

Supporting Information

Computational Mechanistic Study of the Ru-catalyzed CO₂ Reduction by Pinacolborane Reveals the σ - π Coupling Mechanism for CO₂ decarbonylation

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S11. Comparisons of the optimized geometries of $\text{RuH}(\kappa^2\text{-CO}_2\text{H})(\text{CO})(\text{PCy}_3)_2$ (**3**) and $\text{RuH}\{(\mu\text{-H})_2\text{Bpin}\}(\text{CO})(\text{PCy}_3)_2$ (**5**) with their X-ray structures.

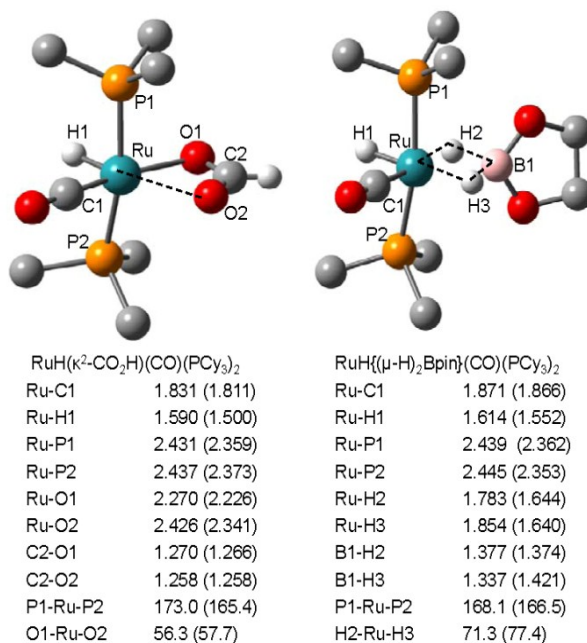


Figure S1. Optimized structures of $\text{RuH}(\kappa^2\text{-CO}_2\text{H})(\text{CO})(\text{PCy}_3)_2$ and $\text{RuH}\{(\mu\text{-H})_2\text{Bpin}\}(\text{CO})(\text{PCy}_3)_2$. Key bond distances and bond angles are given in angstroms and degrees, respectively. Experimental values from X-ray structures are given in the parentheses. For clarity, only the key atoms are presented.

SI2. Free energy profile of HBpin oxidative addition and CO₂ insertion steps in Path_A for the formation of the active catalyst **13**.

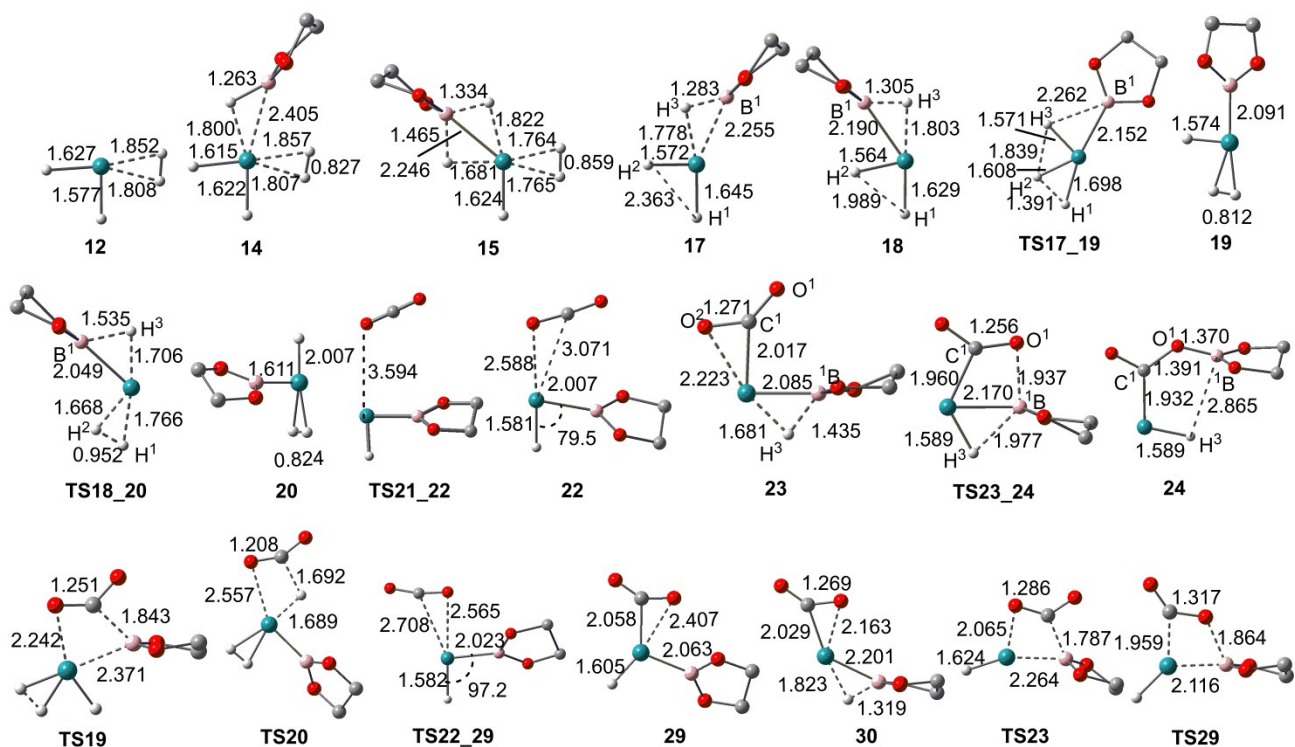
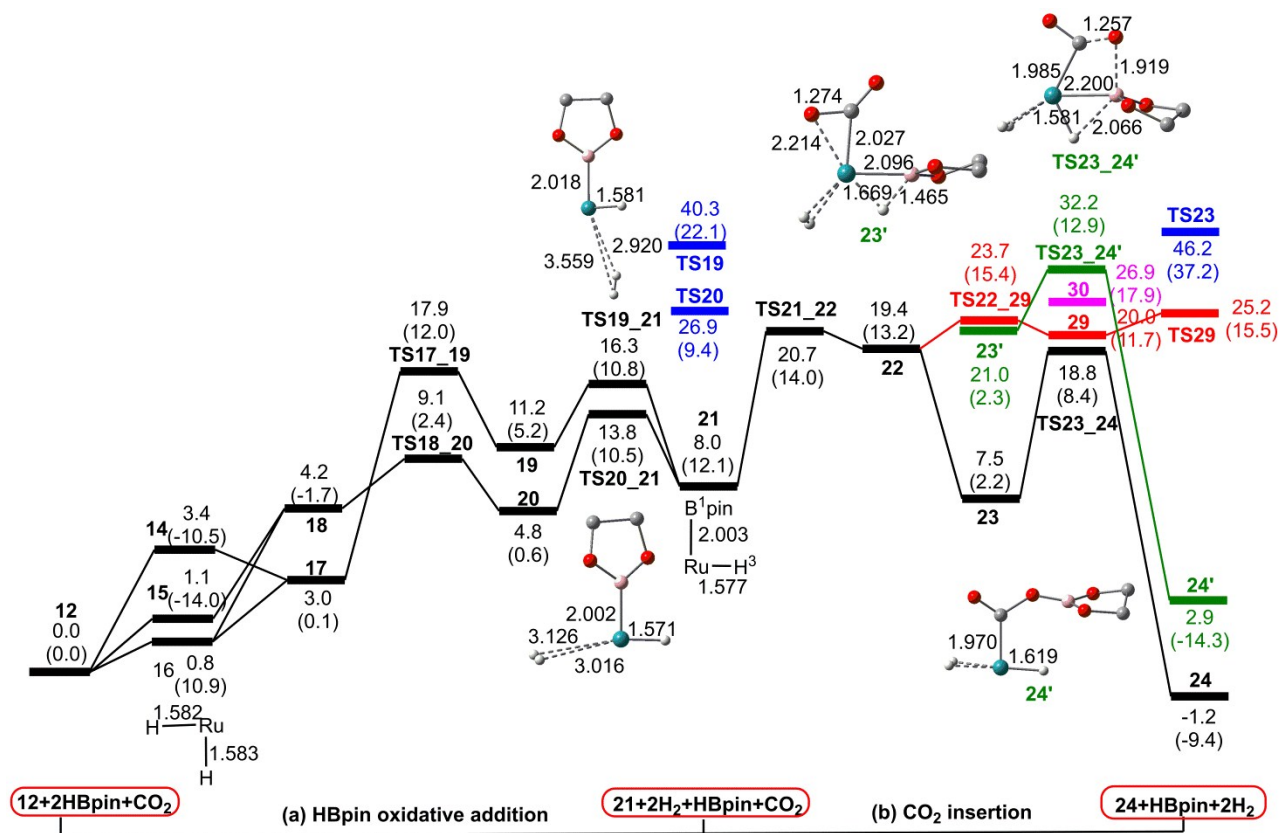


Figure S2. Free energy profile of HBpin oxidative addition and CO₂ insertion steps in Path_A for the formation of the active catalyst **13** via the oxidative insertion mechanism. Free energies and

enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are given in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

SI3. Free energy profile of C-O bond cleavage and σ -bond metathesis steps in Path_A for the formation of the active catalyst **13**.

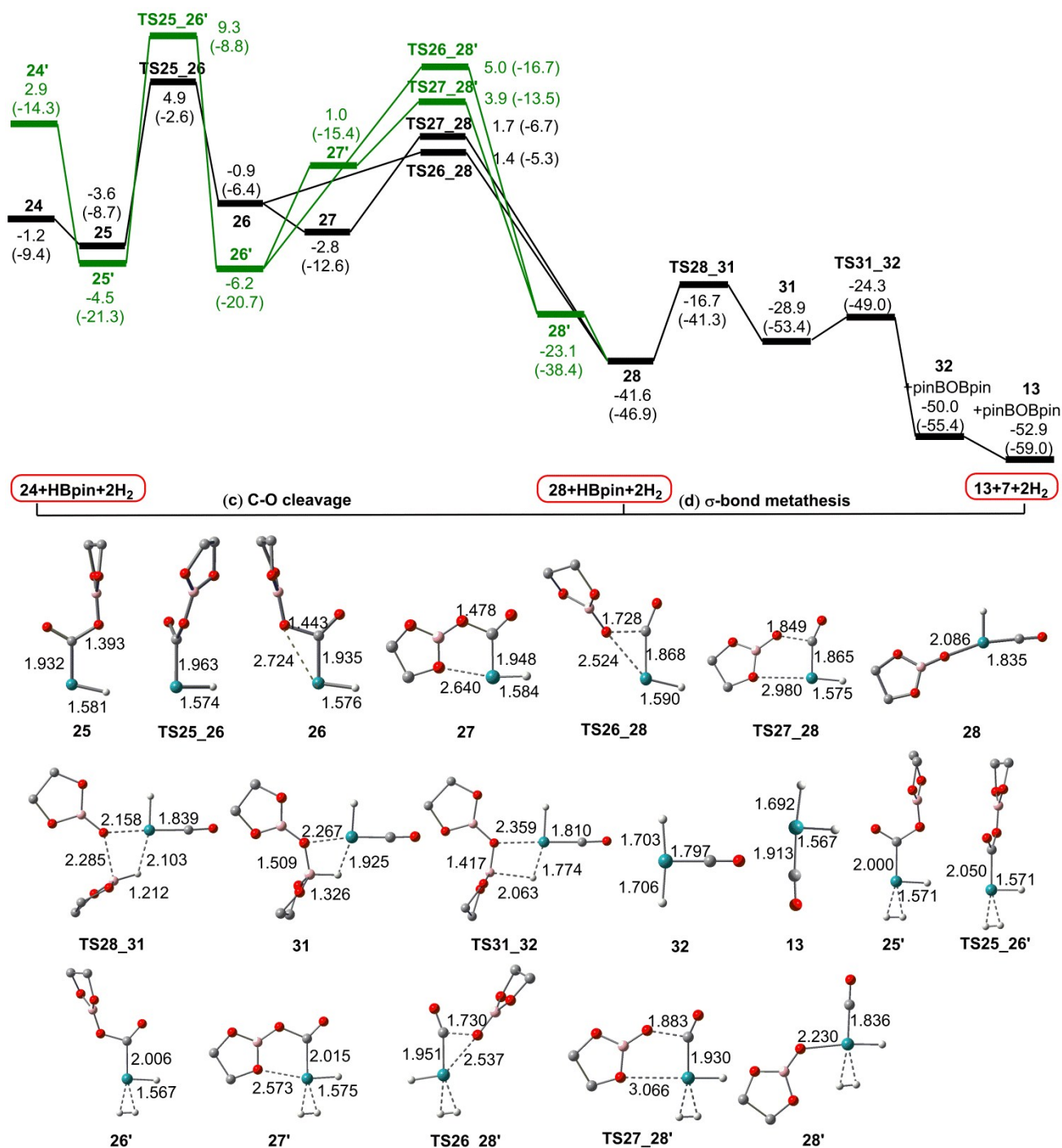
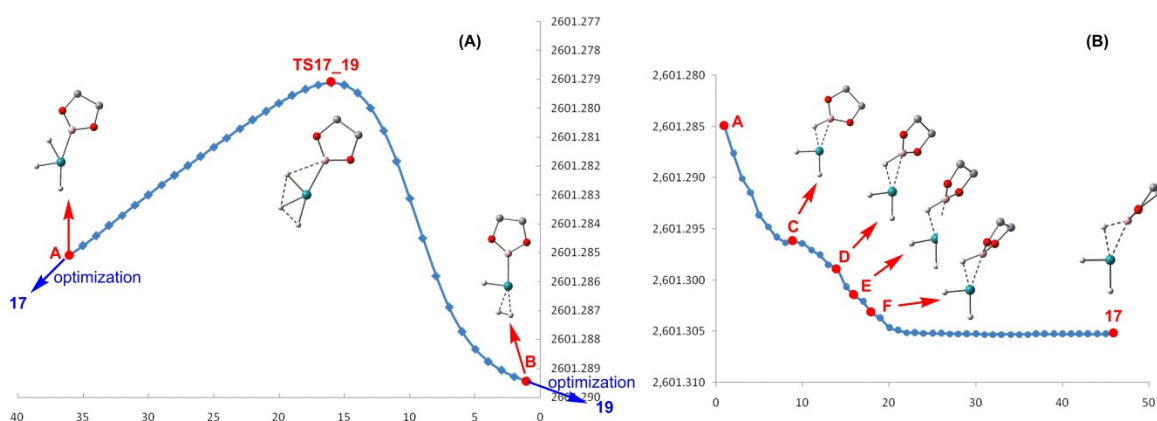


Figure S3. Free energy profile of C-O bond cleavage and σ -bond metathesis steps in Path_A for the formation of the active catalyst **13** via the oxidative insertion mechanism. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are given in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

SI4. IRC result of TS17_19.

IRC calculation of transition state TS17_19 is performed. It can correctly connect intermediates 17 and 19. The following pictures present the results. The IRC result of TS17_19, connecting intermediates A and B, is given in figure A. Optimizations of A and B give intermediates 17 and 19, respectively. The optimization potential energy surface (in a.u.) of A is shown in figure B from which we can see that during optimization the boryl is rotated from coplanar with Ru-H bonds (A) to perpendicular to Ru-H bonds (17 in Figure B) and a shallow minimum (around point C) is shown in the potential energy surface.



SI5. Potential energy surface from 22 to 23, scanned via using the Ru-C bond as reaction coordinate.

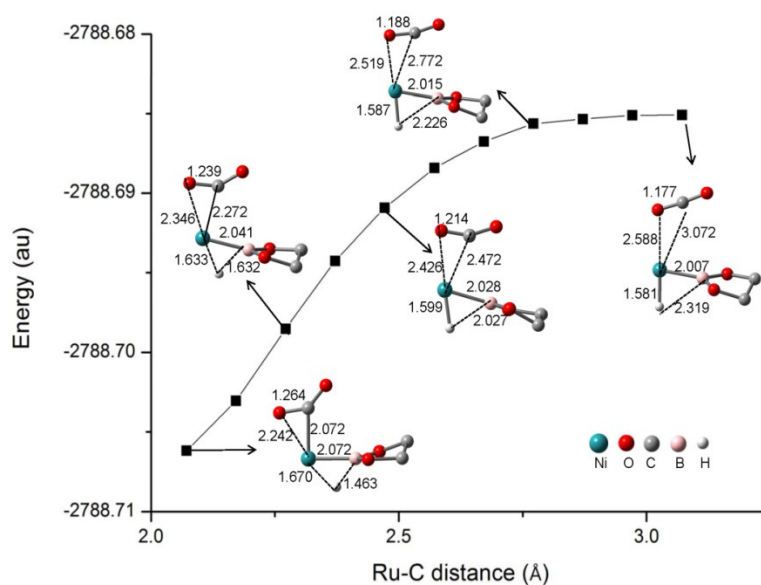


Figure S4. Potential energy surface from 22 to 23 scanned via using the Ru-C bond distance as reaction coordinate varying from 3.072 Å to 2.072 Å.

SI6. Mechanism for the reversible transformation between **1** and **2**.

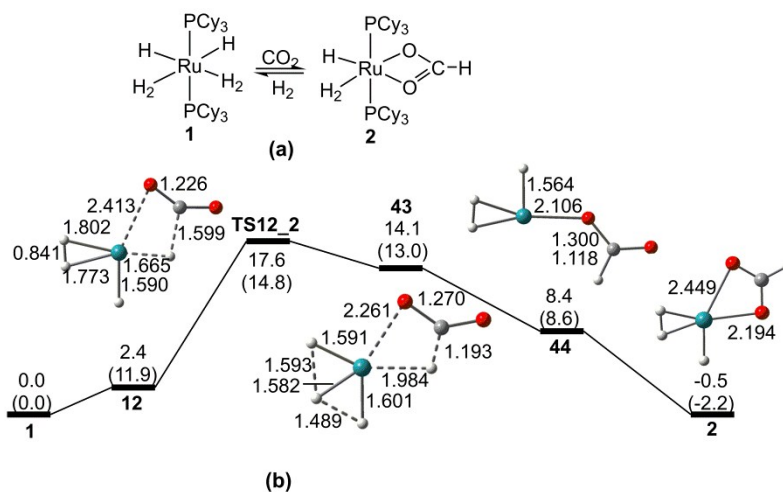


Figure S5. Mechanism for the reversible transformation between **1** and **2** (a), along with the free energy and geometric results (b).

SI7. Free energy profiles of **12** mediated **7-11** formations

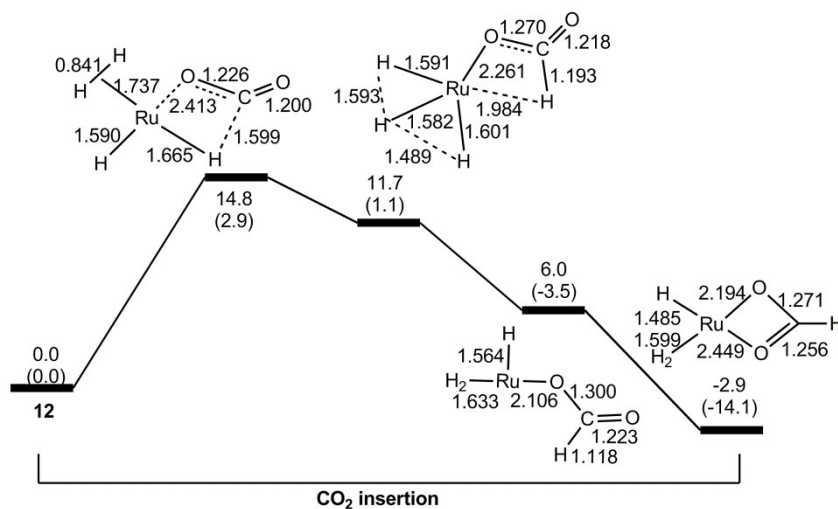


Figure S6. Free energy profile of CO₂ insertion step in pinBOCHO (**7**) formation mediated by **12**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

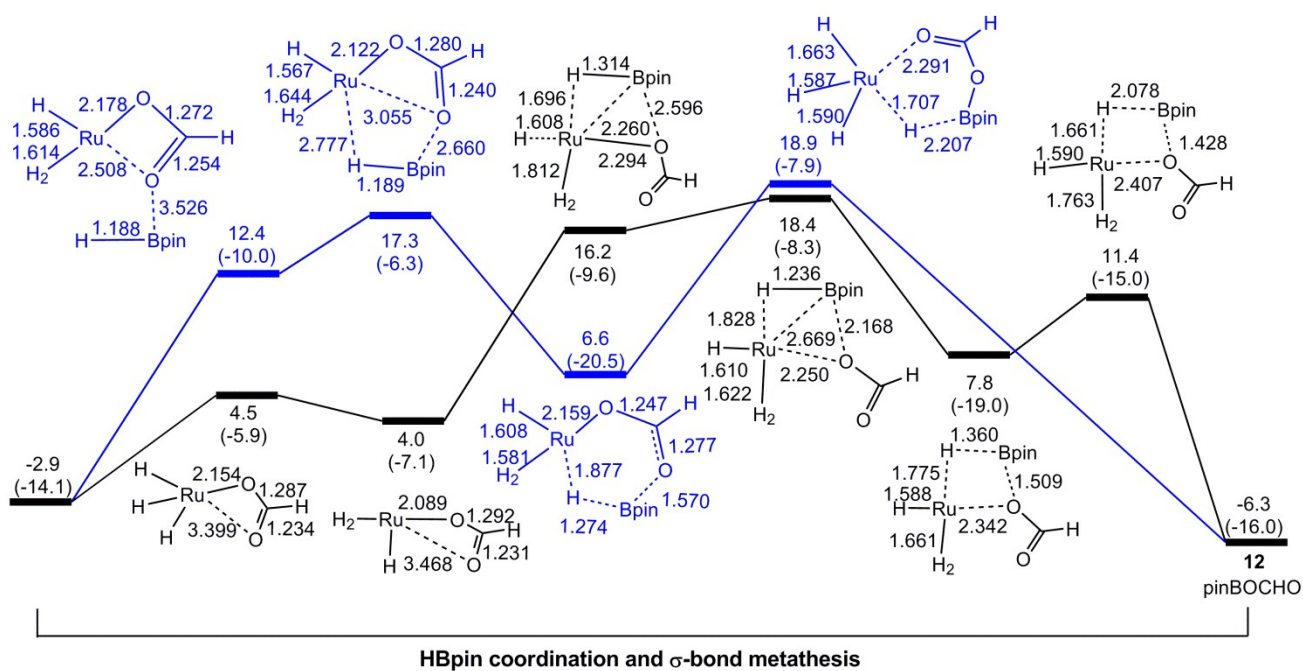


Figure S7. Free energy profile of HBpin coordination and σ -bond metathesis step in pinBOCHO (**7**) formation mediated by **12**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

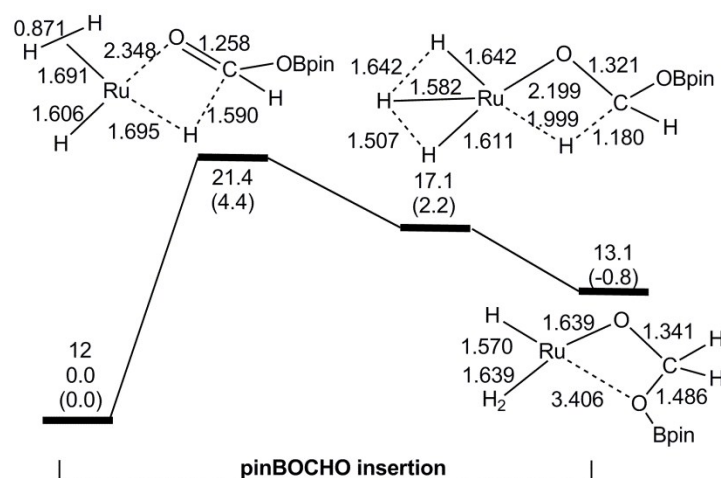


Figure S8. Free energy profile of pinBOCHO insertion step in pinBOCH₂OBpin formation mediated by **12**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

