	-0.97978	-5.06121	-1.34072
H	-0.74731	-3.30944	-2.52954
C	-1.60298	-5.64461	-0.24945
H	-2.98475	-5.34490	1.36354
H	-0.27759	-5.63223	-1.93510
H	-1.39208	-6.67339	0.01308
C	-4.25180	-0.98340	-0.82225
C	-4.55862	-0.14919	0.24486
C	-5.28336	-1.65628	-1.47427
C	-5.87735	0.01892	0.64738
H	-3.75774	0.35603	0.77700
C	-6.59762	-1.48718	-1.07395
H	-5.06871	-2.32423	-2.29902

C	-6.89782	-0.64479	-0.01225
H	-6.10458	0.67092	1.48135
H	-7.38985	-2.01522	-1.58918
H	-7.92600	-0.51242	0.30076
C	-1.64306	1.03182	-3.82115
H	-2.52025	1.26560	-3.20184
H	-1.88956	1.40386	-4.82078
H	-1.36286	-0.81259	-4.92882
H	-0.50679	-0.77409	-3.39699
C	-0.42675	1.80046	-3.28805
H	0.49244	1.23328	-3.46944
H	-0.30429	2.76554	-3.78545
C	-2.60498	-1.25606	-3.22622
H	-2.63499	-2.29880	-3.54854
H	-3.55723	-0.80491	-3.52020
C	2.71464	-2.25716	-1.88721
C	3.45948	-3.34215	-1.41946
C	3.06740	-1.61632	-3.07676
C	4.56041	-3.78072	-2.14579
H	3.18778	-3.81357	-0.48179
C	4.16703	-2.06112	-3.79961
H	2.47828	-0.77044	-3.41526
C	4.91419	-3.14228	-3.33278
H	5.15051	-4.61352	-1.77730
H	4.44536	-1.56508	-4.72378
H	5.77710	-3.48534	-3.89535
C	-1.79931	-0.83149	3.52721
C	-1.12221	-1.85558	4.19047
C	-2.76215	-0.07191	4.19298
C	-1.41971	-2.12556	5.52193
H	-0.35644	-2.40724	3.65584
C	-3.06252	-0.35114	5.52139
H	-3.26159	0.72950	3.65910
C	-2.39217	-1.37836	6.18465
H	-0.89003	-2.91475	6.04613
H	-3.81464	0.23281	6.04259

H	-2.62404	-1.59230	7.22384
O	-0.76110	-1.35843	1.44407
O	-1.88407	0.52526	1.55445
O	1.32278	-2.40228	-0.00243
O	0.94159	-0.73557	-1.47281
C	0.89011	0.95383	1.03350
H	-0.20162	2.28891	2.16536
C	0.77915	1.84204	2.02602
C	1.87907	2.24148	2.98233
H	2.33119	1.34217	3.41963
H	1.43708	2.79313	3.82080
C	2.98038	3.10058	2.35114
H	2.53724	4.01588	1.93758
H	3.41658	2.55726	1.50365
C	4.08137	3.46685	3.34425
H	4.51546	2.54597	3.75499
H	3.64008	4.00355	4.19443
C	5.18183	4.31706	2.71433
H	4.77289	5.25361	2.32004
H	5.96369	4.56958	3.43697
H	5.65332	3.78544	1.88076
O	2.19136	0.39395	0.83161
C	2.63203	-0.57478	1.64718
O	2.02861	-1.01106	2.59927
C	3.96086	-1.09893	1.19858
C	4.45712	-2.23839	1.83277
C	4.67626	-0.51080	0.15311
C	5.66302	-2.79383	1.41847
H	3.87790	-2.67254	2.64129
C	5.88348	-1.06721	-0.25776
H	4.27494	0.37002	-0.33600
C	6.37565	-2.20846	0.37242
H	6.04885	-3.68151	1.91018
H	6.43564	-0.61677	-1.07660
H	7.31573	-2.64402	0.04658
H	0.60076	-2.00829	0.55454

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XYZ

C	-1.73048	-0.12079	-0.03388
C	-0.23397	-0.02386	-0.01238
C	0.44654	1.18807	-0.15045
C	0.48516	-1.21318	0.11857
C	1.83798	1.21152	-0.13712
H	-0.09556	2.11685	-0.31257
C	1.87403	-1.18697	0.14279
H	-0.06644	-2.14384	0.20016
C	2.55111	0.02562	0.01766
H	2.36372	2.15328	-0.25530
H	2.43104	-2.11141	0.25508
H	3.63621	0.04510	0.03218
O	-2.31946	-1.13094	-0.30787
O	-2.41088	1.00440	0.27876
H	-1.80851	1.66977	0.64224