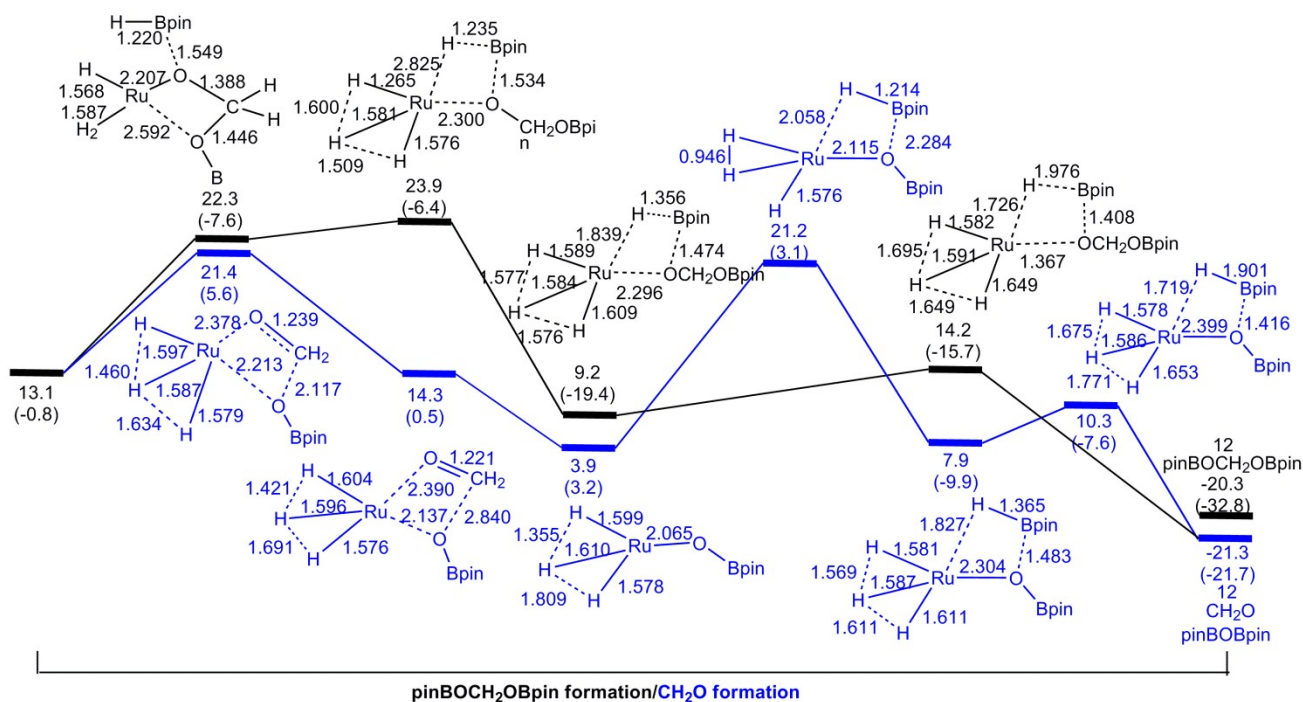


Figure S9. Free energy profile of HBpin metathesis step in pinBOCH₂OBpin formation and CH₂O formation mediated by **12**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

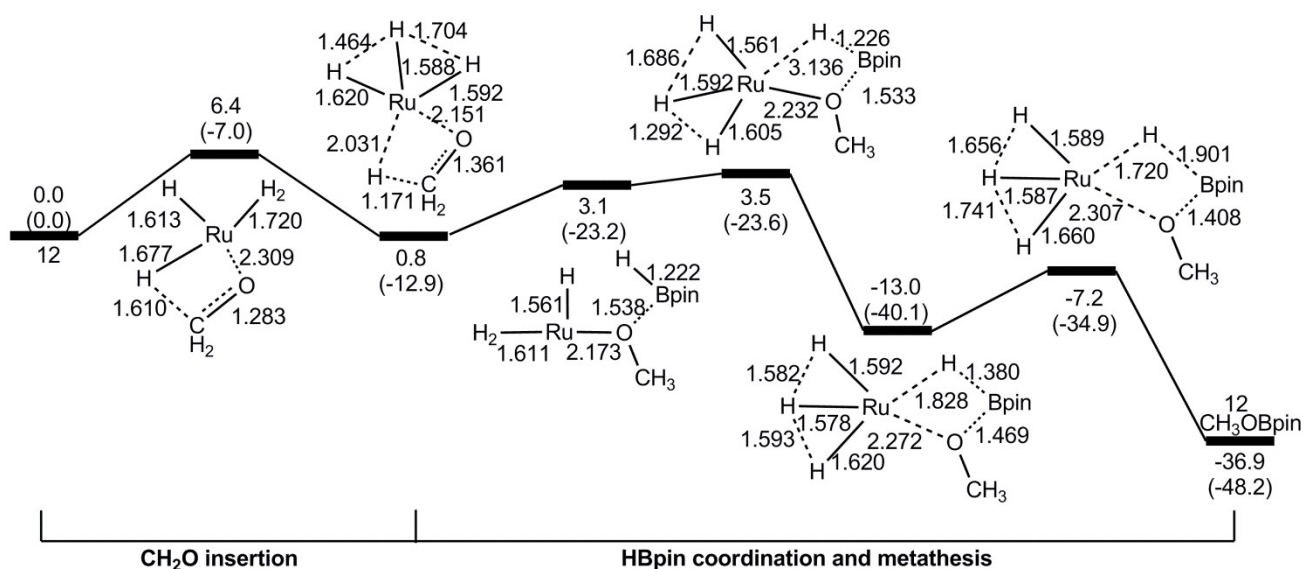


Figure S10. Free energy profile of pinBOCH₃ formation mediated by **12**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

SI8. Free energy profiles of **13** mediated **7-10** formation

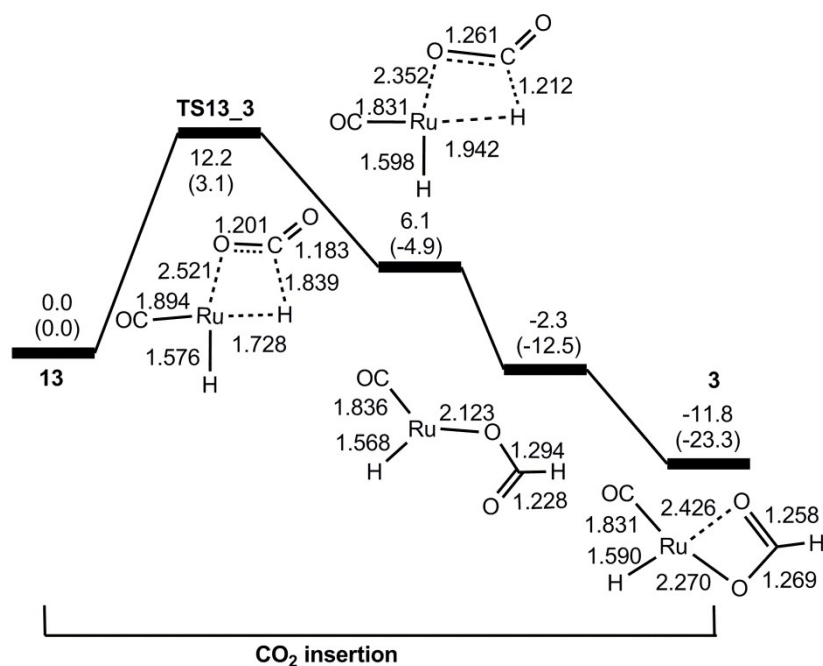


Figure S11. Free energy profile of CO₂ insertion step in pinBOCHO formation mediated by **13**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

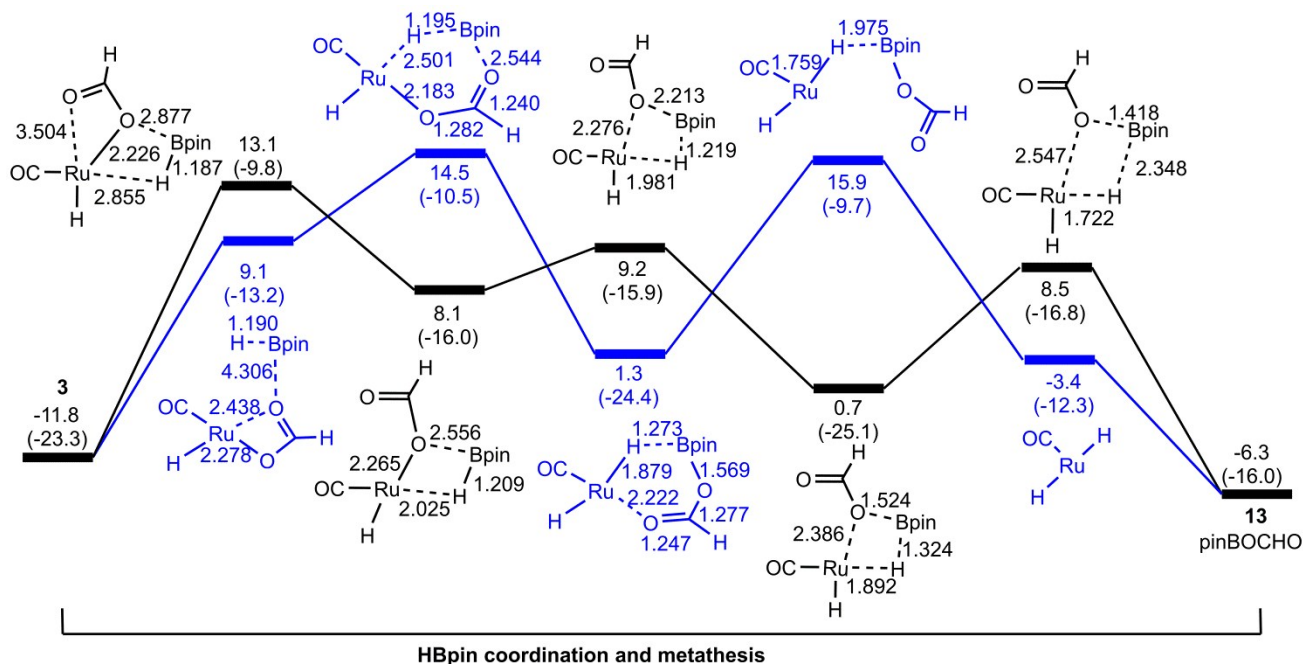


Figure S12. Free energy profile of HBpin coordination and metathesis step in pinBOCHO formation mediated by **13**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

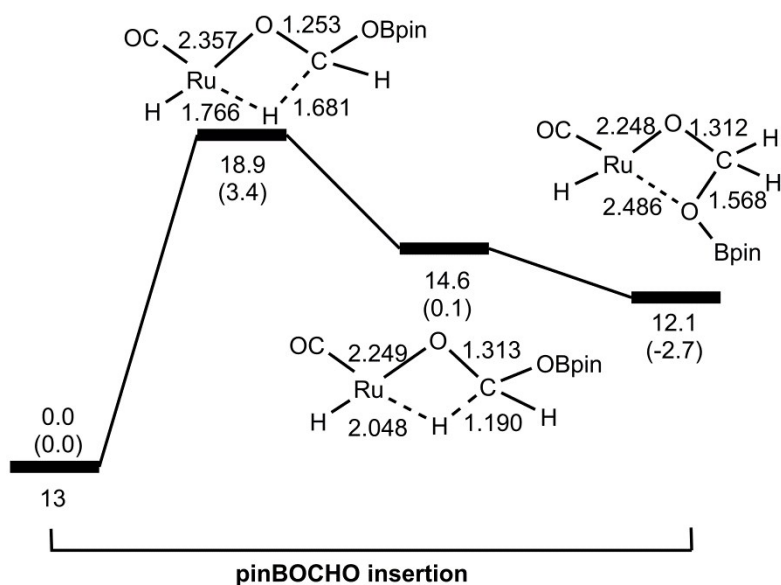


Figure S13. Free energy profile of pinBOCHO insertion step in pinBOCH₂OBpin formation mediated by **13**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

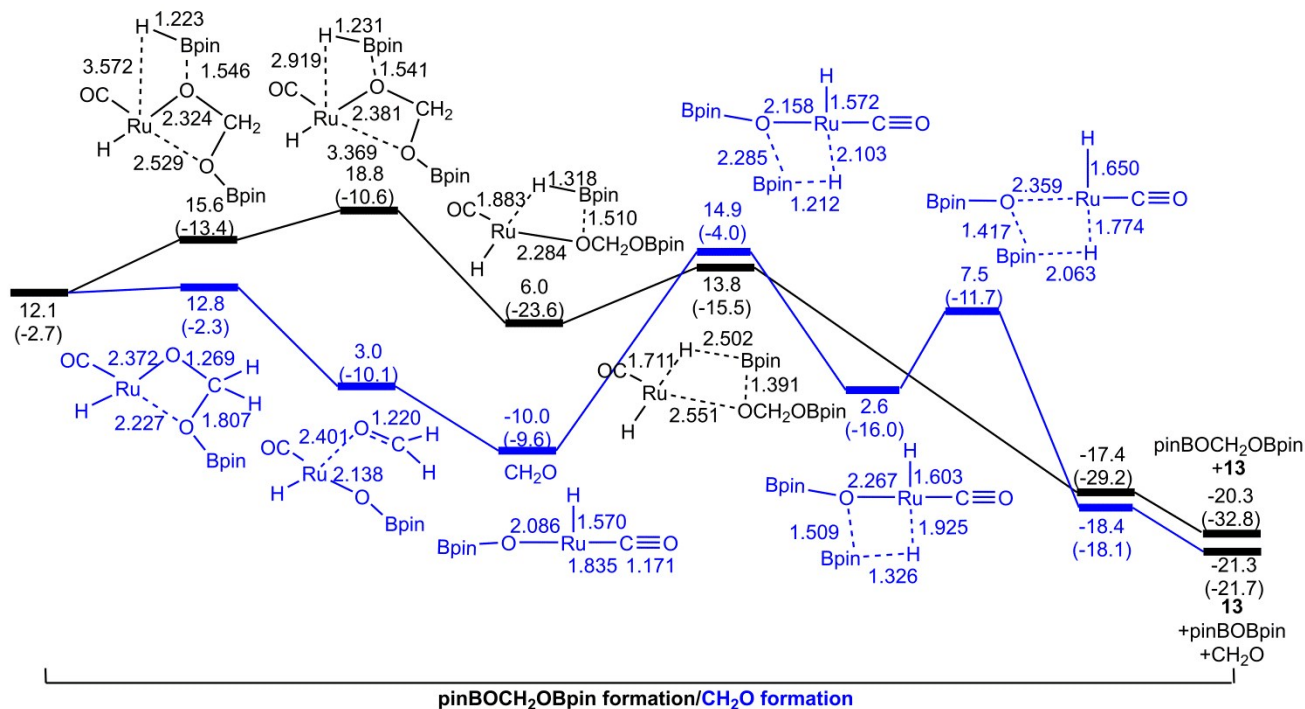


Figure S14. Free energy profile of HBpin metathesis step in pinBOCH₂OBpin formation and CH₂O formation mediated by **13**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

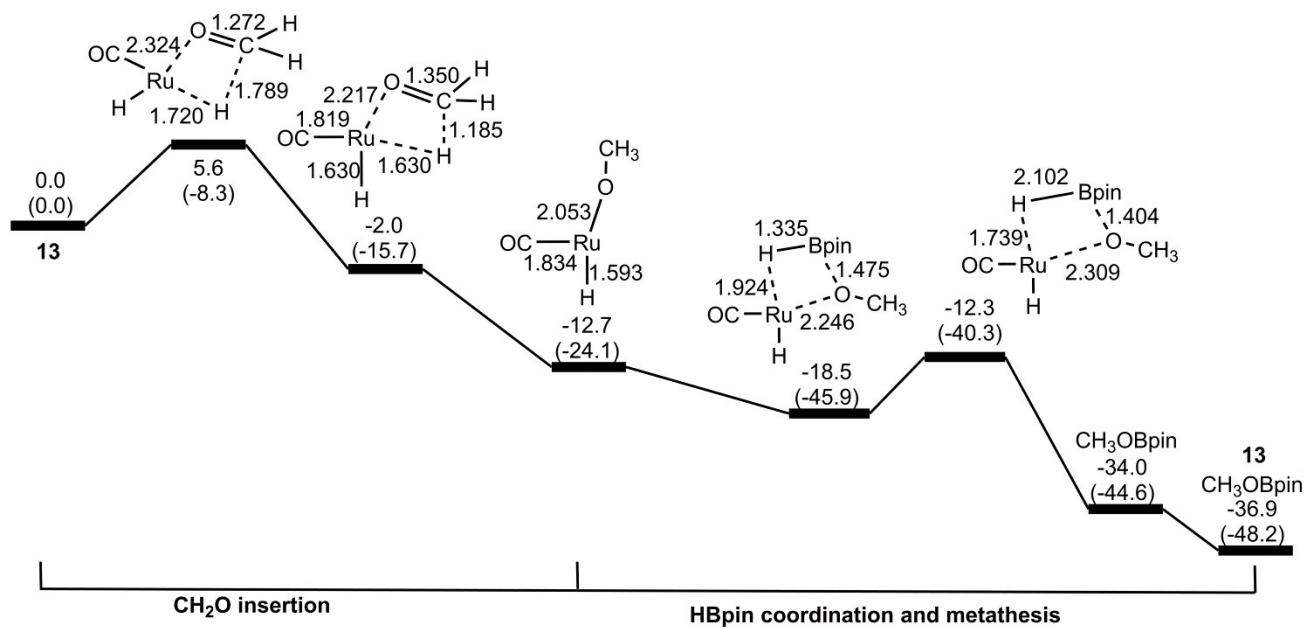


Figure S15. Free energy profile of pinBOCH₃ formation mediated by **13**. Free energies and enthalpies (in parentheses) are given in kcal/mol. The key bond lengths are listed in Å. The two axial PCy₃ ligands on Ru are omitted for clarity.

SI9. Various CO₂ decarbonylation mechanisms reported previously.

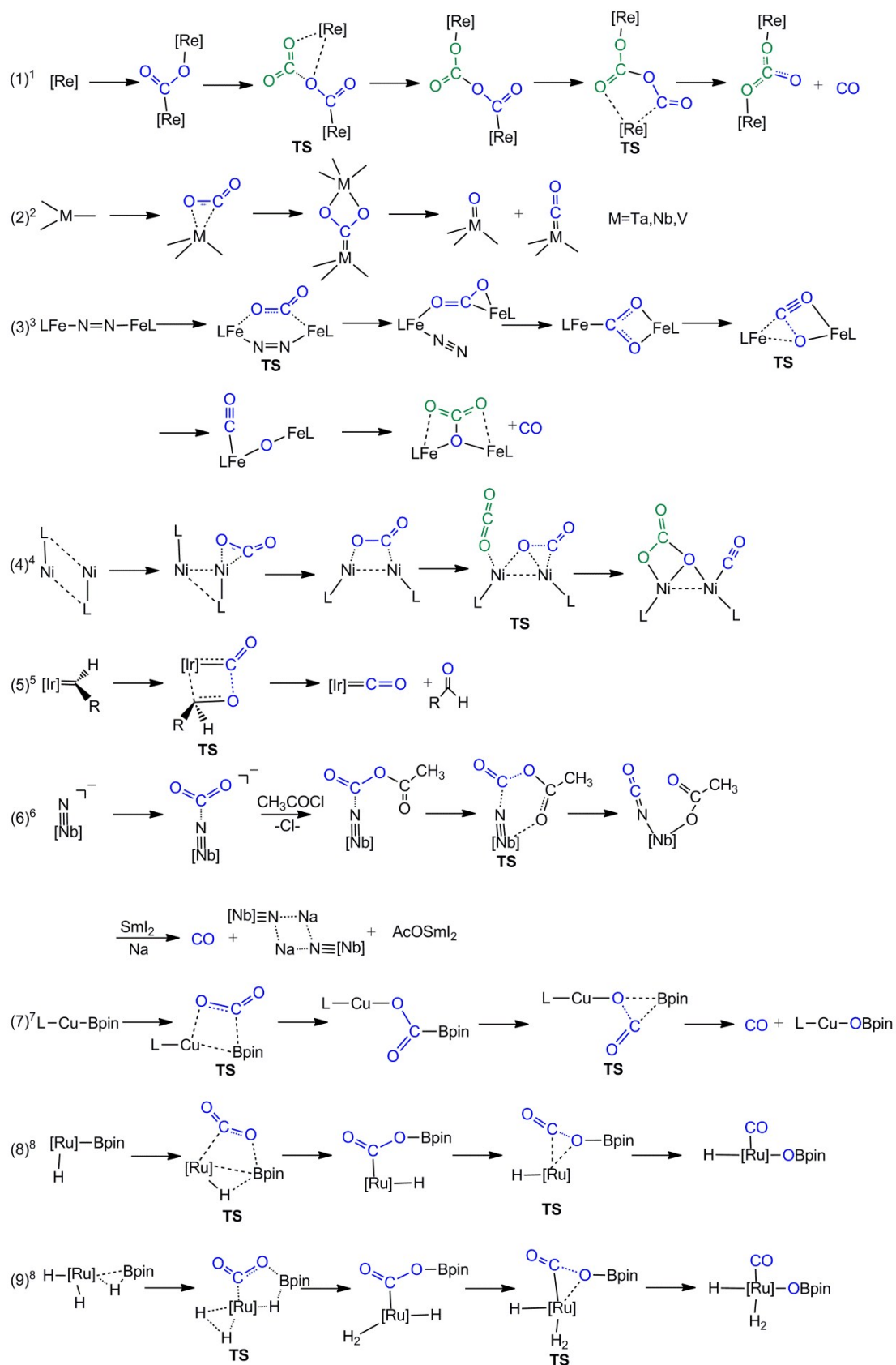


Figure S16. Comparison of CO₂ decarbonylation mechanisms between previously reported and present system.

References

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- (8) We proposed mechanism in present system.

SI10. Complete ref.93

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SI11. Cartesian coordinates of optimized structures

1				C	2.445321	-0.755327	2.686003
Ru	-0.023674	-0.392284	-0.129978	H	-3.608591	-0.950267	-1.811998
P	2.350162	-0.105194	-0.133771	C	-4.732856	0.847004	-1.459607
P	-2.379654	-0.070657	0.053277	C	-2.563365	0.670482	-2.735534
H	0.249331	-1.344787	-1.681214	H	-2.664090	-1.573373	1.881716
H	-0.063449	0.889130	-1.106414	C	-4.728394	-1.368363	1.330414
H	-0.120236	-1.468687	1.353518	C	-3.030057	-2.857035	0.212087
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H	-0.524240	-1.548389	-1.486426	C	-2.518544	1.279389	2.573404
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C	2.861268	1.532587	-0.942757	H	3.287633	-2.880696	0.491308
C	3.216541	-0.020994	1.568847	C	3.950553	-3.854098	-1.328541
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C	2.206213	2.753273	-0.261464	H	1.135075	2.574589	-0.141622
H	3.160080	1.051796	1.806879	H	5.286346	0.094119	0.845635
C	4.707655	-0.426254	1.614435	H	4.804523	-1.499964	1.404611

C	5.324671	-0.143678	2.996822	H	-0.278515	1.912068	-3.265929
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H	1.399491	-0.438041	2.675613	Ru	-0.055028	0.104714	0.009615
H	-5.347631	0.459021	-0.642052	P	-2.458558	-0.060822	0.130499
H	-4.545829	1.905234	-1.233762	P	2.353745	0.070866	-0.001804
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H	-1.976136	-2.980961	-0.057299	C	-2.975516	-0.532226	2.932157
H	-1.235286	2.674734	0.524288	H	-3.175623	0.112147	-2.131877
H	-2.624254	2.871514	-0.529946	C	-2.524431	-1.909608	-2.092539
C	-2.785402	3.958424	1.337676	C	-4.784809	-1.059440	-1.318555
C	-2.969593	2.500542	3.394824	H	-4.283581	1.339213	0.988818
H	-2.960415	0.373491	3.005459	C	-3.771977	2.357147	-0.839656
H	-1.429823	1.166078	2.646758	C	-2.499641	2.526143	1.321732
H	5.014298	-3.683464	-1.104711	H	2.427471	-0.497198	2.300797
H	3.711429	-4.859328	-0.957500	C	2.735265	-2.412330	1.407185
C	3.732797	-3.779321	-2.845780	C	4.519158	-0.689294	1.884937
H	3.771916	-2.304296	-4.445077	H	2.755835	0.156748	-2.325005
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H	1.932563	3.955449	-2.037905	C	2.737714	2.461833	1.470162
H	1.996609	4.894846	-0.549957	H	-1.568221	-2.574287	1.604127
H	6.377990	-0.453857	3.001462	H	-2.858519	-3.038876	0.512004
H	5.317733	0.940998	3.181114	C	-3.290391	-3.454632	2.586955
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H	-6.465949	1.314203	-2.681885	H	-2.584716	-2.803455	-1.458649
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H	-2.748237	1.024603	-4.869264	H	-4.919470	-1.925516	-0.655865
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H	-6.252799	-2.426205	2.463200	H	-2.869129	2.595534	-1.415544
C	-4.960277	-3.894078	1.509942	H	-4.415316	1.744882	-1.479369
H	-2.855023	-4.120982	1.958720	C	-4.517620	3.660938	-0.499791
H	-3.364459	-4.982547	0.509738	C	-3.243598	3.824904	1.674963
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H	-2.338523	4.870852	0.921380	H	-1.584795	2.764465	0.767477
C	-2.414926	3.810871	2.819647	H	1.692665	-2.575124	1.116523
H	-2.654586	2.378053	4.439488	H	3.360018	-2.872270	0.629836
H	-4.069226	2.547198	3.404373	C	3.030828	-3.107523	2.746497
H	2.697660	-4.072213	-3.076590	H	4.757309	0.375426	1.977369
H	4.383192	-4.496991	-3.362342	H	5.181237	-1.092509	1.108310
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H	4.663234	-1.942118	3.996678	H	4.977704	-1.488405	-1.014244
H	4.979804	-0.601973	5.095620	C	5.063051	-1.058840	-3.128904
H	-4.545554	2.376172	-3.829109	C	2.870155	-2.275692	-3.503488
H	-5.267751	1.176989	-4.898453	H	2.715264	-2.747324	-1.402795
H	-5.612887	-3.957882	0.626282	H	1.339799	-1.835630	-2.023180
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H	-1.319663	3.814546	2.919757	H	3.433311	2.188508	-1.939657
H	-2.786617	4.668453	3.395613	C	3.781664	4.006409	-0.826076
				C	3.460907	3.804378	1.674579
				H	1.656473	2.636655	1.389867
				H	2.887554	1.829356	2.354217
2							
C	-0.218561	1.464854	-2.257087				

H	-4.369726	-3.556543	2.397930
H	-2.869295	-4.467230	2.538956
C	-3.078204	-2.850801	3.980448
H	-3.410136	-0.962733	5.011978
H	-4.696664	-1.421069	3.900614
H	-2.966594	-1.388924	-4.146040
H	-2.595273	-3.093318	-3.911010
C	-4.630948	-2.542328	-3.378380
H	-6.450950	-1.652067	-2.581617
H	-5.350460	-0.501095	-3.333979
H	-4.780432	4.184554	-1.428368
H	-5.467685	3.412829	-0.002309
C	-3.690908	4.574979	4.013304
H	-4.124779	3.589938	2.291789
H	-2.595886	4.464377	2.288967
H	2.350294	-2.713670	3.516246
H	2.818632	-4.181310	2.662370
C	4.484265	-2.883952	3.187046
H	5.885845	-1.245064	3.478686
H	4.246591	-0.902598	4.021586
H	4.795489	-0.230438	-3.801549
H	6.156555	-1.150847	-3.167261
C	4.399250	-2.351366	-3.626123
H	2.417005	-3.227474	-3.809878
H	2.485256	-1.510453	-4.193393
H	4.865464	3.824418	-0.763274
H	3.623599	4.650392	-1.700857
C	3.313452	4.718385	0.450566
H	3.070200	4.300741	2.572485
H	4.529149	3.616816	1.861490
H	-2.004010	-2.854165	4.218142
H	-3.571116	-3.464563	4.745377
H	-5.046729	-2.729521	-4.376953
H	-4.779245	-3.466504	-2.799700
H	-2.802187	4.921970	-0.133025
H	-4.267575	5.470050	0.681038
H	4.663196	-3.339014	4.169788
H	5.156758	-3.392453	2.480031
H	4.692122	-2.552777	-4.664728
H	4.768362	-3.197919	-3.027593
H	2.257604	5.003881	0.337708
H	3.877527	5.648327	0.599394
H	-0.006979	0.613719	1.604595
H	-0.002894	-0.353054	1.610211

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C	-0.175906	1.396761	-2.298584
H	-0.211770	1.842145	-3.310035
O	-0.099771	0.132748	-2.212131
O	-0.212782	2.149722	-1.291405
Ru	-0.058888	0.138380	0.057161
C	-0.000844	0.405792	1.868053
P	-2.480138	-0.077286	0.071759
P	2.375194	0.063797	-0.023883
H	0.004350	-1.416481	0.385495
O	0.061819	0.591730	3.021343
C	-3.285088	-1.068910	1.473099
C	-3.126332	-0.904559	-1.499999
C	-3.435347	1.564564	0.130294
C	3.098912	-0.849791	1.474556
C	3.019014	-0.699959	-1.622465
C	3.263928	1.729881	0.050891
H	-4.301932	-1.282631	1.113276
C	-2.569762	-2.416682	1.718577
C	-3.433874	-0.306892	2.810042
H	-2.902446	-0.145061	-2.260512
C	-2.352256	-2.169411	-1.932418

C	-4.644960	-1.183239	-1.537728
H	-4.420601	1.329689	0.562765
C	-3.672786	2.227964	-1.245644
C	-2.717721	2.578949	1.054635
H	2.513350	-0.419659	2.299267
C	2.791867	-2.363673	1.461379
C	4.589337	-0.621005	1.815221
H	2.676829	0.037658	-2.361832
C	4.550567	-0.827981	-1.763421
C	2.332728	-2.028822	-2.010772
H	4.334674	1.506899	0.157327
C	3.100043	2.597008	-1.216565
C	2.812814	2.529016	1.294689
H	-1.543965	-2.218187	2.052376
H	-2.481631	-2.986820	0.788937
C	-3.299236	-3.266533	2.773168
C	-4.164058	-1.160446	3.863601
H	-2.444192	-0.033142	3.195128
H	-3.990493	0.624434	2.665405
H	-1.277806	-1.975840	-1.908573
H	-2.554304	-2.992465	-1.234551
C	-2.781298	-2.603275	-3.345034
C	-5.085456	-1.614443	-2.948748
H	-4.887467	-1.990709	-0.833209
H	-5.223517	-0.307735	-1.219244
H	-2.702406	2.457057	-1.700464
H	-4.203211	1.555579	-1.927241
C	-4.485651	3.528376	-1.102868
C	-3.528577	3.876787	1.209953
H	-2.522420	2.149877	2.042094
H	-1.741012	2.807334	0.612234
H	1.737459	-2.536145	1.222077
H	3.383944	-2.848998	0.673957
C	3.143950	-3.014482	2.809850
H	4.823362	0.446995	1.871679
H	5.224695	-1.041480	1.025495
C	4.952817	-1.279512	3.160075
H	5.054125	0.109290	-1.499199
H	4.919659	-1.591948	-1.065955
C	4.936588	-1.235334	-3.197240
C	2.713998	-2.431886	-3.445630
H	2.639071	-2.826727	-1.323089
H	1.248715	-1.924943	-1.926121
H	2.037552	2.811381	-1.372612
H	3.457540	2.060116	-2.103487
C	3.877421	3.920047	-1.084585
C	3.582537	3.854209	1.426550
H	1.739108	2.741057	1.208060
H	2.941838	1.939475	2.210152
H	-4.291250	-3.551151	2.390877
H	-2.747990	-4.201791	2.935447
C	-3.465046	-2.506198	4.094786
H	-4.233625	-0.597696	4.803347
H	-5.197183	-1.340798	3.529990
H	-2.485392	-1.823002	-4.061232
H	-2.238674	-3.512753	-3.633887
C	-4.296600	-2.838801	-3.436905
H	-6.162533	-1.827105	-2.953792
H	-4.928272	-0.777562	-3.645259
H	-4.626170	3.980985	-2.093210
H	-5.490896	3.286031	-0.725829
C	-3.812934	4.525921	-0.150620
H	-4.480799	3.656794	1.716655
H	-2.983912	4.574022	1.859577
H	2.495473	-2.595525	3.593162
H	2.929911	-4.090319	2.768153
C	4.614189	-2.776281	3.180752

H	6.019757	-1.125583	3.367674
H	4.401829	-0.772448	3.965866
H	4.658009	-0.425022	-3.887169
H	6.026382	-1.346518	-3.270934
C	4.235872	-2.532709	-3.627108
H	2.237419	-3.387404	-3.700324
H	2.309148	-1.685137	-4.144077
H	4.955628	3.706267	-1.026716
H	3.727617	4.523589	-1.989127
C	3.450142	4.710303	0.159758
H	3.217410	4.406086	2.302197
H	4.646108	3.640843	1.612459
H	-2.474177	-2.328059	4.537474
H	-4.028452	-3.110390	4.817544
H	-4.584193	-3.089316	-4.466179
H	-4.564797	-3.707974	-2.817593
H	-2.864825	4.863582	-0.592921
H	-4.440556	5.418223	-0.028130
H	4.835251	-3.201961	4.167936
H	5.258356	-3.303992	2.461332
H	4.483178	-2.769655	-4.669970
H	4.617860	-3.366194	-3.018522
H	2.403153	5.025837	0.044738
H	4.047267	5.626581	0.253592

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C	-0.229198	-2.228464	-0.432436
O	-0.362234	-3.326555	-0.756698
Ru	-0.010955	-0.245879	-0.205323
P	-2.411116	0.282506	-0.041655
P	2.440489	-0.143386	-0.075016
C	0.000747	0.115456	-2.034415
O	-0.030047	-0.345098	1.967346
C	-3.369882	-0.032411	-1.644110
C	-2.728053	2.116082	0.273930
C	-3.262345	-0.559837	1.422263
C	3.162963	0.948050	-1.448967
C	3.378444	-1.765688	-0.306673
C	3.020677	0.443937	1.623901
O	0.002692	0.376779	-3.167620
C	-0.056034	-1.467318	2.602603
H	-2.861787	0.654682	-2.336508
C	-4.868148	0.343943	-1.642876
C	-3.183477	-1.447296	-2.236043
H	-3.817049	2.220436	0.374178
C	-2.082715	2.591921	1.595267
C	-2.280983	3.018921	-0.895943
H	-2.517099	-0.394560	2.210916
C	-4.598509	0.045171	1.911049
C	-3.408315	-2.089323	1.255539
H	2.670978	0.528171	-2.338417
C	2.731122	2.428881	-1.364316
C	4.685823	0.870247	-1.704672
H	4.446453	-1.509295	-0.276843
C	3.089905	-2.398327	-1.687327
C	3.114499	-2.775016	0.833211
H	2.607357	-0.343454	2.268285
C	4.547739	0.485194	1.851355
C	2.376007	1.762310	2.104780
O	-0.112115	-2.611051	2.144949
H	-0.025923	-1.326157	3.705038
H	-5.418710	-0.345373	-0.989489
H	-5.024568	1.351644	-1.242429
C	-5.460085	0.259994	-3.062135
C	-3.775902	-1.534116	-3.653710
H	-3.675271	-2.189871	-1.596308
H	-2.124250	-1.713535	-2.267206

H	-2.426841	1.984802	2.439882
H	-0.998899	2.443679	1.531232
C	-2.386356	4.074523	1.872174
C	-2.577488	4.502241	-0.610164
H	-2.781936	2.729635	-1.827205
H	-1.204290	2.885366	-1.058364
H	-4.516330	1.125851	2.063647
H	-5.379342	-0.108358	1.155932
C	-5.043094	-0.612515	3.231533
C	-3.857211	-2.748227	2.571583
H	-2.463876	-2.537239	0.939101
H	-4.156323	-2.303908	0.480244
H	1.658343	2.506293	-1.166160
H	3.244808	2.909354	-0.521220
C	3.092204	3.182747	-2.655264
C	5.061604	1.627061	-2.993270
H	5.229328	1.310006	-0.859304
H	5.023740	-0.167567	-1.789713
H	2.016652	-2.598383	-1.780471
H	3.349264	-1.702139	-2.493992
C	3.861259	-3.715444	-1.883730
C	3.881852	-4.090765	0.612388
H	2.043118	-2.984802	0.917825
H	3.417234	-2.347829	1.796289
H	5.029355	-0.443159	1.524900
H	4.987177	1.296231	1.255784
C	4.870727	0.731567	3.336991
C	2.699980	2.012537	3.588008
H	2.754446	2.604226	1.510984
H	1.295354	1.713891	1.962397
H	-6.527609	0.513716	-3.031506
H	-4.976985	1.015882	-3.698860
C	-5.256593	-1.130172	-3.679358
H	-3.205318	-0.872356	-4.321752
H	-3.650632	-2.553025	-4.041251
H	-3.466468	4.204737	2.039322
H	-1.888906	4.381492	2.801123
C	-1.943301	4.968647	0.706838
H	-2.217965	5.114172	-1.447471
H	-3.666577	4.651542	-0.559765
H	-4.310160	-0.370707	4.015288
H	-5.999122	-0.179066	3.553284
C	-5.161105	-2.136641	3.100015
H	-3.975901	-3.827889	2.415929
H	-3.057961	-2.629320	3.315892
H	2.786815	4.233388	-2.566381
H	2.517903	2.759606	-3.492304
C	4.593410	3.088877	-2.960889
H	6.147544	1.576351	-3.145286
H	4.601930	1.117847	-3.853186
H	3.600251	-4.148272	-2.857941
H	4.941136	-3.505310	-1.913638
C	3.569234	-4.712497	-0.754894
H	3.633750	-4.792653	1.418198
H	4.963791	-3.900296	0.683267
H	5.958887	0.775032	3.475880
H	4.513634	-0.124728	3.927893
C	4.211957	2.017653	3.854983
H	2.254621	2.964011	3.906553
H	2.222971	1.227351	4.192435
H	-5.843229	-1.867085	-3.110845
H	-5.641138	-1.150129	-4.706951
H	-2.204371	6.016058	0.905614
H	-0.847893	4.928294	0.616278
H	-5.981665	-2.375687	2.406623
H	-5.429969	-2.581798	4.066542
H	4.823410	3.582372	-3.913785

H	5.154062	3.630775	-2.184496
H	4.151243	-5.631830	-0.898943
H	2.508700	-4.999565	-0.789097
H	4.412583	2.141625	4.926977
H	4.666253	2.883387	3.349759
H	0.178177	1.371284	0.020715

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C	0.150200	1.717929	1.548879
O	0.268115	2.531022	2.376654
Ru	0.008381	0.384337	0.244173
P	-2.393832	0.777973	0.013397
P	2.441864	0.324845	0.094431
B	-0.229175	-1.921526	0.060949
H	-0.114329	-0.961418	-0.919456
H	-0.111893	-1.208100	1.185650
H	0.124498	1.526611	-0.890807
C	-2.940868	2.586481	-0.208245
C	-3.193317	-0.099887	-1.465498
C	-3.512554	0.264512	1.474427
C	3.365477	-0.396562	1.582360
C	3.132204	2.100835	0.025909
C	3.122667	-0.673896	-1.355984
O	0.811487	-2.884854	-0.067134
O	-1.479753	-2.594014	-0.068569
H	-4.004469	2.507668	-0.475366
C	-2.214592	3.304416	-1.365291
C	-2.869086	3.450314	1.070874
H	-3.203582	-1.140581	-1.119553
C	-2.364215	-0.098215	-2.768687
C	-4.643680	0.328248	-1.782423
H	-4.348504	0.980832	1.463235
C	-4.111952	-1.156208	1.382333
C	-2.763705	0.413486	2.819563
H	4.424260	-0.147080	1.431282
C	3.274251	-1.931217	1.711781
C	2.902236	0.269637	2.897359
H	2.497105	2.610375	0.762686
C	4.596933	2.333465	0.464751
C	2.880695	2.800033	-1.327784
H	2.805327	-1.688426	-1.078099
C	4.658327	-0.671966	-1.516960
C	2.442580	-0.366585	-2.709665
C	0.235453	-4.123864	-0.523686
C	-1.241280	-4.012909	0.005316
H	-1.144907	3.363374	-1.131131
H	-2.292791	2.725684	-2.290521
C	-2.772336	4.719141	-1.602170
C	-3.432843	4.862742	0.828589
H	-3.429676	2.984137	1.887274
H	-1.830115	3.535209	1.407301
H	-2.322728	0.912187	-3.195659
H	-1.333041	-0.392360	-2.561019
C	-2.989634	-1.048246	-3.805942
C	-5.283157	-0.619342	-2.813950
H	-5.261645	0.361730	-0.877306
H	-4.644124	1.346059	-2.196673
H	-3.296698	-1.884742	1.322132
H	-4.701457	-1.274568	0.467943
C	-5.016862	-1.467891	2.588609
C	-3.673847	0.114687	4.022311
H	-1.915779	-0.283138	2.822867
H	-2.334262	1.414001	2.925283
H	2.227054	-2.234390	1.808876
H	3.644619	-2.419887	0.804672
C	4.082935	-2.434251	2.921395
C	3.710154	-0.233218	4.105730

H	2.976560	1.361481	2.836958
H	1.840308	0.040067	3.052884
H	4.793776	1.887390	1.444320
H	5.285859	1.856034	-0.243660
C	4.915657	3.839311	0.541091
C	3.188883	4.305027	-1.246093
H	3.527700	2.353590	-2.094747
H	1.845333	2.644086	-1.646662
H	4.996072	0.332906	-1.803650
H	5.155615	-0.912457	-0.570322
C	5.104893	-1.670395	-2.600593
C	2.894956	-1.360117	-3.794342
H	1.355476	-0.401662	-2.596142
H	2.691419	0.649115	-3.038670
C	1.048815	-5.282578	0.056609
C	0.313982	-4.154693	-2.058596
C	-1.375531	-4.446656	1.475268
C	-2.293424	-4.729986	-0.842529
H	-2.211105	5.203148	-2.412077
H	-3.815762	4.648202	-1.945230
C	-2.717045	5.571187	-0.328044
H	-4.507059	4.790608	0.600411
H	-3.348423	5.451820	1.750860
H	-2.398404	-1.029247	-4.730864
H	-2.939742	-2.078152	-3.422526
C	-4.452635	-0.687698	-4.103694
H	-5.364044	-1.625707	-2.377502
H	-6.307047	-0.291143	-3.036311
H	-5.894383	-0.803585	2.565263
H	-5.402787	-2.492072	2.498758
C	-4.286457	-1.287827	3.925139
H	-3.099311	0.219658	4.951770
H	-4.480394	0.862428	4.068121
H	3.981778	-3.524541	3.000708
H	5.152259	-2.232372	2.754708
C	3.642533	-1.760952	4.228225
H	3.336255	0.242800	5.021382
H	4.760594	0.077365	3.998803
H	4.308069	4.292361	1.338405
H	5.964901	3.977271	0.833312
C	4.629857	4.559335	-0.782840
H	3.013681	4.771478	-2.224348
H	2.488828	4.779437	-0.542710
H	6.196842	-1.635267	-2.709533
H	4.855236	-2.690793	-2.274360
C	4.422362	-1.385877	-3.945734
H	2.540058	-2.367241	-3.533160
H	2.421775	-1.101397	-4.750669
H	2.062542	-5.267149	-0.358327
H	0.596154	-6.248434	-0.197830
H	1.130260	-5.210981	1.143773
H	-0.262354	-3.335968	-2.500431
H	-0.056367	-5.101139	-2.468043
H	1.358847	-4.038882	-2.364055
H	-0.633126	-3.944052	-2.102974
H	-1.255456	-5.529312	1.593516
H	-2.370500	-4.173328	1.841481
H	-3.286322	-4.577240	-0.405625
H	-2.104632	-5.809644	-0.877266
H	-2.313897	-4.346582	-1.865782
H	-1.666278	5.743429	-0.052104
H	-3.161371	6.558926	-0.506728
H	-4.892048	-1.411990	-4.801773
H	-4.487727	0.290970	-4.605423
H	-4.971568	-1.469123	4.763553
H	-3.485270	-2.037368	4.004794
H	4.262639	-2.106557	5.065563

H	2.608798	-2.058593	4.458038
H	4.816584	5.635965	-0.679116
H	5.326513	4.193405	-1.552066
H	4.765963	-0.411856	-4.325539
H	4.721486	-2.134490	-4.690746

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C	-0.014772	0.461058	-2.093809
O	0.028579	0.464703	-3.253619
Ru	-0.043472	0.414147	-0.148909
P	-2.405429	-0.056787	0.027965
P	2.346675	0.104322	0.082883
H	-0.025913	0.200948	1.501721
H	0.021590	-1.241207	-0.150804
C	-3.137279	-1.383149	-1.129275
C	-2.926799	-0.674172	1.745789
C	-3.591296	1.409185	-0.233569
C	3.380366	1.664510	0.357020
C	3.126652	-0.615515	-1.491561
C	2.810748	-0.946525	1.591520
H	-4.070900	-1.682297	-0.632043
C	-2.238841	-2.634241	-1.245228
C	-3.527707	-0.898488	-2.543693
H	-2.678080	0.192063	2.374558
C	-2.101079	-1.853236	2.300838
C	-4.431240	-0.981740	1.925732
H	-4.576254	0.964947	-0.445156
C	-3.744530	2.323889	1.005487
C	-3.185644	2.280012	-1.446936
H	4.429896	1.343192	0.399272
C	3.059517	2.357773	1.700302
C	3.250246	2.656129	-0.820308
H	2.791106	0.119762	-2.237705
C	4.668126	-0.674409	-1.579402
C	2.532536	-1.974338	-1.924325
H	2.294237	-0.388740	2.386024
C	4.307815	-1.022736	1.966853
C	2.207589	-2.367716	1.599263
H	-1.302210	-2.353483	-1.740348
H	-1.954027	-3.005223	-0.257104
C	-2.923710	-3.755206	-2.045497
C	-4.199134	-2.019585	-3.359505
H	-4.220470	-0.054037	-2.485928
H	-2.634582	-0.547730	-3.077280
H	-2.337854	-2.769758	1.744029
H	-1.035438	-1.656138	2.164397
C	-2.420008	-2.087139	3.788184
C	-4.770148	-1.212642	3.410661
H	-5.062592	-0.180580	1.525882
H	-4.689296	-1.890750	1.365268
H	-2.770682	2.761067	1.258910
H	-4.070771	1.755649	1.881257
C	-4.759389	3.454222	0.748749
C	-4.213866	3.391521	-1.716903
H	-2.212999	2.738617	-1.242574
H	-3.050565	1.676008	-2.347253
H	1.999819	2.631498	1.731999
H	3.228037	1.669798	2.536595
C	3.913242	3.622616	1.903801
C	4.098792	3.920755	-0.597572
H	3.553604	2.179277	-1.759946
H	2.199180	2.942769	-0.941796
H	5.123413	0.279371	-1.292274
H	5.052329	-1.429668	-0.881813
C	5.120133	-1.037451	-3.006970
C	2.971915	-2.334994	-3.353576
H	2.877408	-2.760297	-1.239880

H	1.441837	-1.953067	-1.853731
H	4.848538	-1.613454	1.216403
H	4.773161	-0.032120	1.980739
C	4.494590	-1.682485	3.345730
C	2.384958	-3.032094	2.975769
H	1.149776	-2.326938	1.328062
H	2.708962	-2.986317	0.843221
H	-2.250694	-4.619675	-2.114744
H	-3.819233	-4.098915	-1.506008
C	-3.325830	-3.277008	-3.446327
H	-5.159807	-2.278072	-2.889109
H	-4.435744	-1.646049	-4.364215
H	-1.832750	-2.935205	4.163889
H	-2.102236	-1.206737	4.366317
C	-3.918016	-2.336653	4.017459
H	-4.597265	-0.280392	3.968474
H	-5.838109	-1.444767	3.515376
H	-5.758007	3.012975	0.609832
H	-4.823490	4.094730	1.637918
C	-4.399069	4.289062	-0.486473
H	-3.890852	3.988023	-2.579818
H	-5.179855	2.941296	-1.992120
H	3.631479	4.105280	2.848393
H	4.971805	3.337535	2.001901
C	3.759640	4.603399	0.733974
H	3.947891	4.614864	-1.434280
H	5.165382	3.649524	-0.604679
H	4.824964	-0.228755	-3.691829
H	6.215963	-1.092950	-3.044263
C	4.501375	-2.358295	-3.485333
H	2.551095	-3.309016	-3.635073
H	2.552668	-1.598506	-4.054437
H	5.564344	-1.738792	3.586180
H	4.034944	-1.043143	4.114033
C	3.859938	-3.078630	3.400539
H	1.807427	-2.469016	3.723821
H	1.963123	-4.045413	2.953569
H	-2.418555	-3.049296	-4.024815
H	-3.853772	-4.071543	-3.989369
H	-4.131870	-2.440025	5.089083
H	-4.198701	-3.291889	3.548924
H	-5.171758	5.046012	-0.673396
H	-3.463488	4.833893	-0.294567
H	4.399969	5.481817	0.885816
H	2.723114	4.968232	0.701121
H	4.795266	-2.561406	-4.523171
H	4.902761	-3.184103	-2.878939
H	4.409304	-3.750832	2.724385
H	3.956882	-3.502528	4.408407
C	-0.135651	2.317481	0.231578
O	-0.204005	3.437199	0.531871

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C	2.977953	0.680445	-0.553383
C	3.447878	-0.428573	0.471064
B	1.241464	-0.680011	-0.004583
O	2.342506	-1.371921	0.437024
O	1.529504	0.578904	-0.476014
C	4.727308	-1.168717	0.086730
H	5.579543	-0.480646	0.044531
H	4.946984	-1.934337	0.837674
H	4.630513	-1.665445	-0.881203
C	3.546748	0.081911	1.915307
H	3.671247	-0.774920	2.584621
H	4.401197	0.753198	2.051634
H	2.636981	0.613054	2.212989
C	3.381376	2.109608	-0.196734

H	4.472139	2.217335	-0.186719
H	2.980077	2.800740	-0.944953
H	2.990795	2.407631	0.778740
C	3.365824	0.369587	-2.005534
H	2.837501	1.061293	-2.668991
H	4.441869	0.486887	-2.171434
H	3.081237	-0.649922	-2.285049
C	-2.977706	0.680986	0.552790
C	-3.448050	-0.428982	-0.470397
B	-1.241523	-0.680221	0.004544
O	-2.342911	-1.372482	-0.435699
O	-1.529292	0.579244	0.474887
C	-4.727540	-1.168447	-0.084995
H	-5.579622	-0.480151	-0.043442
H	-4.947555	-1.934885	-0.835009
H	-4.630649	-1.664076	0.883499
C	-3.547220	0.080124	-1.915104
H	-3.671918	-0.777379	-2.583528
H	-4.401686	0.751287	-2.051923
H	-2.637507	0.610927	-2.213551
C	-3.381208	2.109793	0.194913
H	-4.471970	2.217561	0.185099
H	-2.979692	2.801621	0.942375
H	-2.990857	2.406889	-0.780936
C	-3.365096	0.371565	2.005396
H	-2.836924	1.064309	2.667889
H	-4.441148	0.488584	2.171489
H	-3.080004	-0.647478	2.286110
O	-0.000037	-1.239587	-0.000203