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XYZ

C	2.85801	-0.50625	-0.00002
H	2.82763	-1.15221	0.88355
H	2.82781	-1.15150	-0.88412
H	3.81714	0.01898	0.00029
C	1.68464	0.47021	0.00026
H	1.74751	1.12553	-0.87803
H	1.74731	1.12480	0.87910
C	0.33564	-0.24446	-0.00019
H	0.25785	-0.89518	-0.87933
H	0.25753	-0.89576	0.87851
C	-0.84148	0.74104	-0.00013
H	-0.77250	1.39451	-0.87869
H	-0.77246	1.39441	0.87851
C	-2.14111	0.06551	-0.00011
C	-3.19639	-0.51585	0.00014
H	-4.13372	-1.02475	0.00050

I

31

XYZ

C	-1.84261	2.92776	-0.75982
H	-1.07633	3.54299	-1.21653
C	-1.55661	1.72344	-0.28265
C	-2.51874	0.75995	0.35052
H	-3.52488	1.18209	0.25235
H	-2.29971	0.67593	1.42031
C	-2.47241	-0.63178	-0.28848
H	-1.47109	-1.06418	-0.16084
H	-2.63642	-0.54413	-1.37069
C	-3.50783	-1.57807	0.31479
H	-4.50949	-1.14829	0.18513
H	-3.34048	-1.65138	1.39690
C	-3.45863	-2.96874	-0.31194
H	-2.47384	-3.42594	-0.16914
H	-4.20542	-3.63523	0.12885
H	-3.64764	-2.91745	-1.38948
O	-0.25795	1.24466	-0.48993
C	0.45012	0.82333	0.58348
C	1.73685	0.18751	0.18577
C	2.59530	-0.22472	1.20662
C	2.08654	-0.00734	-1.15172
C	3.80504	-0.83012	0.88995
H	2.29543	-0.06122	2.23663
C	3.29780	-0.61592	-1.46356
H	1.41004	0.31703	-1.93447
C	4.15581	-1.02583	-0.44506
H	4.47487	-1.15036	1.68153
H	3.57270	-0.77135	-2.50189
H	5.10074	-1.50032	-0.69190
O	0.07798	0.95542	1.72283
H	-2.85249	3.31435	-0.69747

II

31

XYZ

C	0.79919	-2.05178	0.12112
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C	2.07126	-1.81951	0.42336
C	2.65975	-0.49356	0.80429
H	3.14004	-0.57874	1.78882
H	1.86484	0.25318	0.90322
C	3.70073	-0.01005	-0.21204
H	3.22002	0.10279	-1.19223
H	4.47497	-0.77994	-0.33540
C	4.35726	1.30707	0.19515
H	4.83276	1.18402	1.17683
H	3.58130	2.07284	0.32316
C	5.38987	1.78438	-0.82245
H	4.92766	1.94202	-1.80259
H	5.85342	2.72580	-0.51394
H	6.18561	1.04235	-0.94713
O	-0.12655	-1.02621	0.16724
C	-1.41066	-1.32084	-0.15267
C	-2.29398	-0.12754	-0.05753
C	-3.64428	-0.30200	-0.36678
C	-1.81504	1.12717	0.32448
C	-4.51578	0.77752	-0.29428
H	-3.98690	-1.28864	-0.66068
C	-2.69136	2.20469	0.39551
H	-0.76467	1.25156	0.56295
C	-4.03914	2.03083	0.08688
H	-5.56567	0.64365	-0.53413
H	-2.32334	3.18132	0.69302
H	-4.72001	2.87463	0.14356
O	-1.78143	-2.42176	-0.47542
H	0.39143	-3.01118	-0.17114
H	2.74546	-2.67028	0.36076

III

31

XYZ

C	-0.88258	-0.53806	-0.46817
C	-1.89609	0.27406	-0.73908
C	-3.31210	-0.19936	-0.87996
H	-3.34535	-1.29421	-0.81515

H	-3.69182	0.06712	-1.87614
C	-4.24104	0.40473	0.17917
H	-4.17522	1.50090	0.13829
H	-3.88634	0.11154	1.17573
C	-5.69627	-0.02226	0.00159
H	-5.75753	-1.11792	0.03020
H	-6.04099	0.27962	-0.99596
C	-6.61415	0.57235	1.06636
H	-6.58342	1.66682	1.04067
H	-7.65280	0.26208	0.92041
H	-6.30588	0.25522	2.06813
O	0.39271	-0.02285	-0.34044
C	1.39503	-0.88324	-0.03720
C	2.70879	-0.19133	0.05535
C	3.82546	-0.96775	0.37111
C	2.84345	1.18094	-0.16402
C	5.07693	-0.37174	0.46764
H	3.68932	-2.03161	0.53558
C	4.09830	1.77263	-0.06655
H	1.96935	1.77299	-0.40964
C	5.21310	0.99822	0.24871
H	5.94622	-0.97267	0.71429
H	4.20747	2.83896	-0.23637
H	6.19106	1.46362	0.32555
O	1.22947	-2.06534	0.13477
H	-0.95573	-1.61159	-0.33500
H	-1.69869	1.33958	-0.84477