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C	1.067473	-0.698073	-0.013139
C	0.727329	0.845177	0.032961
B	-1.180095	-0.388100	-0.101764
O	-0.698052	0.835272	0.322146
O	-0.189997	-1.280470	-0.444793
C	1.437594	1.637340	1.128455
H	2.523550	1.620423	0.980935
H	1.109030	2.681422	1.099182
H	1.213901	1.241982	2.121777
C	0.901559	1.543551	-1.322400
H	0.452363	2.540254	-1.268533
H	1.957861	1.656435	-1.588292
H	0.400599	0.989090	-2.122440
C	2.152259	-1.093841	-1.013071
H	3.109952	-0.625237	-0.758378
H	2.290425	-2.179657	-0.992211
H	1.883652	-0.809688	-2.033028
C	1.382063	-1.288612	1.368323
H	1.395975	-2.380055	1.290688
H	2.356678	-0.956345	1.741586
H	0.617361	-1.012479	2.101476
O	-2.491467	-0.716248	-0.188757
C	-3.506001	0.231230	0.122506
H	-3.972317	-0.032361	1.078830
H	-3.106814	1.248145	0.187861
H	-4.269271	0.189504	-0.661213

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C	-1.341974	-0.635282	0.187192
C	-0.902556	0.845070	-0.160792
B	0.889223	-0.532358	-0.176360
O	0.446076	0.650975	-0.686535
O	-0.059966	-1.286155	0.448304
C	-1.739959	1.536590	-1.233202
H	-2.776218	1.658710	-0.898029

H	-1.329199	2.531329	-1.432302
H	-1.739884	0.977622	-2.171617
C	-0.764681	1.747488	1.071422
H	-0.271393	2.677883	0.775165
H	-1.741455	1.993577	1.500883
H	-0.150945	1.277081	1.845756
C	-2.213003	-0.778899	1.432318
H	-3.164374	-0.250185	1.304311
H	-2.434049	-1.836917	1.605448
H	-1.713393	-0.388871	2.321699
C	-1.974950	-1.378898	-0.995058
H	-2.059346	-2.440211	-0.742437
H	-2.975943	-0.997519	-1.221657
H	-1.359187	-1.293639	-1.896063
O	2.186959	-1.017880	-0.339240
C	3.283509	-0.261221	-0.106616
H	4.171923	-0.768102	-0.511390
O	3.304310	0.787053	0.481276

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C	-4.047888	-0.654997	0.550004
C	-3.855024	0.796038	-0.049638
B	-2.008604	-0.472982	-0.426306
O	-2.693698	0.619570	-0.909255
O	-2.694000	-1.184184	0.526740
C	-5.012436	1.307698	-0.904154
H	-5.927290	1.400536	-0.307834
H	-4.765710	2.297939	-1.300561
H	-5.212435	0.646264	-1.750125
C	-3.470533	1.843135	1.003880
H	-3.148867	2.756568	0.494358
H	-4.314841	2.090420	1.656165
H	-2.640150	1.496321	1.626961
C	-4.557781	-0.699159	1.988835
H	-5.555270	-0.251148	2.063979
H	-4.627814	-1.739911	2.321156
H	-3.885662	-0.173217	2.670414
C	-4.898510	-1.570452	-0.340993
H	-4.815155	-2.597963	0.026144
H	-5.955156	-1.283010	-0.326887
H	-4.548290	-1.553416	-1.378110
C	4.047774	0.655518	0.549560
C	3.855195	-0.795980	-0.049079
B	2.008513	0.472417	-0.426619
O	2.693802	-0.620354	-0.908778
O	2.693786	1.184439	0.525907
C	5.012678	-1.307978	-0.903302
H	5.927578	-1.400237	-0.306965
H	4.766126	-2.298533	-1.299033
H	5.212503	-0.647073	-1.749726
C	3.470967	-1.842444	1.005159
H	3.149534	-2.756311	0.496269
H	4.315338	-2.089070	1.657611
H	2.640495	-1.495409	1.627997
C	4.557611	0.700809	1.988375
H	5.555305	0.253305	2.063838
H	4.627159	1.741809	2.320020
H	3.885715	0.175009	2.670282
C	4.898239	1.570516	-0.342055
H	4.814803	2.598245	0.024455
H	5.954915	1.283195	-0.327850
H	4.547945	1.552809	-1.379136
O	0.772948	0.861040	-0.854641
C	-0.000005	-0.000885	-1.660131
H	-0.640318	0.633326	-2.277799
H	0.640422	-0.635621	-2.277139
O	-0.773106	-0.862126	-0.854051

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C	3.981903	-0.067233	0.399686
O	2.995520	0.441522	-0.383151
O	4.591148	0.602852	1.184426
C	2.288738	-0.490337	-1.198970
H	1.835986	0.109783	-1.989343
H	2.982998	-1.227888	-1.615592
O	1.337284	-1.189633	-0.450055
C	-2.056629	-0.523738	0.451087
C	-1.628581	0.829542	-0.249237
B	0.096129	-0.643404	-0.239913
O	-0.385875	0.450386	-0.914859
O	-0.775304	-1.185254	0.663354
C	-2.599495	1.350560	-1.305357
H	-3.569503	1.592732	-0.856695
H	-2.197585	2.264715	-1.753859
H	-2.756847	0.623159	-2.104842
C	-1.273373	1.942484	0.744409
H	-0.801819	2.767145	0.201352
H	-2.163470	2.327760	1.252502
H	-0.566196	1.590535	1.501993
C	-2.743631	-0.362581	1.804940
H	-3.679844	0.197765	1.702552
H	-2.982464	-1.348982	2.215019
H	-2.102888	0.154096	2.522791
C	-2.882766	-1.443795	-0.457193
H	-2.956326	-2.429606	0.011863
H	-3.896051	-1.057867	-0.609880
H	-2.409189	-1.570563	-1.436124
H	4.163375	-1.144156	0.223923

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Ru	-0.006981	-0.163178	-0.259248
P	-2.365452	-0.084714	-0.020766
P	2.349594	0.063388	-0.198600
H	-0.017614	0.888828	0.982307
H	0.036975	-0.846276	-1.932258
H	-0.075668	1.103484	-1.192097
H	-0.057425	-1.542211	-1.494448
C	-2.943211	-1.415533	1.197141
C	-2.983636	1.520680	0.763205
C	-3.529237	-0.260286	-1.528704
C	3.166288	-0.704603	1.343556
C	3.287763	-0.774618	-1.626793
C	2.998295	1.836793	-0.270527
H	-4.041393	-1.434548	1.211058
C	-2.442877	-2.805794	0.741617
C	-2.456126	-1.130717	2.635739
H	-2.402413	1.565683	1.694035
C	-4.481538	1.596933	1.123095
C	-2.573376	2.756104	-0.066451
H	-3.776334	0.784823	-1.768436
C	-4.865621	-1.001469	-1.299813
C	-2.812416	-0.836023	-2.767697
H	3.419397	-1.722757	1.012523
C	4.471454	-0.059107	1.858949
C	2.155642	-0.856813	2.501207
H	2.800585	-0.334893	-2.510096
C	4.804891	-0.517881	-1.750506
C	3.022549	-2.295111	-1.685323
H	4.083973	1.791200	-0.106477
C	2.387955	2.727764	0.833323
C	2.749825	2.480388	-1.653290
H	-1.344598	-2.782945	0.671716
H	-2.803854	-3.036053	-0.268155

C	-2.866062	-3.919317	1.714119
C	-2.873729	-2.245340	3.610880
H	-2.849164	-0.173484	2.995707
H	-1.361302	-1.031792	2.634637
H	-4.786991	0.735198	1.729124
H	-5.084620	1.566881	0.204879
C	-4.806841	2.898767	1.878990
C	-2.906094	4.062942	0.674970
H	-3.103232	2.751697	-1.031043
H	-1.503612	2.705867	-0.290138
H	-5.406550	-0.582484	-0.445113
H	-4.667275	-2.054613	-1.059259
C	-5.762377	-0.944492	-2.550305
C	-3.708321	-0.792872	-4.016760
H	-2.513456	-1.876156	-2.570508
H	-1.888865	-0.278517	-2.951803
H	5.211359	0.025914	1.056129
H	4.267755	0.962590	2.204728
C	5.070049	-0.862696	3.028183
C	2.752066	-1.652823	3.674211
H	1.840525	0.135201	2.849226
H	1.243684	-1.348666	2.137187
H	5.029754	0.553823	-1.724203
H	5.324325	-0.970300	-0.894477
C	5.370830	-1.125614	-3.047771
C	3.577417	-2.913841	-2.980388
H	3.504881	-2.788420	-0.828676
H	1.950326	-2.498712	-1.600835
H	1.299661	2.745320	0.707241
H	2.570915	2.299763	1.826064
C	2.946423	4.160011	0.776400
C	3.294406	3.918286	-1.717057
H	3.211141	1.886441	-2.450985
H	1.669869	2.485132	-1.850267
H	-3.962518	-4.011086	1.706252
H	-2.470294	-4.883761	1.369796
C	-2.391972	-3.625567	3.144545
H	-2.484946	-2.023797	4.613386
H	-3.970658	-2.256176	3.697527
H	-4.278021	2.896159	2.843626
H	-5.879497	2.938193	2.110478
C	-4.387329	4.136675	1.073454
H	-2.283600	4.128196	1.579583
H	-2.637243	4.924148	0.049224
H	-6.693893	-1.494792	-2.362746
H	-6.049910	0.100440	-2.740408
C	-5.047569	-1.505982	-3.787208
H	-3.899966	0.257173	-4.284636
H	-3.178966	-1.238865	-4.868961
H	5.374642	-1.856236	2.666350
H	5.982123	-0.369433	3.389196
C	4.062473	-1.027683	4.174702
H	2.946692	-2.686038	3.348739
H	2.022963	-1.715610	4.492596
H	4.923060	-0.609875	-3.910252
H	6.452263	-0.944033	-3.103407
C	5.077225	-2.629105	-3.146113
H	3.030270	-2.498914	-3.839809
H	3.392492	-3.996039	-2.985312
H	4.025697	4.144332	0.992287
H	2.480422	4.769634	1.561727
C	2.715019	4.797504	-0.600464
H	3.072385	4.353369	-2.700392
H	4.391164	3.895119	-1.626891
H	-1.292440	-3.654668	3.173828
H	-2.743593	-4.405679	3.832054
H	-5.004633	4.200202	0.164643

H	-4.584487	5.050649	1.648743
H	-4.865772	-2.581484	-3.641873
H	-5.688992	-1.414437	-4.673279
H	3.848266	-0.040768	4.611197
H	4.494771	-1.637945	4.978176
H	5.633264	-3.156909	-2.356737
H	5.439582	-3.027388	-4.102655
H	1.634243	4.921428	-0.762666
H	3.155998	5.802246	-0.637927

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Ru	0.137373	0.421839	-0.104932
P	2.461879	-0.035429	0.055788
P	-2.248698	0.150058	-0.152273
H	0.088336	-1.252087	0.137233
C	2.824883	-0.695845	1.799965
C	3.145530	-1.233283	-1.247324
C	3.723460	1.378813	-0.081201
C	-3.300120	1.716985	0.004200
C	-2.850271	-0.882776	1.336711
C	-2.912269	-0.611169	-1.752420
H	3.845000	-0.377553	2.063610
C	2.747410	-2.229436	1.953437
C	1.824574	-0.039646	2.786327
H	3.028066	-0.627303	-2.158138
C	2.291726	-2.498503	-1.476949
C	4.642824	-1.599326	-1.132729
H	4.711865	0.932720	0.105052
C	3.733736	2.003285	-1.495029
C	3.510083	2.470646	0.990468
H	-4.344073	1.398913	0.127616
C	-3.239160	2.619771	-1.247785
C	-2.891251	2.514179	1.263516
H	-2.227069	-0.473583	2.148207
C	-4.323613	-0.738647	1.783963
C	-2.494177	-2.380704	1.219422
H	-2.680760	0.188864	-2.471249
C	-4.433221	-0.869202	-1.819861
C	-2.139201	-1.854799	-2.243198
H	1.755307	-2.570541	1.629960
H	3.479438	-2.720699	1.305571
C	2.991785	-2.671821	3.407629
C	2.057646	-0.480266	4.241575
H	1.866496	1.052062	2.723399
H	0.807372	-0.337255	2.480839
H	2.349092	-3.159181	-0.603805
H	1.241925	-2.215809	-1.582999
C	2.775304	-3.271325	-2.716013
C	5.121024	-2.394913	-2.362227
H	5.262522	-0.702343	-1.029356
H	4.812680	-2.201419	-0.230089
H	2.728557	2.372543	-1.732456
H	3.976172	1.246154	-2.249314
C	4.740098	3.162013	-1.612219
C	4.518016	3.625908	0.854077
H	2.491869	2.870748	0.906097
H	3.603078	2.040911	1.994001
H	-2.198845	2.893405	-1.457153
H	-3.607829	2.080702	-2.127881
C	-4.071889	3.902445	-1.064802
C	-3.726584	3.795036	1.434811
H	-2.985369	1.892958	2.163138
H	-1.830845	2.784821	1.182388
H	-4.600534	0.311962	1.913449
H	-4.988839	-1.146337	1.011794
C	-4.574172	-1.481178	3.110672
C	-2.729737	-3.118336	2.547794

H	-3.124884	-2.843333	0.448004
H	-1.454816	-2.494003	0.898246
H	-4.697389	-1.684086	-1.132280
H	-5.000497	0.011297	-1.496486
C	-4.866608	-1.260530	-3.244925
C	-2.569742	-2.239918	-3.669135
H	-1.064463	-1.658521	-2.208107
H	-2.326036	-2.703738	-1.574163
H	2.915342	-3.764872	3.475403
H	4.021494	-2.412777	3.697027
C	2.011656	-2.006797	4.382469
H	3.038932	-0.112536	4.577512
H	1.309828	-0.010594	4.893767
H	2.165645	-4.174659	-2.848313
H	2.617573	-2.653922	-3.613243
C	4.261465	-3.641432	-2.611451
H	5.076755	-1.743253	-3.247660
H	6.175146	-2.673872	-2.233674
H	5.762292	2.770194	-1.498018
H	4.682555	3.594258	-2.619486
C	4.491466	4.239915	-0.550633
H	4.301540	4.389470	1.612524
H	5.530998	3.252065	1.067339
H	-3.974694	4.531386	-1.959033
H	-5.136714	3.636190	-0.983677
C	-3.650244	4.683569	0.186507
H	-3.380180	4.345006	2.319466
H	-4.776230	3.524587	1.625512
H	-3.991710	-0.993796	3.906889
H	-5.630349	-1.382059	3.393734
C	-4.178396	-2.961741	3.030188
H	-2.479278	-4.180860	2.430996
H	-2.044588	-2.718264	3.310528
H	-5.945491	-1.463496	-3.262546
H	-4.698460	-0.405927	-3.917127
C	-4.084260	-2.475009	-3.764671
H	-2.282178	-1.435958	-4.363230
H	-2.024748	-3.137265	-3.990022
H	0.991822	-2.359764	4.168023
H	2.236293	-2.304098	5.414896
H	4.595725	-4.156849	-3.521157
H	4.400338	-4.350334	-1.781232
H	5.239858	5.038673	-0.633415
H	3.510551	4.704129	-0.726505
H	-4.281215	5.573047	0.311352
H	-2.618763	5.042130	0.059086
H	-4.315772	-3.446471	4.005441
H	-4.849370	-3.477461	2.326952
H	-4.351319	-3.359065	-3.166321
H	-4.374094	-2.699323	-4.799381
C	0.235976	2.280784	-0.545992
O	0.321251	3.395598	-0.885298
H	0.172296	0.120461	-1.641838

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Ru	-0.028200	0.247946	0.193680
P	-2.361503	0.774757	0.072697
P	2.359127	0.409445	0.156344
B	-0.188882	-2.040970	-0.526917
H	0.047164	1.245578	-1.074023
H	-0.171370	-0.942336	-1.148820
H	0.103498	1.615356	1.056926
C	-2.764113	2.614522	0.326824
C	-3.204121	0.372578	-1.587495
C	-3.612300	0.015104	1.321765
C	3.270731	-0.219765	1.696877
C	2.929752	2.225042	0.106329

H	-2.749164	2.252590	0.864194
C	-4.730343	1.760374	0.173385
C	-2.784990	2.536230	-1.251197
H	-3.455779	-0.176072	-2.071836
C	-4.562673	-1.648751	-0.967394
C	-2.255949	-1.943651	-1.965265
H	3.262688	-1.713019	1.070147
C	4.606950	-0.156105	1.683378
C	2.267890	-0.550099	2.568544
H	2.626725	-0.402503	-2.511602
C	4.506785	-1.124308	-1.756555
C	2.273281	-2.317320	-1.638263
H	4.271289	1.611675	-0.350090
C	2.746355	2.801554	0.607012
C	2.933025	2.346624	-1.871083
H	-1.224467	-1.950147	1.903104
H	-2.541395	-2.761960	1.072008
C	-2.747674	-2.729890	3.229836
C	-3.128007	-0.433578	4.216549
H	-3.228027	1.170882	2.770467
H	-1.631339	0.452140	2.917290
H	-5.035781	1.217739	1.076508
H	-5.200712	1.247033	-0.676518
C	-5.266542	3.202839	0.231281
C	-3.327506	3.975380	-1.203564
H	-3.175996	2.041316	-2.153360
H	-1.694395	2.537900	-1.340283
H	-5.280155	-0.946628	-0.530095
H	-4.382771	-2.422806	-0.208892
C	-5.182059	-2.315395	-2.210235
C	-2.870469	-2.620334	-3.202300
H	-1.980041	-2.717613	-1.233570
H	-1.329604	-1.421763	-2.239674
H	5.280183	-0.253487	0.825199
H	4.576759	0.912112	1.936261
C	5.185996	-0.930159	2.882103
C	2.846198	-1.315347	3.770696
H	2.124267	0.504407	2.839755
H	1.268415	-0.935876	2.323440
H	5.010594	-0.150130	-1.785885
H	4.893491	-1.652509	-0.873843
C	4.873241	-1.935393	-3.012898
C	2.644998	-3.136558	-2.886535
H	2.547861	-2.891175	-0.740465
H	1.184775	-2.174497	-1.596089
H	1.658601	2.925664	0.538989
H	2.948009	2.424635	1.617042
C	3.439984	4.160729	0.417058
C	3.616000	3.712399	-2.064382
H	3.296326	1.656325	-2.641546
H	1.849989	2.446635	-2.022729
H	-3.823472	-2.957566	3.190061
H	-2.230653	-3.689645	3.360425
C	-2.468763	-1.804113	4.421229
H	-2.880574	0.237399	5.049507
H	-4.221733	-0.554286	4.227821
H	-4.876299	3.696630	1.133674
H	-6.360089	3.190524	0.330331
C	-4.850147	4.007988	-1.007874
H	-2.844556	4.513399	-0.374248
H	-3.050228	4.507536	-2.122966
H	-6.112551	-2.827996	-1.932619
H	-5.458873	-1.536883	-2.936713
C	-4.206728	-3.300591	-2.870576
H	-3.034117	-1.861131	-3.981610
H	-2.164653	-3.349692	-3.620983
H	5.318757	-1.985744	2.601053

H	6.185017	-0.544801	3.125063
C	4.268332	-0.844740	4.109889
H	2.868093	-2.390656	3.537322
H	2.187511	-1.198155	4.641244
H	4.583369	-1.365492	-3.908156
H	5.961541	-2.069985	-3.067285
C	4.165781	-3.298248	-3.027858
H	2.250663	-2.628090	-3.778731
H	2.159063	-4.120264	-2.847103
H	4.522909	4.047462	0.578738
H	3.083634	4.867231	1.178239
C	3.194080	4.723218	-0.989699
H	3.385656	4.100337	-3.065391
H	4.707892	3.579080	-2.025846
H	-1.381833	-1.671259	4.528927
H	-2.822039	-2.262994	5.353723
H	-5.338893	3.579630	-1.895990
H	-5.204434	5.043825	-0.926054
H	-4.024630	-4.141711	-2.184718
H	-4.653110	-3.728982	-3.777316
H	4.230439	0.197313	4.460759
H	4.680279	-1.438079	4.936370
H	4.543765	-3.910152	-2.194940
H	4.406546	-3.843529	-3.949550
H	2.123874	4.948836	-1.105713
H	3.731981	5.670726	-1.124677

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Ru	-0.090831	0.234960	-0.016511
P	-2.432794	0.684874	0.031585
P	2.274842	0.480295	0.090679
B	-0.036715	-1.925995	-0.659889
H	0.033375	1.141256	-1.295275
H	-0.324068	-0.895657	-1.368289
H	0.027060	1.487496	1.042566
C	-2.911507	2.513201	0.208102
C	-3.484749	0.088601	-1.431856
C	-3.332078	-0.068569	1.537786
C	3.065256	-0.084978	1.718656
C	2.742017	2.326001	0.067925
C	3.323176	-0.430077	-1.197687
O	-1.061539	-2.709616	-0.128897
O	1.041107	-2.721273	-1.038991
H	-4.008235	2.542896	0.126600
C	-2.313634	3.371168	-0.927186
C	-2.537776	3.120054	1.577683
H	-3.515360	-0.996122	-1.257022
C	-2.824605	0.272447	-2.816500
C	-4.938974	0.604523	-1.479202
H	-4.116355	0.647580	1.827964
C	-4.010306	-1.433533	1.287709
C	-2.333265	-0.206626	2.712090
H	4.134665	0.165141	1.675688
C	2.951800	-1.609943	1.920360
C	2.452303	0.646350	2.933899
H	2.013508	2.722488	0.788083
C	4.149664	2.739337	0.555352
C	2.440417	3.016115	-1.279481
H	3.108839	-1.474610	-0.938297
C	4.854057	-0.241795	-1.167684
C	2.798225	-0.249937	-2.639576
C	-0.587016	-4.074651	0.016886
C	0.635116	-4.112282	-0.981510
H	-1.220223	3.287089	-0.888337
H	-2.618896	2.983925	-1.904411
C	-2.725739	4.848908	-0.819471
C	-2.952334	4.598929	1.681126

H	-3.016952	2.562325	2.389993
H	-1.453944	3.029052	1.723810
H	-2.775999	1.337958	-3.075465
H	-1.792073	-0.087662	-2.793315
C	-3.626066	-0.462129	-3.906068
C	-5.752305	-0.125115	-2.564053
H	-5.433539	0.492710	-0.506715
H	-4.937619	1.680028	-1.704321
H	-3.255919	-2.148763	0.937933
H	-4.766948	-1.357790	0.500110
C	-4.686622	-1.972290	2.562271
C	-3.006298	-0.738466	3.988139
H	-1.538712	-0.903562	2.405034
H	-1.838961	0.746653	2.918664
H	1.888770	-1.886066	1.916373
H	3.412943	-2.149929	1.086167
C	3.591589	-2.066130	3.243069
C	3.096110	0.196687	4.256656
H	2.554991	1.732041	2.828656
H	1.372776	0.447093	2.961874
H	4.388200	2.283794	1.522304
H	4.912307	2.389597	-0.151090
C	4.258660	4.270968	0.684144
C	2.545244	4.546411	-1.158607
H	3.158062	2.674433	-2.037834
H	1.443448	2.733715	-1.632285
H	5.108005	0.779953	-1.478455
H	5.251891	-0.370333	-0.153802
C	5.547355	-1.231842	-2.122778
C	3.486030	-1.234883	-3.600028
H	1.714885	-0.396090	-2.663153
H	2.988912	0.774534	-2.984974
C	-1.736863	-5.020838	-0.335538
C	-0.192115	-4.276808	1.486069
C	0.240991	-4.513332	-2.411318
C	1.825639	-4.952469	-0.518969
H	-2.253144	5.422782	-1.627407
H	-3.812709	4.937052	-0.968902
C	-2.355758	5.441098	0.546166
H	-4.049977	4.673565	1.647133
H	-2.644063	4.997713	2.656618
H	-3.153241	-0.306582	-4.884664
H	-3.591316	-1.544729	-3.710884
C	-5.090849	-0.000286	-3.944243
H	-5.837059	-1.188808	-2.295743
H	-6.775768	0.271481	-2.594664
H	-5.513783	-1.302672	2.843028
H	-5.139041	-2.950590	2.351572
C	-3.707028	-2.079932	3.737809
H	-2.260479	-0.838175	4.787800
H	-3.745038	-0.003128	4.341554
H	3.464285	-3.150502	3.362401
H	4.675894	-1.883723	3.201997
C	2.998752	-1.322937	4.447752
H	2.618647	0.718210	5.096572
H	4.155284	0.495420	4.266081
H	3.567604	4.615233	1.468107
H	5.268829	4.543847	1.017355
C	3.921349	4.980225	-0.634602
H	2.344704	5.011344	-2.132933
H	1.764036	4.906959	-0.472863
H	6.633775	-1.072506	-2.102317
H	5.374522	-2.257655	-1.764650
C	5.015080	-1.098841	-3.557550
H	3.200638	-2.258899	-3.319236
H	3.120058	-1.075746	-4.623143
H	-2.542766	-4.910875	0.397602

H	-1.404345	-6.065369	-0.315195
H	-2.149588	-4.805983	-1.323813
H	0.622418	-3.609386	1.778941
H	0.118297	-5.308951	1.682150
H	-1.055776	-4.054638	2.121237
H	-0.600070	-3.913652	-2.773215
H	-0.030859	-5.572333	-2.478908
H	1.091683	-4.333547	-3.076196
H	2.630024	-4.886219	-1.259087
H	1.545986	-6.007773	-0.419067
H	2.220404	-4.604531	0.438352
H	-1.260488	5.461719	0.647037
H	-2.698108	6.481634	0.619964
H	-5.655049	-0.575164	-4.690123
H	-5.128262	1.051051	-4.266844
H	-4.229696	-2.416944	4.642513
H	-2.949667	-2.845078	3.509631
H	3.506134	-1.626895	5.372536
H	1.941567	-1.605359	4.562756
H	3.956887	6.069516	-0.502266
H	4.687667	4.731270	-1.384207
H	5.301017	-0.113615	-3.955843
H	5.486316	-1.846664	-4.208959

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Ru	0.010876	0.273595	0.097010
P	-2.307716	0.880791	0.043516
P	2.407679	0.205037	0.104026
B	-0.374334	-1.881511	0.131498
H	-0.034250	-0.332160	-1.344774
H	-0.144423	-1.152753	1.189610
H	0.192949	1.582155	-0.856058
C	-2.607271	2.746243	-0.188047
C	-3.463585	0.074644	-1.221816
C	-3.229640	0.614692	1.701929
C	3.134202	-0.359387	1.762338
C	3.071371	1.991763	-0.015121
C	3.319559	-0.880943	-1.144274
O	0.598373	-2.837287	-0.191814
O	-1.653621	-2.445765	-0.014690
H	-3.691528	2.896504	-0.073401
C	-2.195447	3.260874	-1.584347
C	-1.900522	3.574128	0.908646
H	-3.608513	-0.923953	-0.792156
C	-2.812041	-0.155815	-2.602733
C	-4.846552	0.743240	-1.380908
H	-3.927379	1.460366	1.807000
C	-4.052868	-0.688782	1.800084
C	-2.230383	0.662544	2.883225
H	4.199589	-0.092390	1.775785
C	3.040406	-1.881899	1.996189
C	2.436139	0.400191	2.914113
H	2.318852	2.531959	0.580506
C	4.453028	2.318320	0.595827
C	2.985919	2.569355	-1.444487
H	3.014618	-1.883985	-0.815266
C	4.861388	-0.815560	-1.117632
C	2.797201	-0.731563	-2.590761
C	-0.052688	-3.979195	-0.794732
C	-1.508340	-3.872848	-0.209061
H	-1.135659	3.028940	-1.745870
H	-2.752884	2.736598	-2.366848
C	-2.422812	4.774715	-1.741439
C	-2.118530	5.087924	0.738329
H	-2.257599	3.281033	1.901052
H	-0.822813	3.355152	0.876409
H	-2.587161	0.801852	-3.088485

H	-1.854805	-0.667272	-2.470254
C	-3.736389	-0.976429	-3.519392
C	-5.766149	-0.087226	-2.294609
H	-5.329424	0.890268	-0.406848
H	-4.727672	1.742478	-1.820512
H	-3.387616	-1.546473	1.641113
H	-4.811074	-0.731082	1.012002
C	-4.758049	-0.815716	3.163531
C	-2.935348	0.556706	4.245794
H	-1.528893	-0.175122	2.774927
H	-1.625311	1.575537	2.853757
H	1.997962	-2.207352	1.905527
H	3.597097	-2.421913	1.222293
C	3.591558	-2.278037	3.377844
C	2.986598	-0.001766	4.293062
H	2.536482	1.484888	2.781571
H	1.358790	0.177915	2.879537
H	4.528099	1.959238	1.627171
H	5.244296	1.810698	0.029331
C	4.719048	3.836004	0.584647
C	3.239277	4.086291	-1.452442
H	3.742655	2.087677	-2.078414
H	2.006380	2.347147	-1.878737
H	5.194348	0.177142	-1.448680
H	5.243373	-0.951539	-0.098666
C	5.481663	-1.875306	-2.046763
C	3.426258	-1.784557	-3.519720
H	1.706838	-0.819962	-2.599073
H	3.035236	0.266312	-2.978211
C	0.716430	-5.241055	-0.400161
C	-0.005494	-3.797921	-2.319356
C	-1.653216	-4.535252	1.171003
C	-2.619655	-4.368104	-1.134589
H	-2.089138	5.092636	-2.737969
H	-3.500660	4.992608	-1.689916
C	-1.696521	5.573712	-0.652911
H	-3.183399	5.318911	0.892937
H	-1.567033	5.627643	1.519611
H	-3.267639	-1.100124	-4.504637
H	-3.854845	-1.986528	-3.099820
C	-5.121886	-0.330972	-3.666661
H	-5.975140	-1.054847	-1.814268
H	-6.733313	0.419735	-2.410254
H	-5.506473	-0.014283	3.258044
H	-5.312031	-1.763042	3.203229
C	-3.774493	-0.723974	4.337491
H	-2.190506	0.585100	5.052034
H	-3.586340	1.432180	4.390863
H	3.481869	-3.361154	3.520236
H	4.671275	-2.067434	3.413859
C	2.894533	-1.517495	4.513943
H	2.442366	0.535437	5.080884
H	4.038352	0.312931	4.369690
H	3.996338	4.329741	1.251582
H	5.714679	4.039102	1.000717
C	4.595587	4.434017	-0.822911
H	3.187531	4.465914	-2.481313
H	2.435883	4.588649	-0.892906
H	6.576498	-1.793941	-2.026059
H	5.234455	-2.877478	-1.665953
C	4.960277	-1.737599	-3.484366
H	3.092120	-2.786090	-3.210996
H	3.063423	-1.637507	-4.545482
H	1.719198	-5.214141	-0.839714
H	0.211594	-6.141442	-0.770067
H	0.827580	-5.323640	0.683634
H	-0.547004	-2.899346	-2.629707

H	-0.430349	-4.660897	-2.843898
H	1.036874	-3.687215	-2.632934
H	-0.867294	-4.199998	1.855131
H	-1.614818	-5.628300	1.106248
H	-2.619714	-4.253128	1.600913
H	-3.592731	-4.229822	-0.650956
H	-2.501627	-5.436619	-1.350959
H	-2.632513	-3.821620	-2.080208
H	-0.610290	5.443876	-0.770233
H	-1.899306	6.647112	-0.762079
H	-5.773540	-0.959500	-4.287607
H	-5.020384	0.630131	-4.192938
H	-4.313723	-0.764387	5.292928
H	-3.103625	-1.595543	4.317301
H	3.332394	-1.789860	5.483031
H	1.835747	-1.813668	4.552572
H	4.737020	5.522105	-0.788296
H	5.400742	4.034120	-1.457530
H	5.303967	-0.779712	-3.903060
H	5.383221	-2.525990	-4.120558

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Ru	-0.021163	0.449352	-0.003132
P	-2.378595	0.756703	0.035576
P	2.371182	0.424760	0.035945
B	-0.219383	-1.669787	-0.323339
H	0.083103	1.867132	-0.753525
H	-0.004957	0.214785	-1.556128
H	0.149511	2.016537	0.627788
C	-3.013887	2.548146	0.065225
C	-3.456856	-0.062265	-1.292147
C	-3.094403	0.106864	1.677805
C	3.042605	0.085129	1.774924
C	3.073346	2.153764	-0.332894
C	3.303005	-0.841931	-1.019394
O	-0.374065	-2.525078	0.784835
O	-0.210775	-2.436763	-1.489496
H	-4.110464	2.470927	0.098963
C	-2.624591	3.329366	-1.208180
C	-2.573701	3.332235	1.320856
H	-3.458086	-1.114781	-0.978066
C	-2.828881	-0.043207	-2.703895
C	-4.926176	0.409840	-1.342054
H	-3.894880	0.799785	1.979269
C	-3.698717	-1.312137	1.621714
C	-1.977311	0.144900	2.749729
H	4.128916	0.249778	1.753490
C	2.799860	-1.369262	2.232725
C	2.428864	1.069514	2.797031
H	2.370969	2.776700	0.237502
C	4.495615	2.515379	0.151844
C	2.905864	2.551466	-1.815114
H	3.003339	-1.784711	-0.538966
C	4.844734	-0.778639	-0.987977
C	2.795736	-0.929125	-2.476911
C	-0.260714	-3.910615	0.357570
C	-0.551995	-3.812328	-1.187261
H	-1.530126	3.353286	-1.288303
H	-2.990184	2.815826	-2.103469
C	-3.167255	4.769588	-1.198155
C	-3.119919	4.771845	1.322227
H	-2.915714	2.826573	2.230805
H	-1.477414	3.357194	1.362862
H	-2.745065	0.988461	-3.069814
H	-1.813749	-0.446189	-2.655788
C	-3.670970	-0.859329	-3.701224
C	-5.754082	-0.430261	-2.330442

H	-5.385116	0.371733	-0.345922
H	-4.965637	1.459049	-1.663268
H	-2.929951	-2.013627	1.274776
H	-4.528045	-1.355597	0.907642
C	-4.207948	-1.764988	3.002634
C	-2.476754	-0.311016	4.131002
H	-1.170885	-0.529908	2.423517
H	-1.545670	1.148046	2.825200
H	1.727118	-1.596416	2.185116
H	3.292904	-2.072937	1.552415
C	3.317718	-1.613578	3.661268
C	2.953676	0.822797	4.221322
H	2.626300	2.107597	2.505909
H	1.335873	0.955794	2.788886
H	4.625951	2.270476	1.211811
H	5.247510	1.936462	-0.397617
C	4.775260	4.017017	-0.056495
C	3.184649	4.049018	-2.027470
H	3.608189	1.973647	-2.430866
H	1.897150	2.303615	-2.163716
H	5.180481	0.142041	-1.481848
H	5.218375	-0.737246	0.042363
C	5.470795	-1.980111	-1.718773
C	3.433530	-2.119595	-3.214369
H	1.707733	-1.030472	-2.485284
H	3.041434	-0.005995	-3.016729
C	-1.258539	-4.750672	1.157885
C	1.164265	-4.382058	0.682101
C	-2.033158	-4.006886	-1.545902
C	0.298283	-4.728626	-2.070203
H	-2.838371	5.292015	-2.106027
H	-4.267041	4.745282	-1.233189
C	-2.720937	5.535010	0.053386
H	-4.217682	4.745145	1.396797
H	-2.760079	5.298264	2.216033
H	-3.225736	-0.788086	-4.702185
H	-3.631482	-1.921518	-3.418902
C	-5.137141	-0.404466	-3.735495
H	-5.803252	-1.469708	-1.972983
H	-6.787491	-0.060184	-2.357869
H	-5.043044	-1.117461	3.310246
H	-4.615036	-2.782078	2.928047
C	-3.104433	-1.709381	4.067407
H	-1.645993	-0.295755	4.848809
H	-3.222828	0.408208	4.501786
H	3.097534	-2.646880	3.960404
H	4.413537	-1.513140	3.672532
C	2.712577	-0.625484	4.667096
H	2.474610	1.523427	4.917649
H	4.032393	1.038227	4.255136
H	4.095789	4.600373	0.582626
H	5.794817	4.252693	0.276074
C	4.579760	4.439403	-1.519557
H	3.082324	4.299600	-3.091475
H	2.423385	4.635989	-1.492625
H	6.565592	-1.898220	-1.697897
H	5.216595	-2.904730	-1.179056
C	4.967207	-2.079832	-3.165536
H	3.082285	-3.054835	-2.754428
H	3.085029	-2.137655	-4.255143
H	-0.996937	-4.715876	2.220997
H	-1.234141	-5.799875	0.839537
H	-2.281313	-4.382248	1.051918
H	1.912041	-3.799888	0.136236
H	1.305039	-5.440942	0.437791
H	1.349624	-4.249638	1.752697
H	-2.679585	-3.361300	-0.944226

H	-2.353862	-5.045302	-1.405131
H	-2.178979	-3.742388	-2.597903
H	0.060369	-4.542696	-3.122690
H	0.092479	-5.784757	-1.858211
H	1.366870	-4.548855	-1.933450
H	-1.628228	5.660233	0.032747
H	-3.153039	6.544174	0.060849
H	-5.718607	-1.036511	-4.419272
H	-5.191485	0.619927	-4.133813
H	-3.505664	-1.995164	5.048480
H	-2.324374	-2.442662	3.817221
H	3.131071	-0.793624	5.667900
H	1.629792	-0.804533	4.745121
H	4.739792	5.519987	-1.628068
H	5.341526	3.946750	-2.142487
H	5.326724	-1.207785	-3.732438
H	5.390258	-2.966266	-3.656024

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Ru	0.010470	0.298715	-0.067072
P	-2.336614	0.801929	-0.002238
P	2.406815	0.236293	0.113901
B	-0.289712	-1.727666	-0.122196
H	0.081277	0.412768	-1.729291
H	-0.113150	-0.888623	1.151073
H	0.136822	1.333303	-1.492753
C	-2.677282	2.669558	-0.165695
C	-3.477327	0.015388	-1.295096
C	-3.261202	0.463032	1.641456
C	3.018550	-0.188844	1.854086
C	3.046527	2.023215	-0.103729
C	3.428304	-0.914644	-0.980845
O	0.719909	-2.692262	-0.320401
O	-1.542855	-2.379486	-0.171817
H	-3.763922	2.793506	-0.041767
C	-2.285724	3.251132	-1.541121
C	-1.984162	3.474518	0.956930
H	-3.606513	-0.995091	-0.889891
C	-2.808508	-0.178444	-2.673240
C	-4.869688	0.662739	-1.452907
H	-3.968978	1.299036	1.757977
C	-4.077749	-0.847601	1.684415
C	-2.288437	0.483559	2.843613
H	4.088703	0.056295	1.904215
C	2.872698	-1.686269	2.200250
C	2.272084	0.674979	2.896216
H	2.248265	2.598457	0.392786
C	4.377741	2.419819	0.575173
C	3.061350	2.485860	-1.578305
H	3.156284	-1.893544	-0.564925
C	4.962435	-0.767398	-0.911403
C	2.945938	-0.940654	-2.447549
C	0.116349	-3.934970	-0.743257
C	-1.336790	-3.809584	-0.158002
H	-1.214122	3.082082	-1.708217
H	-2.811453	2.728015	-2.345884
C	-2.582267	4.757886	-1.639101
C	-2.261408	4.984441	0.852360
H	-2.313774	3.126156	1.940465
H	-0.898448	3.297785	0.907174
H	-2.598916	0.792104	-3.142249
H	-1.845281	-0.678939	-2.538324
C	-3.709724	-1.001453	-3.610400
C	-5.766818	-0.166818	-2.389766
H	-5.363250	0.783128	-0.480494
H	-4.765146	1.672281	-1.872855
H	-3.401240	-1.693991	1.516275

H	-4.819246	-0.874214	0.880100
C	-4.811511	-1.017870	3.027814
C	-3.024934	0.338279	4.185578
H	-1.576295	-0.341416	2.724720
H	-1.685241	1.397743	2.849759
H	1.828039	-1.990254	2.068236
H	3.461591	-2.298178	1.508043
C	3.324624	-1.983468	3.641262
C	2.724309	0.370271	4.334549
H	2.412543	1.743423	2.689401
H	1.195371	0.476704	2.801342
H	4.381317	2.142401	1.633657
H	5.209814	1.878819	0.107498
C	4.632097	3.934619	0.462009
C	3.303354	4.000825	-1.690122
H	3.862905	1.962799	-2.117181
H	2.119877	2.221646	-2.070610
H	5.259196	0.203344	-1.330450
H	5.312035	-0.780730	0.128088
C	5.668237	-1.879185	-1.709093
C	3.660663	-2.047451	-3.242358
H	1.863516	-1.098270	-2.466840
H	3.139353	0.024396	-2.933476
C	0.943654	-5.096333	-0.189285
C	0.139746	-3.969735	-2.279801
C	-1.437058	-4.280553	1.302307
C	-2.434907	-4.474736	-0.989359
H	-2.270992	5.130249	-2.623892
H	-3.668330	4.922569	-1.572564
C	-1.882474	5.544688	-0.523827
H	-3.331837	5.164631	1.032557
H	-1.719223	5.514186	1.646687
H	-3.231237	-1.101794	-4.593611
H	-3.810764	-2.019654	-3.205766
C	-5.105338	-0.378394	-3.759257
H	-5.964826	-1.145220	-1.927140
H	-6.740900	0.326303	-2.507415
H	-5.568745	-0.225225	3.127032
H	-5.358573	-1.970114	3.028257
C	-3.855574	-0.950496	4.225676
H	-2.298642	0.350537	5.008979
H	-3.686537	1.204429	4.340050
H	3.177511	-3.049417	3.859495
H	4.405092	-1.793725	3.731614
C	2.576322	-1.120427	4.665694
H	2.145712	0.979839	5.041017
H	3.777443	0.666041	4.456642
H	3.859871	4.470576	1.034206
H	5.593566	4.183048	0.930373
C	4.607022	4.416609	-0.994816
H	3.323603	4.296043	-2.747372
H	2.457877	4.536039	-1.232413
H	6.755968	-1.734808	-1.666773
H	5.462584	-2.850170	-1.234527
C	5.188565	-1.914766	-3.167239
H	3.367233	-3.026709	-2.836444
H	3.327198	-2.029638	-4.288331
H	1.940225	-5.090224	-0.644025
H	0.475260	-6.060451	-0.421399
H	1.068540	-5.021287	0.893532
H	-0.445403	-3.146716	-2.701408
H	-0.253047	-4.914309	-2.672553
H	1.172774	-3.860671	-2.623911
H	-0.667223	-3.809671	1.921431
H	-1.337353	-5.368377	1.389311
H	-2.414986	-3.995769	1.703926
H	-3.407643	-4.313672	-0.511961

H	-2.273319	-5.556867	-1.064091
H	-2.482908	-4.059459	-1.998930
H	-0.792752	5.472293	-0.658624
H	-2.136119	6.610836	-0.586632
H	-5.740522	-1.008253	-4.395685
H	-5.016244	0.592419	-4.269923
H	-4.416191	-1.020496	5.167049
H	-3.177483	-1.816132	4.197468
H	2.942732	-1.325446	5.680049
H	1.509634	-1.388540	4.655504
H	4.736201	5.505745	-1.039138
H	5.459405	3.978064	-1.535079
H	5.498030	-0.986975	-3.671802
H	5.671729	-2.739413	-3.707318

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Ru	0.006649	0.497954	0.022082
P	-2.369931	0.737429	0.006387
P	2.397688	0.396956	0.072127
B	-0.159735	-1.573198	-0.214756
H	0.206421	2.308597	-0.347637
H	0.055621	0.544059	-1.550696
H	0.119257	2.360915	0.457819
C	-3.045891	2.512934	-0.170466
C	-3.410152	-0.231208	-1.251615
C	-3.156546	0.282556	1.689493
C	3.059603	-0.159589	1.758517
C	3.167644	2.139788	-0.067888
C	3.285493	-0.751685	-1.136489
O	-1.034860	-2.389819	0.532118
O	0.556412	-2.400219	-1.094092
H	-4.139992	2.406112	-0.147123
C	-2.661695	3.172584	-1.512451
C	-2.669059	3.445931	1.001499
H	-3.403877	-1.242954	-0.824263
C	-2.750540	-0.345109	-2.644731
C	-4.881698	0.216272	-1.393095
H	-3.932043	1.038842	1.884206
C	-3.832251	-1.102030	1.783177
C	-2.075435	0.400534	2.790370
H	4.150784	-0.031793	1.761231
C	2.760166	-1.641777	2.056351
C	2.470801	0.725636	2.880370
H	2.499265	2.714415	0.589894
C	4.602731	2.377210	0.454862
C	3.022060	2.747728	-1.479879
H	2.904487	-1.730335	-0.818090
C	4.826248	-0.794873	-1.076410
C	2.808429	-0.584567	-2.596746
C	-0.791259	-3.792379	0.266931
C	0.046084	-3.752032	-1.072034
H	-1.568463	3.251556	-1.578083
H	-2.972698	2.545009	-2.353546
C	-3.287168	4.570212	-1.667269
C	-3.303684	4.839563	0.844415
H	-2.986837	3.016557	1.957500
H	-1.578377	3.555637	1.053419
H	-2.683438	0.644297	-3.115608
H	-1.721405	-0.702017	-2.540529
C	-3.553725	-1.279416	-3.567901
C	-5.676454	-0.735979	-2.304054
H	-5.369299	0.286102	-0.413056
H	-4.919799	1.222225	-1.832072
H	-3.092823	-1.875105	1.549950
H	-4.639459	-1.192069	1.048319
C	-4.413844	-1.347839	3.187989
C	-2.643823	0.146349	4.197005

H	-1.291114	-0.341036	2.577482
H	-1.597468	1.386877	2.761042
H	1.675787	-1.801477	2.000697
H	3.211257	-2.286942	1.293636
C	3.270834	-2.062259	3.445809
C	2.981415	0.310959	4.270698
H	2.703329	1.782695	2.705877
H	1.373434	0.643163	2.858920
H	4.724771	1.985976	1.470304
H	5.328955	1.847879	-0.173492
C	4.944496	3.879820	0.456917
C	3.356802	4.249416	-1.481299
H	3.708556	2.237468	-2.168226
H	2.009948	2.581643	-1.865417
H	5.238021	0.159765	-1.429481
H	5.180889	-0.927676	-0.046768
C	5.381336	-1.924496	-1.964060
C	3.368171	-1.706590	-3.486921
H	1.716542	-0.592892	-2.625893
H	3.139941	0.382494	-2.996278
C	-2.140841	-4.509935	0.161407
C	-0.022531	-4.361505	1.469646
C	-0.798900	-3.936267	-2.341295
C	1.228662	-4.724579	-1.118830
H	-2.964481	5.016303	-2.617016
H	-4.381746	4.472007	-1.724330
C	-2.925634	5.489362	-0.493318
H	-4.398469	4.747862	0.905679
H	-2.997500	5.480286	1.681793
H	-3.082789	-1.314225	-4.558974
H	-3.514303	-2.304179	-3.169905
C	-5.023747	-0.853736	-3.688381
H	-5.725062	-1.731142	-1.837412
H	-6.712299	-0.383712	-2.397152
H	-5.220977	-0.624508	3.380592
H	-4.874849	-2.343875	3.225113
C	-3.346388	-1.215121	4.282177
H	-1.838692	0.210556	4.940941
H	-3.362468	0.942187	4.445519
H	3.013604	-3.113418	3.631349
H	4.369484	-2.003203	3.461715
C	2.699980	-1.170296	4.556718
H	2.520036	0.944160	5.039804
H	4.065288	0.492456	4.326077
H	4.290095	4.395556	1.175730
H	5.972944	4.025188	0.812903
C	4.766358	4.510553	-0.930636
H	3.264225	4.650808	-2.498927
H	2.619366	4.785128	-0.864704
H	6.478781	-1.925826	-1.922803
H	5.051439	-2.893724	-1.561594
C	4.899660	-1.788253	-3.415988
H	2.935200	-2.663320	-3.161990
H	3.044309	-1.552884	-4.524919
H	-2.662892	-4.454332	1.122691
H	-2.007468	-5.569905	-0.086061
H	-2.784274	-4.056823	-0.596407
H	0.947565	-3.874781	1.595368
H	0.141682	-5.440882	1.374872
H	-0.607221	-4.183741	2.378421
H	-1.639306	-3.238424	-2.365247
H	-1.189811	-4.956258	-2.430533
H	-0.172071	-3.731007	-3.215089
H	1.767733	-4.600366	-2.063971
H	0.887557	-5.765249	-1.062206
H	1.934742	-4.547672	-0.303924
H	-1.843346	5.687046	-0.507339

H	-3.422654	6.462228	-0.600551
H	-5.578207	-1.565891	-4.313274
H	-5.080621	0.119999	-4.197712
H	-3.795063	-1.353259	5.274642
H	-2.600835	-2.014359	4.158980
H	3.116361	-1.457773	5.530757
H	1.612727	-1.325047	4.621653
H	4.968622	5.588647	-0.888389
H	5.507611	4.080076	-1.620530
H	5.331869	-0.875509	-3.853651
H	5.269078	-2.627950	-4.019338

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Ru	-0.001545	0.449759	-0.072939
P	-2.373170	0.752724	-0.031308
P	2.387415	0.359040	0.051462
B	-0.192463	-1.551683	-0.247327
H	0.439544	3.169978	-1.038930
H	0.066410	0.545361	-1.649872
H	0.507720	3.885924	-0.848158
C	-3.009337	2.538396	-0.218944
C	-3.489182	-0.227255	-1.210106
C	-3.091538	0.369921	1.702938
C	2.958073	-0.065774	1.810346
C	3.185396	2.080759	-0.196434
C	3.339859	-0.884900	-1.009002
O	-1.149826	-2.323882	0.450725
O	0.574091	-2.424445	-1.040257
H	-4.095321	2.485615	-0.049949
C	-2.777984	3.127742	-1.626978
C	-2.425246	3.480378	0.857274
H	-3.479440	-1.227473	-0.757134
C	-2.889699	-0.385929	-2.625559
C	-4.958085	0.241765	-1.298989
H	-3.817589	1.168065	1.921496
C	-3.826867	-0.977957	1.864531
C	-1.951412	0.453780	2.745293
H	4.048211	0.057827	1.865308
C	2.631553	-1.521391	2.200057
C	2.311160	0.901355	2.827940
H	2.455924	2.736179	0.302600
C	4.556400	2.363440	0.460605
C	3.227996	2.512307	-1.679542
H	2.938153	-1.834526	-0.633049
C	4.874081	-0.917295	-0.851157
C	2.951197	-0.844512	-2.504161
C	-0.899605	-3.735775	0.256758
C	-0.004607	-3.748161	-1.041338
H	-1.705637	3.121889	-1.854045
H	-3.254707	2.501279	-2.386879
C	-3.323727	4.562164	-1.748196
C	-2.975139	4.912021	0.728470
H	-2.649739	3.104036	1.861088
H	-1.330957	3.503621	0.768949
H	-2.833466	0.588963	-3.126769
H	-1.859176	-0.747222	-2.553548
C	-3.741619	-1.337335	-3.484742
C	-5.803813	-0.722292	-2.150158
H	-5.401409	0.343245	-0.301237
H	-5.001515	1.237578	-1.759252
H	-3.134605	-1.789519	1.618089
H	-4.670640	-1.049883	1.170267
C	-4.351464	-1.162010	3.300676
C	-2.460239	0.263063	4.184444
H	-1.218124	-0.331742	2.511019
H	-1.424500	1.412975	2.668067
H	1.550234	-1.681720	2.098275

H	3.118208	-2.223266	1.512831
C	3.059945	-1.839433	3.643365
C	2.735430	0.588797	4.273634
H	2.558555	1.943365	2.592071
H	1.216717	0.818508	2.748136
H	4.546975	2.105286	1.523926
H	5.331626	1.742527	-0.004610
C	4.947781	3.846199	0.316030
C	3.611081	3.994592	-1.826956
H	3.977307	1.909705	-2.208477
H	2.266836	2.313864	-2.165442
H	5.307116	0.007110	-1.255924
H	5.165240	-0.963455	0.205214
C	5.481929	-2.114692	-1.604747
C	3.564006	-2.036583	-3.259152
H	1.863069	-0.858005	-2.596249
H	3.308649	0.083181	-2.967067
C	-2.243029	-4.458589	0.122573
C	-0.176520	-4.252397	1.510447
C	-0.806968	-3.893260	-2.343392
C	1.124032	-4.783122	-1.032489
H	-3.108352	4.954579	-2.750604
H	-4.419736	4.541241	-1.650426
C	-2.742065	5.490113	-0.673696
H	-4.054981	4.902463	0.939784
H	-2.514464	5.554583	1.490375
H	-3.315106	-1.408838	-4.493825
H	-3.697996	-2.350005	-3.056556
C	-5.209803	-0.892531	-3.555652
H	-5.849217	-1.702457	-1.652555
H	-6.836970	-0.355657	-2.212969
H	-5.113165	-0.395920	3.512129
H	-4.857299	-2.133092	3.385204
C	-3.227575	-1.056978	4.339757
H	-1.616635	0.301768	4.886529
H	-3.123230	1.101557	4.446698
H	2.787568	-2.873835	3.890917
H	4.155996	-1.779012	3.719019
C	2.428923	-0.867024	4.649301
H	2.232471	1.277157	4.965397
H	3.815084	0.772362	4.380540
H	4.232114	4.462763	0.880641
H	5.931699	4.014762	0.773411
C	4.955633	4.296976	-1.150984
H	3.650097	4.263112	-2.890798
H	2.828303	4.620749	-1.374886
H	6.574913	-2.106889	-1.497481
H	5.128689	-3.048127	-1.141806
C	5.089101	-2.104289	-3.088705
H	3.113816	-2.965413	-2.881206
H	3.304160	-1.973718	-4.324277
H	-2.804344	-4.370183	1.058997
H	-2.098671	-5.526428	-0.081289
H	-2.854522	-4.033768	-0.677091
H	0.791102	-3.762220	1.645289
H	-0.013419	-5.335324	1.470723
H	-0.791090	-4.031651	2.389650
H	-1.618920	-3.163574	-2.394780
H	-1.232962	-4.897111	-2.452987
H	-0.139193	-3.708759	-3.190971
H	1.701593	-4.706059	-1.959601
H	0.723381	-5.802203	-0.971819
H	1.809356	-4.630987	-0.195116
H	-1.662109	5.611295	-0.842962
H	-3.184824	6.491513	-0.752283
H	-5.800610	-1.613883	-4.135057
H	-5.273124	0.066166	-4.092000

H	-3.634238	-1.145925	5.355653
H	-2.530562	-1.897215	4.204740
H	2.784068	-1.082507	5.665287
H	1.338683	-1.014904	4.659817
H	5.188573	5.367425	-1.220642
H	5.756942	3.766728	-1.687090
H	5.547723	-1.230039	-3.575346
H	5.493937	-2.990317	-3.595374

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Ru	0.011958	0.331775	-0.245254
P	-2.321849	0.769491	-0.005508
P	2.382577	0.234698	0.080965
B	-0.252769	-1.656858	-0.298232
H	0.475284	0.432591	-2.032785
H	-0.009410	0.195701	1.359847
H	-0.339602	0.552287	-2.050632
C	-2.610735	2.646531	-0.140816
C	-3.549394	0.033843	-1.261650
C	-3.227929	0.419634	1.652349
C	2.959026	-0.256173	1.818282
C	3.046740	2.015386	-0.054284
C	3.430494	-0.923872	-1.001388
O	0.668324	-2.594063	-0.804473
O	-1.410791	-2.348763	0.110808
H	-3.695367	2.814107	-0.066484
C	-2.130063	3.209489	-1.496201
C	-1.939243	3.420950	1.015893
H	-3.706657	-0.972499	-0.854845
C	-2.973845	-0.185592	-2.675360
C	-4.918612	0.741241	-1.350153
H	-3.915647	1.271542	1.776300
C	-4.080513	-0.869921	1.687858
C	-2.262272	0.404995	2.858059
H	4.057305	-0.217194	1.811926
C	2.541089	-1.698385	2.175992
C	2.462800	0.714948	2.911820
H	2.356413	2.545224	0.621775
C	4.478451	2.318081	0.441896
C	2.842949	2.636659	-1.454378
H	3.058927	-1.900305	-0.664501
C	4.963051	-0.908589	-0.814513
C	3.084213	-0.852488	-2.503219
C	0.016331	-3.874681	-0.964808
C	-1.168215	-3.774608	0.064994
H	-1.058892	2.991158	-1.616239
H	-2.638805	2.705016	-2.324054
C	-2.351070	4.727501	-1.608763
C	-2.149170	4.940656	0.897971
H	-2.330031	3.083489	1.980837
H	-0.861732	3.198351	1.023640
H	-2.756999	0.775913	-3.160781
H	-2.023346	-0.721942	-2.603921
C	-3.957949	-0.976387	-3.556213
C	-5.905317	-0.049464	-2.228659
H	-5.351063	0.892339	-0.353712
H	-4.787230	1.741838	-1.785069
H	-3.423468	-1.730909	1.518683
H	-4.825078	-0.875731	0.886372
C	-4.824234	-1.026206	3.027904
C	-3.011260	0.278831	4.195036
H	-1.577102	-0.441573	2.737720
H	-1.628879	1.296461	2.868301
H	1.446297	-1.758493	2.146055
H	2.913301	-2.408468	1.429480
C	3.045674	-2.109569	3.569971
C	2.969285	0.306768	4.306531

H	2.783986	1.741407	2.700954
H	1.366128	0.721270	2.903529
H	4.652396	1.900829	1.439098
H	5.208410	1.845435	-0.225773
C	4.744009	3.834738	0.471172
C	3.112665	4.151919	-1.440819
H	3.526222	2.161826	-2.171717
H	1.826383	2.441246	-1.814248
H	5.375233	0.035019	-1.195767
H	5.239465	-0.966914	0.244273
C	5.625510	-2.069557	-1.579179
C	3.754687	-1.998370	-3.282087
H	2.000556	-0.911607	-2.632095
H	3.414498	0.107014	-2.925053
C	1.032723	-4.983207	-0.684408
C	-0.455955	-3.967399	-2.424570
C	-0.778411	-4.222060	1.482308
C	-2.457589	-4.481303	-0.358214
H	-1.974175	5.085485	-2.575816
H	-3.430818	4.939566	-1.596873
C	-1.675571	5.482276	-0.456740
H	-3.218826	5.167007	1.022403
H	-1.626744	5.449221	1.718865
H	-3.538702	-1.100258	-4.563386
H	-4.076553	-1.988492	-3.140464
C	-5.333429	-0.298287	-3.631510
H	-6.122750	-1.014852	-1.747727
H	-6.860321	0.488438	-2.294716
H	-5.562285	-0.215321	3.126045
H	-5.395527	-1.964204	3.020213
C	-3.875030	-0.987389	4.231360
H	-2.288760	0.272710	5.021934
H	-3.651199	1.161802	4.347029
H	2.707798	-3.128939	3.799221
H	4.145910	-2.139966	3.565541
C	2.571605	-1.133606	4.655111
H	2.577265	1.003814	5.058906
H	4.065806	0.397847	4.339083
H	4.075745	4.304296	1.208552
H	5.769305	4.025626	0.814350
C	4.514647	4.476119	-0.904102
H	2.987064	4.561285	-2.451745
H	2.358950	4.644696	-0.807981
H	6.714208	-2.033139	-1.440266
H	5.286515	-3.024401	-1.150876
C	5.275457	-2.028499	-3.072559
H	3.322651	-2.952043	-2.944901
H	3.519163	-1.908454	-4.350889
H	1.826321	-4.954377	-1.439136
H	0.561800	-5.972582	-0.730923
H	1.497876	-4.865545	0.297258
H	-1.184932	-3.184199	-2.655004
H	-0.908101	-4.939992	-2.649390
H	0.406075	-3.829627	-3.085400
H	0.142708	-3.732440	1.811244
H	-0.638305	-5.307239	1.544511
H	-1.576238	-3.939542	2.176902
H	-3.225839	-4.340268	0.409828
H	-2.295859	-5.559629	-0.476071
H	-2.847164	-4.084673	-1.299137
H	-0.584334	5.361492	-0.535369
H	-1.877530	6.558575	-0.531503
H	-6.028467	-0.906427	-4.224858
H	-5.233967	0.664095	-4.155914
H	-4.442890	-1.044456	5.169379
H	-3.219472	-1.870424	4.205179
H	2.981425	-1.418528	5.632958

H	1.476902	-1.194306	4.741936
H	4.660980	5.562569	-0.849244
H	5.267881	4.094316	-1.609456
H	5.721670	-1.128369	-3.521972
H	5.717141	-2.888292	-3.593120

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Ru	-0.009630	0.358134	-0.113559
P	-2.342715	0.706624	0.049467
P	2.365642	0.318591	0.143361
B	-0.203662	-1.630023	-0.242796
H	0.567782	1.272268	-2.929541
H	-0.037346	0.291427	1.455964
H	-0.127719	1.122060	-3.142539
C	-2.708182	2.569204	0.205430
C	-3.457402	0.161070	-1.396765
C	-3.320110	0.051599	1.562380
C	3.008333	-0.131003	1.869350
C	3.067700	2.075058	-0.065494
C	3.334240	-0.880105	-0.969176
O	0.238215	-2.329882	-1.390275
O	-0.804819	-2.546545	0.638773
H	-3.801569	2.686180	0.184077
C	-2.113977	3.362895	-0.978332
C	-2.203530	3.161512	1.540129
H	-3.635310	-0.898238	-1.167975
C	-2.737867	0.171046	-2.761362
C	-4.832374	0.852248	-1.502769
H	-4.056769	0.838542	1.790432
C	-4.106244	-1.258891	1.330901
C	-2.407173	-0.133370	2.796223
H	4.105803	-0.070120	1.831502
C	2.619110	-1.578444	2.238426
C	2.527841	0.842119	2.968123
H	2.672391	2.572984	0.832558
C	4.599102	2.262079	-0.050605
C	2.451848	2.826670	-1.265201
H	2.751031	-1.801304	-0.830295
C	4.806091	-1.200652	-0.629242
C	3.195463	-0.522245	-2.464051
C	-0.311200	-3.668372	-1.375971
C	-0.601302	-3.895939	0.155964
H	-1.025907	3.200675	-1.006554
H	-2.503655	2.987225	-1.930490
C	-2.394696	4.871590	-0.872328
C	-2.482474	4.671398	1.642915
H	-2.677420	2.654942	2.386755
H	-1.123413	2.979119	1.633751
H	-2.489980	1.199928	-3.055714
H	-1.790179	-0.372329	-2.677202
C	-3.611347	-0.461384	-3.859506
C	-5.703433	0.214014	-2.600321
H	-5.361796	0.819284	-0.542177
H	-4.692379	1.915294	-1.743242
H	-3.397443	-2.056141	1.075635
H	-4.805722	-1.161663	0.494655
C	-4.909321	-1.666040	2.581142
C	-3.211794	-0.514735	4.049851
H	-1.681470	-0.920676	2.565256
H	-1.822751	0.770008	2.991577
H	1.526525	-1.670366	2.207311
H	3.011880	-2.281124	1.493878
C	3.134213	-1.980411	3.631047
C	3.043852	0.434697	4.359735
H	2.861225	1.864641	2.755438
H	1.430621	0.860175	2.971701
H	5.047451	1.751780	0.809909

H	5.032355	1.803855	-0.949590
C	4.979948	3.753749	-0.026850
C	2.835021	4.316397	-1.254533
H	2.790510	2.374493	-2.206827
H	1.359615	2.724045	-1.248227
H	5.429688	-0.308945	-0.766265
H	4.913717	-1.497957	0.419443
C	5.347745	-2.327414	-1.529432
C	3.745421	-1.641624	-3.364371
H	2.143143	-0.344733	-2.705154
H	3.742218	0.407255	-2.678868
C	0.708861	-4.626505	-1.994339
C	-1.582910	-3.653130	-2.238268
C	0.594061	-4.487433	0.917652
C	-1.852127	-4.722527	0.463703
H	-1.929957	5.395391	-1.717959
H	-3.478234	5.044254	-0.955531
C	-1.891732	5.446387	0.458066
H	-3.570003	4.836205	1.674897
H	-2.082105	5.055981	2.590131
H	-3.090717	-0.409695	-4.824767
H	-3.749630	-1.529710	-3.637056
C	-4.986050	0.215252	-3.958240
H	-5.942734	-0.821792	-2.316782
H	-6.661070	0.746259	-2.673091
H	-5.686654	-0.909561	2.769068
H	-5.436563	-2.609304	2.385114
C	-4.021925	-1.797524	3.824773
H	-2.529972	-0.638338	4.901712
H	-3.895963	0.306470	4.314637
H	2.807634	-3.002651	3.862835
H	4.234862	-1.998036	3.624319
C	2.652293	-1.005781	4.713316
H	2.656350	1.133011	5.113245
H	4.140383	0.527418	4.383600
H	4.633044	4.200263	0.916927
H	6.072658	3.859950	-0.038819
C	4.357623	4.513082	-1.207706
H	2.413093	4.816596	-2.136059
H	2.381054	4.797352	-0.374850
H	6.399794	-2.524505	-1.284116
H	4.797734	-3.255620	-1.313592
C	5.200442	-1.987345	-3.019005
H	3.117063	-2.534742	-3.239581
H	3.663406	-1.344779	-4.418408
H	0.865371	-4.367414	-3.047155
H	0.353590	-5.663318	-1.952348
H	1.675392	-4.571391	-1.487494
H	-2.335049	-2.977165	-1.820036
H	-2.026875	-4.650511	-2.333024
H	-1.326957	-3.294363	-3.240493
H	1.511060	-3.929488	0.710913
H	0.761234	-5.539619	0.660728
H	0.396638	-4.423278	1.992600
H	-1.990022	-4.788597	1.548384
H	-1.756463	-5.743348	0.074225
H	-2.752545	-4.273285	0.038139
H	-0.793806	5.377800	0.490156
H	-2.140996	6.512654	0.534202
H	-5.603923	-0.283470	-4.716110
H	-4.855465	1.254462	-4.296001
H	-4.632802	-2.031186	4.706816
H	-3.328905	-2.640272	3.687530
H	3.063414	-1.284850	5.692287
H	1.557944	-1.072761	4.799080
H	4.602554	5.581251	-1.146632
H	4.798701	4.144584	-2.146097

H	5.845229	-1.128126	-3.258518
H	5.552833	-2.823056	-3.637575

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Ru	-0.016848	0.304616	0.018547
P	-2.317749	0.769819	0.084249
P	2.354381	0.239565	0.154848
B	-0.264962	-1.677519	-0.121889
H	-0.043503	0.289459	1.595325
C	-2.604010	2.617097	0.441796
C	-3.212830	0.488257	-1.568377
C	-3.498356	-0.017939	1.359992
C	3.145073	-0.330254	1.777441
C	2.979464	2.033316	0.032327
C	3.228870	-0.845622	-1.128928
O	0.041858	-2.344817	-1.331092
O	-0.775933	-2.613747	0.792736
H	-3.667111	2.823248	0.248392
C	-1.757652	3.504738	-0.497021
C	-2.315937	2.987679	1.913421
H	-3.472890	-0.577786	-1.523641
C	-2.260215	0.632584	-2.776203
C	-4.516543	1.277015	-1.800069
H	-4.239137	0.760900	1.601304
C	-4.276649	-1.251148	0.851493
C	-2.746126	-0.400549	2.656504
H	4.234386	-0.227040	1.666111
C	2.833339	-1.814456	2.061580
C	2.707729	0.539287	2.976887
H	2.421189	2.498332	0.860331
C	4.473332	2.332589	0.279005
C	2.507689	2.744560	-1.255273
H	2.838754	-1.836290	-0.853059
C	4.768530	-0.932523	-1.111887
C	2.720075	-0.587318	-2.564068
C	-0.517942	-3.678201	-1.298802
C	-0.649700	-3.949974	0.248398
H	-0.694432	3.251848	-0.362270
H	-1.992761	3.294135	-1.545579
C	-1.954201	5.006137	-0.223833
C	-2.513572	4.490244	2.181501
H	-2.968379	2.420390	2.584776
H	-1.284551	2.701934	2.163110
H	-1.915629	1.671021	-2.871329
H	-1.368990	0.013270	-2.612390
C	-2.953121	0.216250	-4.086432
C	-5.205389	0.852716	-3.109733
H	-5.205548	1.146436	-0.955753
H	-4.292450	2.351374	-1.854350
H	-3.557859	-2.032449	0.573050
H	-4.860936	-1.010969	-0.043084
C	-5.236222	-1.797838	1.925353
C	-3.711705	-0.916752	3.736522
H	-2.012510	-1.175707	2.410515
H	-2.174766	0.447944	3.043518
H	1.744965	-1.949240	2.096640
H	3.202615	-2.445537	1.244095
C	3.457795	-2.294971	3.383146
C	3.336268	0.055047	4.295396
H	2.979746	1.589501	2.816403
H	1.613682	0.505568	3.054834
H	4.825342	1.851313	1.198057
H	5.075010	1.920573	-0.540966
C	4.725157	3.850016	0.363611
C	2.752676	4.261142	-1.177363
H	3.052060	2.343208	-2.120033
H	1.444079	2.541040	-1.435594

H	5.198099	0.031924	-1.412341	P	-2.373927	0.752586	-0.040175
H	5.141649	-1.141057	-0.102218	P	2.344561	0.352757	0.055971
C	5.273151	-2.018960	-2.079747	B	-0.170382	-1.636977	-0.567411
C	3.227374	-1.667553	-3.534699	H	0.035234	0.616486	-1.444396
H	1.625150	-0.572096	-2.572065	C	-2.637677	2.331373	1.003776
H	3.066408	0.393892	-2.915332	C	-3.058684	1.274456	-1.736667
C	0.422978	-4.624555	-2.047472	C	-3.760223	-0.414726	0.562932
C	-1.870629	-3.628345	-2.026815	C	3.283962	-0.147719	1.628945
C	0.606579	-4.586441	0.861843	C	2.854085	2.184684	-0.091633
C	-1.875556	-4.767139	0.663070	C	3.256183	-0.640845	-1.286573
H	-1.310657	5.591121	-0.893907	O	-1.094789	-2.146085	-1.503649
H	-2.991068	5.284214	-0.465514	O	0.671005	-2.694921	-0.156607
C	-1.666092	5.356416	1.241151	H	-3.475120	2.887315	0.559059
H	-3.575588	4.745569	2.046716	C	-1.368971	3.213079	0.912581
H	-2.271057	4.711205	3.229139	C	-2.988595	2.094419	2.487451
H	-2.270427	0.364710	-4.933234	H	-3.037805	0.325160	-2.290248
H	-3.174129	-0.860685	-4.047917	C	-2.159075	2.255429	-2.518199
C	-4.259908	0.992068	-4.311838	C	-4.507505	1.813976	-1.747593
H	-5.531798	-0.194449	-3.024283	H	-4.608354	0.218833	0.864247
H	-6.112856	1.450664	-3.266480	C	-4.259434	-1.403788	-0.516116
H	-6.017873	-1.047598	2.119156	C	-3.294554	-1.223747	1.793142
H	-5.750538	-2.687580	1.538012	H	4.354614	0.014193	1.443023
C	-4.513748	-2.125956	3.238134	C	3.078596	-1.645296	1.946967
H	-3.146895	-1.181068	4.640279	C	2.893676	0.709678	2.852917
H	-4.406805	-0.113524	4.026803	H	2.488588	2.583789	0.867062
H	3.183640	-3.343531	3.558535	C	4.360448	2.510984	-0.169828
H	4.555084	-2.268768	3.299919	C	2.088471	2.963618	-1.185399
C	3.021187	-1.421987	4.566490	H	2.768968	-1.620611	-1.185911
H	2.979287	0.680933	5.123932	C	4.777905	-0.859903	-1.125026
H	4.427917	0.189270	4.251040	C	2.944587	-0.121220	-2.707490
H	4.205722	4.252474	1.246071	C	-0.697203	-3.476328	-1.906121
H	5.795100	4.042035	0.517415	C	0.178397	-3.948791	-0.686250
C	4.228517	4.579001	-0.893798	H	-0.517729	2.645839	1.328260
H	2.432923	4.740558	-2.111806	H	-1.118131	3.426571	-0.130549
H	2.128712	4.686717	-0.377029	C	-1.514373	4.534490	1.687124
H	6.370797	-2.047081	-2.068602	C	-3.156277	3.420606	3.251131
H	4.931984	-3.003087	-1.725258	H	-3.910866	1.510879	2.578696
C	4.758309	-1.787338	-3.507606	H	-2.190795	1.509685	2.967039
H	2.778707	-2.631411	-3.256118	H	-2.169154	3.240015	-2.027951
H	2.881928	-1.444172	-4.552788	H	-1.124354	1.901860	-2.511349
H	0.474040	-4.332590	-3.102012	C	-2.656005	2.425037	-3.964840
H	0.062869	-5.659538	-2.001930	C	-5.027588	1.978624	-3.188013
H	1.436604	-4.592426	-1.641012	H	-5.188388	1.168138	-1.183889
H	-2.570840	-2.958572	-1.518461	H	-4.534317	2.796064	-1.254933
H	-2.332653	-4.619158	-2.103024	H	-3.410825	-2.004226	-0.861060
H	-1.712318	-3.244901	-3.040272	H	-4.641273	-0.874220	-1.393589
H	1.508824	-4.037453	0.580336	C	-5.373654	-2.318389	0.025609
H	0.724584	-5.631866	0.555092	C	-4.400212	-2.137830	2.348515
H	0.521704	-4.556643	1.953044	H	-2.437312	-1.836689	1.484336
H	-1.908376	-4.847288	1.754941	H	-2.938143	-0.560411	2.586245
H	-1.828861	-5.783131	0.252443	H	2.007688	-1.839302	2.076724
H	-2.808421	-4.304359	0.333337	H	3.385234	-2.269164	1.101079
H	-0.599569	5.185696	1.452362	C	3.844296	-2.073714	3.210236
H	-1.855095	6.421932	1.424917	C	3.654900	0.276642	4.119431
H	-4.755286	0.645491	-5.227961	H	3.098034	1.770015	2.666289
H	-4.027107	2.056502	-4.466208	H	1.813679	0.621116	3.029492
H	-5.236354	-2.451839	3.997985	H	4.921650	1.982483	0.609512
H	-3.827354	-2.968585	3.072428	H	4.758630	2.166047	-1.133303
H	3.511943	-1.754900	5.490426	C	4.611967	4.025452	-0.047494
H	1.938923	-1.538790	4.723223	C	2.335361	4.477675	-1.063293
H	4.372715	5.662012	-0.788712	H	2.410493	2.630218	-2.179843
H	4.835720	4.264876	-1.755928	H	1.018488	2.741458	-1.122167
H	5.201436	-0.861142	-3.904049	H	5.307964	0.098480	-1.185446
H	5.090395	-2.598754	-4.168316	H	5.011378	-1.284763	-0.143599
				C	5.328164	-1.798766	-2.215206
				C	3.504593	-1.054422	-3.795360
				H	1.863355	0.004003	-2.832598

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Ru -0.046836 0.253379 0.084902

H	3.397585	0.870337	-2.841750	B	0.115665	-1.740719	0.248516
C	0.100377	-3.336188	-3.211456	H	0.010573	0.294395	1.355108
C	-1.949528	-4.315983	-2.169751	C	2.807904	2.269545	-0.907293
C	1.375237	-4.831388	-1.047370	C	3.060390	0.960428	1.745126
C	-0.638389	-4.628596	0.423057	C	3.800888	-0.522431	-0.682118
H	-0.579619	5.106869	1.623387	C	-3.472623	0.000439	-1.526360
H	-2.289372	5.148212	1.203908	C	-2.721121	2.247263	0.196880
C	-1.899457	4.295191	3.152726	C	-3.147033	-0.587382	1.354817
H	-4.014832	3.969926	2.836762	O	1.160052	-2.422542	0.907384
H	-3.396317	3.213156	4.302170	O	-0.930630	-2.660982	0.017099
H	-2.009762	3.133622	-4.499619	H	3.694110	2.699397	-0.420080
H	-2.564682	1.462090	-4.488599	C	1.630174	3.253738	-0.719058
C	-4.116702	2.896782	-4.015516	C	3.136998	2.146890	-2.410471
H	-5.080880	0.989277	-3.666067	H	3.052167	-0.049920	2.177736
H	-6.052383	2.372780	-3.171439	C	2.133671	1.817844	2.632431
H	-6.254648	-1.707224	0.274801	C	4.498745	1.518981	1.847044
H	-5.691818	-3.013946	-0.762214	H	4.647988	0.128946	-0.946585
C	-4.930931	-3.093664	1.273015	C	4.311485	-1.576525	0.327212
H	-4.014072	-2.704404	3.206165	C	3.325920	-1.250285	-1.958786
H	-5.227421	-1.519313	2.728224	H	-4.504414	0.177182	-1.192171
H	3.653725	-3.135093	3.417052	C	-3.356537	-1.485009	-1.933460
H	4.926067	-1.981426	3.029791	C	-3.233010	0.912855	-2.749901
C	3.463181	-1.215038	4.423480	H	-2.418256	2.667597	-0.774656
H	3.329176	0.886540	4.972324	C	-4.194821	2.645811	0.422940
H	4.727401	0.480814	3.981471	C	-1.822018	2.936179	1.248608
H	4.306777	4.362436	0.954551	H	-2.686059	-1.571859	1.203230
H	5.687172	4.231987	-0.130912	C	-4.680533	-0.781628	1.325400
C	3.832601	4.815675	-1.108253	C	-2.716060	-0.094438	2.754068
H	1.801875	5.007370	-1.863521	C	0.693372	-3.718995	1.345178
H	1.911213	4.837953	-0.113412	C	-0.493136	-3.998498	0.351379
H	6.411755	-1.919714	-2.084658	H	0.728470	2.817679	-1.179499
H	4.885292	-2.797886	-2.087045	H	1.401624	3.385706	0.342705
C	5.012172	-1.283506	-3.625121	C	1.903648	4.626159	-1.358966
H	2.986841	-2.022934	-3.747664	C	3.426361	3.520717	-3.043056
H	3.289356	-0.635847	-4.787342	H	4.004272	1.496470	-2.565256
H	-0.523271	-2.828911	-3.954594	H	2.291698	1.684428	-2.937200
H	0.399917	-4.308762	-3.618481	H	2.131194	2.857561	2.274484
H	0.996769	-2.729384	-3.058731	H	1.105719	1.452582	2.563869
H	-2.610308	-4.350841	-1.300372	C	2.610202	1.805660	4.096186
H	-1.682677	-5.344326	-2.442218	C	4.999006	1.499764	3.303458
H	-2.512456	-3.883020	-3.003625	H	5.197322	0.966597	1.209761
H	2.055202	-4.328761	-1.739781	H	4.510898	2.558436	1.490637
H	1.048382	-5.773254	-1.504520	H	3.466619	-2.197384	0.641670
H	1.938185	-5.076538	-0.140266	H	4.708852	-1.101620	1.228766
H	-0.008513	-4.746496	1.310414	C	5.418475	-2.456839	-0.282897
H	-0.993415	-5.620189	0.120051	C	4.428035	-2.125174	-2.580583
H	-1.504556	-4.023583	0.707533	H	2.472677	-1.882776	-1.683541
H	-1.068149	3.791888	3.668812	H	2.968203	-0.534286	-2.706180
H	-2.055816	5.251049	3.669053	H	-2.318512	-1.706360	-2.206454
H	-4.468389	2.947582	-5.054249	H	-3.571246	-2.138038	-1.081613
H	-4.179331	3.919736	-3.614479	C	-4.284942	-1.836647	-3.107672
H	-5.760507	-3.694760	1.667440	C	-4.156403	0.548330	-3.927026
H	-4.134846	-3.800666	0.996673	H	-3.398485	1.963937	-2.487926
H	4.054574	-1.505231	5.301629	H	-2.186967	0.834807	-3.071501
H	2.409536	-1.396853	4.681759	H	-4.848935	2.185382	-0.326434
H	3.987451	5.893762	-0.971298	H	-4.526785	2.272896	1.400854
H	4.227336	4.566801	-2.104657	C	-4.372837	4.175275	0.388736
H	5.545136	-0.335255	-3.792661	C	-1.994327	4.464438	1.211781
H	5.381753	-1.987598	-4.381952	H	-2.073895	2.573690	2.252300
C	-0.553607	-1.902857	3.597215	H	-0.774433	2.664703	1.083647
O	-0.288821	-0.764438	3.523666	H	-5.189114	0.181311	1.462859
O	-0.818864	-3.036583	3.689874	H	-5.011712	-1.175738	0.359765
				C	-5.139346	-1.750106	2.432624
				C	-3.171469	-1.061371	3.860806
22				H	-1.629764	0.037721	2.790077
Ru	0.064443	0.209749	-0.223201	H	-3.166166	0.888159	2.951733
P	2.420139	0.623694	-0.016321	C	0.242040	-3.567010	2.806307
P	-2.330666	0.400348	-0.055993				

C	1.847610	-4.720427	1.270774	H	0.020469	-0.669038	1.258772
C	-1.672848	-4.768657	0.948263	C	2.954738	2.181646	-0.907492
C	-0.046723	-4.680213	-0.951395	C	2.946383	0.868952	1.778205
H	1.029592	5.277529	-1.227694	C	3.835138	-0.594720	-0.648370
H	2.736201	5.110713	-0.827059	C	-3.501907	-0.072738	-1.571607
C	2.259847	4.497345	-2.845299	C	-2.649271	2.283880	-0.005080
H	4.334295	3.943936	-2.587752	C	-3.244760	-0.431773	1.357871
H	3.643352	3.395701	-4.112039	O	1.206297	-2.615851	0.548985
H	1.945817	2.429358	4.708885	O	-1.081131	-2.628516	0.464278
H	2.527518	0.781788	4.490053	H	3.936456	2.447297	-0.489146
C	4.061953	2.287707	4.230140	C	1.972994	3.333046	-0.600079
H	5.062398	0.457023	3.648518	C	3.130218	2.039020	-2.437177
H	6.017103	1.908016	3.354154	H	3.048070	-0.157794	2.156923
H	6.299906	-1.834065	-0.500185	C	1.851710	1.533786	2.642509
H	5.740947	-3.202443	0.455990	C	4.292764	1.591540	2.001587
C	4.962935	-3.149993	-1.573127	H	4.659700	0.073825	-0.941422
H	4.037395	-2.632061	-3.472864	C	4.395519	-1.584493	0.395780
H	5.254247	-1.483517	-2.922502	C	3.368030	-1.375651	-1.897900
H	-4.148510	-2.890347	-3.383737	H	-4.535501	0.140091	-1.262884
H	-5.333431	-1.730591	-2.790118	C	-3.387518	-1.588469	-1.852490
C	-4.032038	-0.929646	-4.318873	C	-3.234881	0.745743	-2.856444
H	-3.930206	1.194257	-4.785706	H	-2.332683	2.598226	-1.010594
H	-5.199095	0.758868	-3.645651	C	-4.081266	2.810552	0.220085
H	-4.137929	4.542008	-0.621872	C	-1.667342	2.960314	0.978224
H	-5.423586	4.432599	0.576766	H	-2.858046	-1.452569	1.250595
C	-3.461029	4.875464	1.406468	C	-4.787510	-0.517417	1.368909
H	-1.364135	4.928568	1.981864	C	-2.740239	0.095098	2.719444
H	-1.636505	4.846304	0.243278	C	0.801877	-3.962262	0.912328
H	-6.231679	-1.857941	2.399473	C	-0.679658	-4.020609	0.383023
H	-4.720777	-2.747280	2.230900	H	0.979898	3.059877	-0.980103
C	-4.689122	-1.286269	3.823970	H	1.872715	3.480845	0.480720
H	-2.658431	-2.025973	3.734688	C	2.411178	4.657798	-1.249601
H	-2.865939	-0.672608	4.841231	C	3.569708	3.366940	-3.080613
H	1.081639	-3.187322	3.397591	H	3.880189	1.276106	-2.668196
H	-0.080017	-4.520786	3.239538	H	2.183902	1.709088	-2.880672
H	-0.578609	-2.848488	2.891443	H	1.701590	2.575916	2.330621
H	2.288149	-4.756569	0.271449	H	0.894104	1.019511	2.501375
H	1.510087	-5.729137	1.538294	C	2.240788	1.516262	4.131948
H	2.634188	-4.432400	1.976598	C	4.692721	1.574514	3.488034
H	-2.104806	-4.249441	1.807404	H	5.089824	1.143774	1.396443
H	-1.367561	-5.772518	1.267447	H	4.204162	2.636667	1.674902
H	-2.458194	-4.881751	0.192912	H	3.583038	-2.233129	0.739598
H	-0.877462	-4.665883	-1.663978	H	4.784397	-1.056665	1.272821
H	0.245403	-5.723303	-0.784893	C	5.534396	-2.434254	-0.201023
H	0.794253	-4.152110	-1.409924	C	4.509723	-2.210722	-2.501253
H	1.382219	4.130055	-3.398210	H	2.542204	-2.031384	-1.606245
H	2.506921	5.480138	-3.267084	H	2.965128	-0.701599	-2.659161
H	4.399005	2.207217	5.271853	H	-2.347818	-1.828875	-2.096616
H	4.112487	3.355205	3.967311	H	-3.632537	-2.164267	-0.952698
H	5.787303	-3.727226	-2.011833	C	-4.302339	-2.020924	-3.010510
H	4.165980	-3.869555	-1.335012	C	-4.152632	0.293288	-4.006221
H	-4.728641	-1.168963	-5.132750	H	-3.401493	1.813708	-2.671955
H	-3.020059	-1.120069	-4.707698	H	-2.187366	0.642395	-3.157432
H	-3.568222	5.965144	1.328095	H	-4.781920	2.354402	-0.489227
H	-3.779648	4.602315	2.423686	H	-4.422212	2.528183	1.225404
H	-5.200505	-0.344594	4.074655	C	-4.134715	4.344034	0.090508
H	-4.989080	-2.016982	4.586438	C	-1.717650	4.491817	0.846128
C	0.182336	-0.973163	-3.055480	H	-1.909809	2.681222	2.010633
O	0.169736	0.177377	-2.808594	H	-0.643692	2.606754	0.793071
O	0.190711	-2.088995	-3.397356	H	-5.225935	0.483694	1.471396
				H	-5.165119	-0.931810	0.428831
				C	-5.279180	-1.402187	2.530927
				C	-3.224548	-0.795242	3.876745
				H	-1.645557	0.151173	2.726098
				H	-3.115722	1.114373	2.884252
				C	0.906592	-4.062966	2.441716
				C	1.755374	-4.961724	0.258802
23							
Ru	0.035580	0.161799	-0.198781				
P	2.456947	0.567994	-0.031140				
P	-2.401544	0.413415	-0.113717				
B	0.062091	-1.829268	0.404883				

C	-1.638982	-4.851319	1.236402	C	3.006463	2.404193	-0.664784
C	-0.783625	-4.448082	-1.088200	C	3.260320	0.631751	1.737346
H	1.671531	5.438025	-1.026457	C	3.794978	-0.371819	-0.996719
H	3.359123	4.988228	-0.798496	C	-3.422992	-0.213851	-1.564289
C	2.594998	4.508084	-2.764657	C	-3.081241	2.184855	0.125111
H	4.572343	3.635930	-2.714109	C	-3.268051	-0.645652	1.342885
H	3.660825	3.231910	-4.166041	O	1.369459	-2.433540	0.453537
H	1.460197	2.008960	4.726187	O	-0.912895	-2.572875	0.438560
H	2.286542	0.473177	4.478504	H	4.061607	2.521570	-0.377342
C	3.598988	2.191934	4.371727	C	2.208908	3.547265	-0.003854
H	4.872658	0.535710	3.802370	C	2.932856	2.542833	-2.203274
H	5.640895	2.110558	3.624757	H	3.409976	-0.445968	1.885486
H	6.384670	-1.777493	-0.440409	C	2.322669	1.083681	2.878047
H	5.895641	-3.143542	0.555733	C	4.630630	1.329884	1.888709
C	5.102366	-3.180125	-1.470590	H	4.565932	0.355593	-1.294271
H	4.137834	-2.761406	-3.374624	C	4.507648	-1.492838	-0.207906
H	5.302455	-1.540994	-2.869045	C	3.167099	-0.965492	-2.275479
H	-4.166426	-3.093211	-3.202937	H	-4.476314	-0.009478	-1.327679
H	-5.355779	-1.886452	-2.719516	C	-3.298697	-1.731529	-1.820793
C	-4.020610	-1.210132	-4.282213	C	-3.086081	0.558414	-2.863247
H	-3.916707	0.871795	-4.908699	H	-2.371662	2.719550	-0.524874
H	-5.198537	0.523871	-3.750847	C	-4.506824	2.512421	-0.387326
H	-3.896200	4.626578	-0.945414	C	-2.943144	2.779266	1.546185
H	-5.155577	4.698409	0.283517	H	-2.994890	-1.659433	1.027445
C	-3.143868	5.027811	1.044341	C	-4.806932	-0.576008	1.457140
H	-1.033709	4.951851	1.571184	C	-2.630234	-0.454409	2.738031
H	-1.356851	4.778937	-0.152525	C	1.053927	-3.811731	-0.783360
H	-6.376658	-1.431244	2.533341	C	-0.434712	-3.936160	0.291233
H	-4.939318	-2.434454	2.361838	H	1.151104	3.446315	-0.278121
C	-4.754745	-0.914407	3.888281	H	2.263520	3.483229	1.089469
H	-2.780090	-1.795553	3.770836	C	2.707716	4.929835	-0.459756
H	-2.865300	-0.391121	4.832330	C	3.421288	3.928359	-2.664508
H	1.931020	-3.824097	2.745674	H	3.548757	1.778982	-2.687657
H	0.670140	-5.070509	2.801037	H	1.902245	2.376085	-2.535168
H	0.234084	-3.352291	2.932843	H	2.119278	2.161254	2.801701
H	1.821339	-4.804774	-0.819992	H	1.358887	0.573369	2.798249
H	1.426318	-5.991374	0.442656	C	2.949608	0.792220	4.254267
H	2.759580	-4.851279	0.681628	C	5.264486	1.029970	3.258840
H	-1.685759	-4.491775	2.267473	H	5.319221	1.033593	1.089169
H	-1.338664	-5.905793	1.248448	H	4.496941	2.416244	1.796999
H	-2.647238	-4.795986	0.812397	H	3.759254	-2.209454	0.144205
H	-1.819809	-4.326305	-1.419381	H	5.017092	-1.096036	0.675757
H	-0.507086	-5.499823	-1.221655	C	5.555441	-2.209356	-1.082239
H	-0.157538	-3.822417	-1.729456	C	4.217203	-1.667827	-3.152348
H	1.621633	4.291382	-3.227990	H	2.393627	-1.680837	-1.983047
H	2.950934	5.449898	-3.202122	H	2.658135	-0.195594	-2.861392
H	3.879296	2.121294	5.430503	H	-2.258724	-1.966066	-2.063451
H	3.513602	3.264552	4.141647	H	-3.554011	-2.303737	-0.922326
H	5.953571	-3.725750	-1.898652	C	-4.219110	-2.167194	-2.975886
H	4.345200	-3.931901	-1.208255	C	-4.033137	0.138680	-4.000858
H	-4.702329	-1.511513	-5.088261	H	-3.140178	1.642034	-2.713379
H	-3.000388	-1.426475	-4.629000	H	-2.059523	0.344364	-3.164683
H	-3.165371	6.115506	0.900075	H	-4.676354	2.122847	-1.392944
H	-3.456963	4.843855	2.082982	H	-5.251350	2.035951	0.263539
H	-5.191654	0.070372	4.112614	C	-4.751077	4.033639	-0.404308
H	-5.081244	-1.590562	4.688893	C	-3.160115	4.302843	1.542151
C	0.071597	-0.470878	-2.115652	H	-3.695793	2.320883	2.200468
O	0.067576	0.780473	-2.334341	H	-1.970404	2.551260	1.992078
O	0.073878	-1.496909	-2.760800	H	-5.109664	0.421135	1.804349
				H	-5.286238	-0.729159	0.484302
				C	-5.336169	-1.627126	2.450900
				C	-3.155132	-1.508321	3.729127
				H	-1.541186	-0.524007	2.666387
				H	-2.861324	0.543298	3.131252
				C	1.207736	-3.954249	2.305366
				C	2.043121	-4.735065	0.072856
				C	-1.318544	-4.855792	1.134548
23'							
Ru	0.047755	0.339429	-0.057908				
P	2.525764	0.676669	-0.019004				
P	-2.467389	0.376067	-0.037866				
B	0.179145	-1.706594	0.379913				
H	0.094099	-0.592018	1.326625				

C	-0.551761	-4.312888	-1.192792	H	-0.033557	0.506534	1.192658
H	2.108620	5.714407	0.020863	C	-2.890163	-2.217217	-0.921078
H	3.743955	5.074486	-0.118988	C	-2.947663	-0.935194	1.781088
C	2.649319	5.067434	-1.986576	C	-3.873632	0.548093	-0.604168
H	4.492701	4.032488	-2.434439	C	3.454771	-0.086105	-1.624802
H	3.328713	4.001488	-3.755683	C	2.632820	-2.289374	0.154419
H	2.275392	1.140426	5.047591	C	3.239551	0.535305	1.266291
H	3.042715	-0.296788	4.379929	O	-1.194876	2.688071	0.233015
C	4.332747	1.439606	4.407678	O	1.106933	2.680638	0.161531
H	5.481390	-0.046138	3.330070	H	-3.816409	-2.592293	-0.463014
H	6.227985	1.549167	3.343581	C	-1.779342	-3.269941	-0.705019
H	6.357226	-1.499299	-1.336061	C	-3.158042	-2.046768	-2.433462
H	6.026775	-3.012496	-0.499952	H	-3.022520	0.082994	2.187277
C	4.951362	-2.767933	-2.376465	C	-1.865833	-1.646273	2.622306
H	3.727262	-2.086139	-4.040568	C	-4.309226	-1.632799	1.991795
H	4.948343	-0.929749	-3.517014	H	-4.709588	-0.130984	-0.835334
H	-4.090570	-3.242055	-3.160287	C	-4.372021	1.560485	0.451626
H	-5.269666	-2.026143	-2.677480	C	-3.489752	1.313312	-1.892661
C	-3.946778	-1.371894	-4.260364	H	4.485477	-0.341475	-1.337719
H	-3.780939	0.696733	-4.911750	C	3.424371	1.412514	-2.005348
H	-5.069334	0.409020	-3.743518	C	3.085275	-0.960596	-2.845243
H	-4.064874	4.496250	-1.128987	H	2.298990	-2.695227	-0.812467
H	-5.767600	4.237250	-0.765200	C	4.070586	-2.795051	0.390050
C	-4.538312	4.669315	0.974876	C	1.677910	-2.880903	1.215304
H	-3.049624	4.694703	2.561656	H	2.863124	1.545576	1.064007
H	-2.374332	4.777514	0.936098	C	4.783835	0.593486	1.257574
H	-6.428125	-1.544823	2.530178	C	2.739095	0.150290	2.675908
H	-5.125742	-2.631649	2.055609	C	-0.762588	3.903741	0.889615
C	-4.686611	-1.479729	3.833419	C	0.720434	4.060225	0.378346
H	-2.831176	-2.504612	3.394882	H	-0.838851	-2.879010	-1.122508
H	-2.703145	-1.345658	4.716491	H	-1.605919	-3.440109	0.362910
H	2.222986	-3.658390	2.589386	C	-2.103345	-4.611388	-1.385384
H	1.047726	-4.986107	2.636969	C	-3.484353	-3.392071	-3.107031
H	0.504894	-3.305447	2.837608	H	-3.996864	-1.363168	-2.596703
H	2.074339	-4.537072	-1.000776	H	-2.278477	-1.599391	-2.911721
H	1.773309	-5.786654	0.226374	H	-1.744170	-2.684580	2.284684
H	3.050337	-4.586905	0.476644	H	-0.898791	-1.148774	2.488629
H	-1.356066	-4.541496	2.180687	C	-2.248029	-1.657176	4.113575
H	-0.955939	-5.889862	1.094680	C	-4.703090	-1.645088	3.480076
H	-2.340312	-4.845568	0.740691	H	-5.098503	-1.152574	1.402052
H	-1.603242	-4.261076	-1.491010	H	-4.244761	-2.671313	1.639167
H	-0.198639	-5.333423	-1.377227	H	-3.539717	2.219305	0.721475
H	0.003973	-3.614275	-1.824140	H	-4.700860	1.055540	1.365552
H	1.599136	5.037348	-2.311682	C	-5.550939	2.393767	-0.087475
H	3.048409	6.041236	-2.298675	C	-4.680778	2.116118	-2.442202
H	4.776223	1.169770	5.374622	H	-2.670648	1.997313	-1.654976
H	4.221872	2.534276	4.408587	H	-3.115995	0.635252	-2.664510
H	5.734550	-3.229338	-2.996991	H	2.398076	1.708014	-2.246732
H	4.240828	-3.568980	-2.127910	H	3.722759	2.034267	-1.154258
H	-4.651761	-1.667573	-5.048499	C	4.338504	1.705130	-3.207169
H	-2.939047	-1.613299	-4.625623	C	3.996179	-0.652265	-4.047649
H	-4.651945	5.759335	0.916412	H	3.177441	-2.025578	-2.600082
H	-5.317480	4.309795	1.663412	H	2.038678	-0.786296	-3.118109
H	-5.001349	-0.524737	4.280578	H	4.753000	-2.397463	-0.369958
H	-5.040010	-2.270964	4.507191	H	4.432825	-2.431804	1.360983
C	0.025585	-0.199287	-2.012282	C	4.123723	-4.333838	0.385672
O	0.013768	1.067664	-2.148427	C	1.728143	-4.418295	1.215304
O	-0.012940	-1.157002	-2.762352	H	1.946284	-2.513033	2.212726
H	0.340928	1.951905	1.119142	H	0.648467	-2.544840	1.031582
H	-0.406166	1.788166	1.246156	H	5.205266	-0.399092	1.462257
				H	5.162295	0.899358	0.277284
				C	5.301443	1.581638	2.320363
				C	3.251443	1.139542	3.737054
				H	1.643923	0.117586	2.693518
				H	3.097499	-0.855228	2.936953
				C	-0.856821	3.662639	2.405068
				C	-1.703246	5.040727	0.487084

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Ru	-0.052866	-0.206872	-0.226672
P	-2.464234	-0.594730	-0.022140
P	2.375897	-0.431547	-0.112133
B	-0.055719	1.961594	-0.145463

C	1.687351	4.681307	1.387230	C	-3.155290	-0.659991	1.777833
C	0.825451	4.807821	-0.960728	C	-3.823086	0.426299	-0.896276
H	-1.274916	-5.314301	-1.226455	C	3.429625	0.102773	-1.636433
H	-2.987345	-5.056185	-0.903997	C	3.052218	-2.221514	0.133760
C	-2.377772	-4.429953	-2.883105	C	3.284259	0.639520	1.262322
H	-4.431656	-3.781501	-2.703553	O	-1.298006	2.502644	0.182437
H	-3.645528	-3.230984	-4.180590	O	1.004603	2.585246	0.209032
H	-1.475915	-2.181649	4.691433	H	-4.135214	-2.417405	-0.435604
H	-2.268537	-0.622206	4.485518	C	-2.367290	-3.568535	-0.038196
C	-3.619929	-2.308083	4.343468	C	-2.949279	-2.462126	-2.227869
H	-4.859475	-0.611006	3.821296	H	-3.257304	0.415807	1.973923
H	-5.662219	-2.163743	3.606927	C	-2.173454	-1.187018	2.846634
H	-6.413580	1.730087	-0.252484	C	-4.539312	-1.319339	1.973878
H	-5.861488	3.119892	0.675679	H	-4.617944	-0.293801	-1.145922
C	-5.208834	3.110116	-1.400149	C	-4.469543	1.547532	-0.050474
H	-4.375596	2.644673	-3.354257	C	-3.305745	1.043688	-2.215201
H	-5.489560	1.428334	-2.734284	H	4.476849	-0.143797	-1.412589
H	4.271931	2.769692	-3.466137	C	3.379946	1.616153	-1.941484
H	5.386646	1.515768	-2.928179	C	3.017067	-0.707172	-2.888147
C	3.972138	0.836664	-4.417884	H	2.335893	-2.761785	-0.504982
H	3.687595	-1.264911	-4.904547	C	4.469166	-2.600881	-0.364445
H	5.029073	-0.947982	-3.807146	C	2.888871	-2.769285	1.571581
H	3.858467	-4.701352	-0.616642	H	3.045753	1.650411	0.911922
H	5.149997	-4.671284	0.579979	C	4.818917	0.512749	1.382745
C	3.160352	-4.935366	1.419607	C	2.626711	0.509102	2.654511
H	1.065671	-4.812892	1.996643	C	-0.941839	3.750476	0.822548
H	1.340043	-4.792433	0.256201	C	0.556050	3.952469	0.376551
H	6.399260	1.591813	2.310499	H	-1.298055	-3.546068	-0.284659
H	4.976876	2.597742	2.052339	H	-2.442415	-3.528357	1.054304
C	4.783348	1.237712	3.723295	C	-2.948840	-4.900582	-0.543852
H	2.821172	2.131986	3.539660	C	-3.501190	-3.802145	-2.748459
H	2.896833	0.835516	4.730711	H	-3.499128	-1.650321	-2.711605
H	-1.883597	3.376003	2.655573	H	-1.899773	-2.343327	-2.523840
H	-0.604760	4.560872	2.980005	H	-2.011438	-2.266585	2.719643
H	-0.193772	2.849866	2.716841	H	-1.200227	-0.702517	2.727790
H	-1.768087	5.140324	-0.598716	C	-2.716607	-0.933145	4.265069
H	-1.367586	5.996525	0.907315	C	-5.088261	-1.062705	3.388990
H	-2.710254	4.842656	0.870155	H	-5.260712	-0.965293	1.228652
H	1.737469	4.101883	2.312492	H	-4.448010	-2.403987	1.826334
H	1.390042	5.707249	1.635110	H	-3.695788	2.276618	0.208637
H	2.693793	4.719800	0.956199	H	-4.883121	1.162020	0.886215
H	1.847854	4.709118	-1.339935	C	-5.607983	2.237022	-0.827474
H	0.606254	5.875018	-0.841436	C	-4.450426	1.697408	-3.007009
H	0.150214	4.385477	-1.707456	H	-2.557848	1.801925	-1.971638
H	-1.457798	-4.092995	-3.382653	H	-2.800192	0.301432	-2.838113
H	-2.652442	-5.389260	-3.340381	H	2.348924	1.919443	-2.143437
H	-3.894255	-2.256715	5.404901	H	3.709909	2.197622	-1.073943
H	-3.559675	-3.376576	4.087442	C	4.270734	1.960170	-3.149106
H	-6.089899	3.641512	-1.783388	C	3.916602	-0.361264	-4.087612
H	-4.438762	3.870617	-1.208578	H	3.065051	-1.785337	-2.694502
H	4.658519	1.032556	-5.252039	H	1.974879	-0.492531	-3.137675
H	2.965088	1.107397	-4.765601	H	4.645364	-2.249999	-1.383498
H	3.180421	-6.031319	1.367276	H	5.226370	-2.120612	0.267902
H	3.500494	-4.663931	2.430181	C	4.674632	-4.127757	-0.329679
H	5.209933	0.274032	4.040452	C	3.067489	-4.296969	1.615327
H	5.126136	1.984891	4.450649	H	3.648547	-2.309886	2.216542
C	-0.150290	0.697715	-1.962622	H	1.919987	-2.500498	2.004807
O	-0.195788	-0.279631	-2.725680	H	5.082242	-0.490924	1.742423
O	-0.138522	1.947588	-2.081028	H	5.305143	0.635461	0.408715

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Ru	-0.037498	-0.377508	-0.141413
P	-2.512393	-0.661365	-0.011392
P	2.464671	-0.406073	-0.086590
B	-0.115628	1.820431	-0.154942
H	-0.047369	0.329160	1.273425
C	-3.066617	-2.357498	-0.690223

C	-3.155290	-0.659991	1.777833
C	-3.823086	0.426299	-0.896276
C	3.429625	0.102773	-1.636433
C	3.052218	-2.221514	0.133760
C	3.284259	0.639520	1.262322
O	-1.298006	2.502644	0.182437
O	1.004603	2.585246	0.209032
H	-4.135214	-2.417405	-0.435604
C	-2.367290	-3.568535	-0.038196
C	-2.949279	-2.462126	-2.227869
H	-3.257304	0.415807	1.973923
C	-2.173454	-1.187018	2.846634
C	-4.539312	-1.319339	1.973878
H	-4.617944	-0.293801	-1.145922
C	-4.469543	1.547532	-0.050474
C	-3.305745	1.043688	-2.215201
H	4.476849	-0.143797	-1.412589
C	3.379946	1.616153	-1.941484
C	3.017067	-0.707172	-2.888147
H	2.335893	-2.761785	-0.504982
C	4.469166	-2.600881	-0.364445
C	2.888871	-2.769285	1.571581
H	3.045753	1.650411	0.911922
C	4.818917	0.512749	1.382745
C	2.626711	0.509102	2.654511
C	-0.941839	3.750476	0.822548
C	0.556050	3.952469	0.376551
H	-1.298055	-3.546068	-0.284659
H	-2.442415	-3.528357	1.054304
C	-2.948840	-4.900582	-0.543852
C	-3.501190	-3.802145	-2.748459
H	-3.499128	-1.650321	-2.711605
H	-1.899773	-2.343327	-2.523840
H	-2.011438	-2.266585	2.719643
H	-1.200227	-0.702517	2.727790
C	-2.716607	-0.933145	4.265069
C	-5.088261	-1.062705	3.388990
H	-5.260712	-0.965293	1.228652
H	-4.448010	-2.403987	1.826334
H	-3.695788	2.276618	0.208637
H	-4.883121	1.162020	0.886215
C	-5.607983	2.237022	-0.827474
C	-4.450426	1.697408	-3.007009
H	-2.557848	1.801925	-1.971638
H	-2.800192	0.301432	-2.838113
H	2.348924	1.919443	-2.143437
H	3.709909	2.197622	-1.073943
C	4.270734	1.960170	-3.149106
C	3.916602	-0.361264	-4.087612
H	3.065051	-1.785337	-2.694502
H	1.974879	-0.492531	-3.137675
H	4.645364	-2.249999	-1.383498
H	5.226370	-2.120612	0.267902
C	4.674632	-4.127757	-0.329679
C	3.067489	-4.296969	1.615327
H	3.648547	-2.309886	2.216542
H	1.919987	-2.500498	2.004807
H	5.082242	-0.490924	1.742423
H	5.305143	0.635461	0.408715
C	5.389312	1.549061	2.368527
C	3.206804	1.536814	3.642566
H	1.546037	0.648387	2.561267
H	2.786267	-0.496335	3.063033
C	-1.100465	3.546140	2.338113
C	-1.901515	4.843501	0.347389
C	1.446929	4.633975	1.416135
C	0.696259	4.683239	-0.969560

H	-2.427971	-5.737216	-0.060124	C	3.393535	-1.868176	0.972963
H	-4.005335	-4.974692	-0.245838	C	3.023034	-0.773559	-1.795177
C	-2.839183	-5.007967	-2.070138	C	3.717970	1.013626	0.465382
H	-4.586124	-3.839587	-2.567191	C	-3.248646	-0.819516	1.718649
H	-3.365614	-3.853393	-3.836282	C	-2.374379	-2.743410	-0.312532
H	-2.012421	-1.332507	5.006549	C	-3.157733	0.133184	-1.097527
H	-2.769616	0.151920	4.438106	O	0.556002	3.512733	0.121985
C	-4.108786	-1.547517	4.466612	O	-1.717648	3.362214	0.418242
H	-5.268831	0.014806	3.517495	H	4.423711	-1.959097	0.597031
H	-6.061020	-1.558106	3.504924	C	2.660434	-3.203024	0.709990
H	-6.419701	1.511860	-0.992018	C	3.467442	-1.596758	2.492962
H	-6.032419	3.041110	-0.211504	H	2.935721	0.227835	-2.237127
C	-5.142977	2.789079	-2.181185	C	1.988088	-1.641417	-2.542740
H	-4.055621	2.117317	-3.940867	C	4.453169	-1.284623	-2.060158
H	-5.188343	0.932205	-3.294175	H	4.693202	0.556417	0.697387
H	4.196824	3.034534	-3.362210	C	3.937849	2.032803	-0.674806
H	5.323935	1.764191	-2.894638	C	3.215457	1.770853	1.716713
C	3.891648	1.143156	-4.391650	H	-4.234899	-1.230450	1.453493
H	3.591733	-0.933839	-4.965893	C	-3.453829	0.630668	2.214820
H	4.951638	-0.672231	-3.875703	C	-2.666195	-1.678166	2.865889
H	3.980053	-4.596325	-1.042688	H	-2.121097	-3.235214	0.637865
H	5.687005	-4.368886	-0.678758	C	-3.763922	-3.262712	-0.733645
C	4.439047	-4.714310	1.068150	C	-1.300308	-3.201359	-1.323486
H	2.941525	-4.654746	2.645444	H	-2.862766	1.150791	-0.802703
H	2.273799	-4.771340	1.019035	C	-4.702311	0.074179	-1.073677
H	6.477311	1.424193	2.446967	C	-2.645142	-0.086662	-2.538165
H	5.217709	2.559251	1.968936	C	-0.029256	4.407439	-0.862809
C	4.734399	1.431556	3.751002	C	-1.494515	4.603225	-0.304070
H	2.940135	2.548481	3.306517	H	1.605688	-3.092235	1.004682
H	2.743590	1.401577	4.628866	H	2.660422	-3.440137	-0.359478
H	-2.126151	3.223298	2.546085	C	3.278209	-4.378217	1.486909
H	-0.914835	4.469327	2.898692	C	4.080643	-2.780691	3.261870
H	-0.421019	2.771099	2.705277	H	4.072820	-0.706213	2.687724
H	-1.927371	4.906535	-0.742813	H	2.461135	-1.384176	2.877911
H	-1.610967	5.822264	0.747886	H	1.984189	-2.665172	-2.146611
H	-2.916314	4.627770	0.699061	H	0.982963	-1.230967	-2.382125
H	1.473397	4.078229	2.356257	C	2.294488	-1.694186	-4.050230
H	1.096913	5.652224	1.624004	C	4.758435	-1.340510	-3.568144
H	2.471267	4.705335	1.034255	H	5.193312	-0.652501	-1.554023
H	1.737830	4.614973	-1.300060	H	4.566829	-2.293699	-1.640239
H	0.436729	5.743989	-0.876613	H	2.969846	2.473155	-0.948406
H	0.071298	4.228224	-1.739943	H	4.341569	1.549089	-1.570093
H	-1.776972	-5.046856	-2.353657	C	4.910200	3.150811	-0.252569
H	-3.292690	-5.943264	-2.422658	C	4.209128	2.859705	2.154344
H	-4.491739	-1.307307	5.466704	H	2.261106	2.243586	1.470107
H	-4.031377	-2.644025	4.416465	H	3.012813	1.090484	2.546417
H	-5.993758	3.211509	-2.731930	H	-2.485245	1.067773	2.475564
H	-4.435282	3.613426	-2.012723	H	-3.871399	1.266035	1.426594
H	4.569232	1.376428	-5.223482	C	-4.371123	0.670160	3.449483
H	2.880925	1.427676	-4.716855	C	-3.571422	-1.635761	4.110452
H	4.526412	-5.808011	1.043975	H	-2.545316	-2.722755	2.554446
H	5.223080	-4.352691	1.749946	H	-1.669051	-1.301817	3.124389
H	5.002725	0.462021	4.197369	H	-4.530015	-2.963544	-0.008739
H	5.124699	2.204425	4.425706	H	-4.046846	-2.816095	-1.695350
C	-0.126770	0.571937	-1.882497	C	-3.761800	-4.795060	-0.885372
O	-0.172139	-0.430718	-2.615942	C	-1.302032	-4.731175	-1.492307
O	-0.111484	1.814200	-2.074352	H	-1.470386	-2.728417	-2.299165
H	0.435949	-2.011423	0.864042	H	-0.307917	-2.873675	-0.983396
H	-0.340175	-2.050502	0.874081	H	-5.049521	-0.923784	-1.365988
				H	-5.088640	0.256563	-0.065967
				C	-5.303924	1.109502	-2.042841
				C	-3.253164	0.930478	-3.518702
				H	-1.551240	-0.024061	-2.558833
				H	-2.916487	-1.097037	-2.874513
				C	0.015340	3.687531	-2.216955
				C	0.813776	5.681222	-0.920375
				C	-2.580538	4.760557	-1.365590
24							
Ru	0.180436	-0.478306	0.255017				
P	2.572512	-0.443170	0.017369				
P	-2.190614	-0.910641	0.153964				
B	-0.477005	2.871893	0.770569				
H	0.032859	0.601569	-0.901355				

C	-1.602719	5.735148	0.728293	C	3.570264	1.331970	0.427191
H	2.704441	-5.292863	1.287381	C	-3.234091	-0.924896	1.758231
H	4.297677	-4.561421	1.115028	C	-2.272066	-2.951467	-0.138080
C	3.332729	-4.091759	2.992222	C	-3.122726	-0.155415	-1.122472
H	5.134086	-2.900501	2.965877	O	0.206797	3.514380	0.044352
H	4.082295	-2.554273	4.335732	O	-2.051036	3.209231	0.358251
H	1.564887	-2.339641	-4.556555	H	4.793192	-1.300605	0.478759
H	2.170531	-0.687651	-4.476916	C	3.477812	-3.004165	0.475594
C	3.723183	-2.187751	-4.322509	C	3.806103	-1.388373	2.391333
H	4.757678	-0.318501	-3.975497	H	2.612404	0.462552	-2.235426
H	5.768382	-1.739425	-3.729716	C	2.026238	-1.564325	-2.469160
H	5.905858	2.712161	-0.085864	C	4.410082	-0.710176	-2.263419
H	5.022171	3.867705	-1.077203	H	4.616713	1.008988	0.543968
C	4.453921	3.867648	1.024525	C	3.535051	2.413521	-0.675154
H	3.821339	3.370674	3.044766	C	3.125699	1.984287	1.759035
H	5.163922	2.397231	2.449349	H	-4.184748	-1.424510	1.514524
H	-4.488666	1.708702	3.784657	C	-3.549304	0.543137	2.128966
H	-5.375733	0.313653	3.173498	C	-2.622605	-1.639100	2.987269
C	-3.817104	-0.197968	4.587409	H	-2.017708	-3.371661	0.845953
H	-3.117758	-2.231674	4.913008	C	-3.636916	-3.554369	-0.533405
H	-4.536216	-2.110767	3.874645	C	-1.182051	-3.455758	-1.115059
H	-3.571047	-5.255189	0.095451	H	-2.893496	0.892694	-0.883388
H	-4.754320	-5.139360	-1.203943	C	-4.665702	-0.287125	-1.147523
C	-2.690265	-5.259902	-1.882423	C	-2.542572	-0.440174	-2.526427
H	-0.556895	-5.024385	-2.243326	C	-0.449438	4.373238	-0.926171
H	-0.991317	-5.196092	-0.544797	C	-1.913499	4.471865	-0.343654
H	-6.399679	1.044585	-2.020603	H	2.457527	-3.257511	0.794489
H	-5.042971	2.120317	-1.696558	H	3.505041	-3.142096	-0.610826
C	-4.787586	0.914362	-3.475705	C	4.458093	-3.988905	1.137649
H	-2.893234	1.937354	-3.262079	C	4.767843	-2.386105	3.059787
H	-2.897255	0.723615	-4.536665	H	4.105439	-0.375839	2.672814
H	1.054023	3.433693	-2.450939	H	2.791236	-1.529061	2.786249
H	-0.371679	4.321624	-3.021969	H	2.265800	-2.564170	-2.080835
H	-0.556045	2.755378	-2.191950	H	0.983713	-1.351864	-2.196517
H	0.923277	6.140055	0.065057	C	2.168222	-1.574479	-4.001740
H	0.366129	6.415279	-1.600506	C	4.543727	-0.714878	-3.797087
H	1.814767	5.443013	-1.294520	H	5.056723	0.066673	-1.837633
H	-2.612374	3.903775	-2.041909	H	4.782731	-1.668166	-1.878787
H	-2.416920	5.667589	-1.958849	H	2.499507	2.753665	-0.802472
H	-3.558428	4.846776	-0.880328	H	3.870950	2.019613	-1.639511
H	-2.579478	5.674782	1.218147	C	4.433176	3.611192	-0.310342
H	-1.510369	6.721404	0.261200	C	4.053272	3.148439	2.144423
H	-0.832831	5.642792	1.500903	H	2.112501	2.370721	1.632723
H	2.308225	-4.013548	3.384979	H	3.073703	1.259571	2.573724
H	3.811418	-4.924406	3.523696	H	-2.619911	1.063718	2.370657
H	3.932849	-2.174849	-5.399789	H	-3.984148	1.083463	1.281939
H	3.810943	-3.236045	-3.999626	C	-4.500753	0.619509	3.335412
H	5.196898	4.617887	1.325705	C	-3.561643	-1.560777	4.204586
H	3.517630	4.406003	0.821962	H	-2.416194	-2.694741	2.771926
H	-4.504307	-0.192841	5.443731	H	-1.663862	-1.168081	3.234181
H	-2.868289	0.231884	4.938077	H	-4.426780	-3.221199	0.150044
H	-2.676245	-6.355541	-1.944861	H	-3.916918	-3.208131	-1.535148
H	-2.948725	-4.892804	-2.886943	C	-3.587207	-5.092778	-0.551067
H	-5.149319	-0.050719	-3.861469	C	-1.128769	-4.993341	-1.153963
H	-5.197140	1.687761	-4.138406	H	-1.378089	-3.069995	-2.124892
C	0.098231	0.662653	1.811440	H	-0.197750	-3.069741	-0.818988
O	0.335724	0.168834	2.908761	H	-4.959560	-1.314914	-1.374381
O	-0.316110	1.990889	1.806643	H	-5.095441	-0.046427	-0.170337
24'				C	-5.281500	0.639821	-2.211731
Ru	0.217252	-0.576227	0.344568	C	-3.173158	0.464136	-3.599373
P	2.617112	-0.278698	0.024422	H	-1.454697	-0.305053	-2.513843
P	-2.142647	-1.077624	0.214733	H	-2.732190	-1.488186	-2.797479
B	-0.773538	2.796539	0.702884	C	-0.381578	3.660663	-2.282594
H	0.028495	0.600050	-0.726088	C	0.307537	5.698975	-0.995073
C	3.786084	-1.538611	0.850313	C	-3.024059	4.583622	-1.385189
C	2.943724	-0.502686	-1.829430	C	-2.070678	5.580406	0.708588
				H	4.193581	-5.015805	0.853535

H	5.472341	-3.809136	0.750111	C	0.822373	-0.781001	0.311786
C	4.463456	-3.835905	2.663163	O	0.990640	-1.281604	1.428307
H	5.800648	-2.142421	2.767821	O	1.755614	-1.080080	-0.677923
H	4.715851	-2.267635	4.149576	C	5.348372	-3.196905	-1.567972
H	1.533974	-2.361996	-4.429317	H	6.411165	-3.427967	-1.438604
H	1.794855	-0.620024	-4.401382	H	4.918753	-3.926819	-2.261292
C	3.628126	-1.768523	-4.437567	H	5.262063	-2.206124	-2.025845
H	4.282288	0.279799	-4.187806	C	4.714339	-4.660438	0.372304
H	5.589197	-0.895328	-4.079315	H	4.431662	-5.414268	-0.369811
H	5.481639	3.277281	-0.292247	H	5.747614	-4.858710	0.680134
H	4.364796	4.371780	-1.100496	H	4.061378	-4.779736	1.239713
C	4.073821	4.222918	1.050039	C	4.607434	-2.383086	2.213151
H	3.720559	3.581874	3.096166	H	5.305165	-3.118519	-2.627978
H	5.074307	2.771583	2.311667	H	4.692937	-1.460022	2.795037
H	-4.697315	1.671416	3.579329	H	3.585002	-2.754073	2.329180
H	-5.471755	0.173031	3.069716	C	6.330430	-1.500028	0.611679
C	-3.921229	-0.110508	4.554448	H	6.446015	-0.650764	1.292993
H	-3.088253	-2.054042	5.063443	H	7.082395	-2.251716	0.878408
H	-4.483659	-2.122460	3.989659	H	6.532911	-1.148455	-0.402705
H	-3.395668	-5.462129	0.467315	P	0.524377	2.427376	0.051641
H	-4.565355	-5.491981	-0.849320	P	-2.205081	-1.444666	-0.231290
C	-2.493781	-5.606249	-1.497549	C	1.968751	2.749993	-1.147164
H	-0.372238	-5.320363	-1.878927	C	-0.659144	3.857225	-0.368215
H	-0.801854	-5.364106	-0.170930	C	1.153566	2.934784	1.771497
H	-6.372598	0.518664	-2.218970	C	-1.969814	-2.750845	-1.573063
H	-5.085649	1.686346	-1.938074	C	-3.894542	-0.706207	-0.652086
C	-4.704985	0.361943	-3.607096	C	-2.311257	-2.454284	1.361200
H	-2.884190	1.506472	-3.405788	H	1.907207	3.820574	-1.391260
H	-2.766140	0.206905	-4.586229	C	1.792076	1.949403	-2.458313
H	0.666173	3.467628	-2.532736	C	3.382734	2.502690	-0.578023
H	-0.817772	4.271848	-3.080437	H	-1.470371	3.727575	0.363917
H	-0.899073	2.698523	-2.249667	C	-1.302114	3.720707	-1.766718
H	0.408650	6.158817	-0.009284	C	-0.098959	5.286154	-0.190503
H	-0.204348	6.404986	-1.659521	H	1.779946	3.832474	1.656386
H	1.313260	5.531304	-1.394092	C	-0.016197	3.280400	2.723977
H	-3.014689	3.740271	-2.078756	C	2.003040	1.815473	2.419705
H	-2.927437	5.510520	-1.962325	H	-2.850295	-3.410841	-1.533412
H	-3.996855	4.598530	-0.882705	C	-0.708660	-3.608571	-1.322253
H	-3.032489	5.453744	1.215221	C	-1.899838	-2.132761	-2.987144
H	-2.047421	6.577156	0.255171	H	-3.791115	-0.499008	-1.726939
H	-1.282160	5.524957	1.465839	C	-5.151002	-1.581071	-0.474646
H	3.477939	-4.123095	3.059195	C	-4.086787	0.666987	0.030342
H	5.193686	-4.519651	3.115026	H	-1.250938	-2.706880	1.510074
H	3.708242	-1.729193	-5.531471	C	-3.115406	-3.771907	1.378222
H	3.965335	-2.771362	-4.135074	C	-2.707535	-1.566992	2.562256
H	4.780789	5.023760	1.304439	H	1.836031	0.880858	-2.223063
H	3.078633	4.683623	0.987013	H	0.801300	2.122982	-2.889716
H	-4.632346	-0.086286	5.390690	C	2.876721	2.307225	-3.488842
H	-3.016045	0.413570	4.891126	C	4.466695	2.870133	-1.607657
H	-2.440647	-6.702164	-1.463812	H	3.543940	3.091326	0.332008
H	-2.758593	-5.338631	-2.531533	H	3.495978	1.446248	-0.305944
H	-5.000056	-0.649063	-3.926305	H	-0.532685	3.852710	-2.539706
H	-5.130479	1.057480	-4.342102	H	-1.707871	2.711788	-1.903566
C	0.044078	0.650344	1.867761	C	-2.402204	4.774883	-1.980220
O	0.357297	0.372392	3.011368	C	-1.193983	6.347837	-0.403026
O	-0.563997	1.908576	1.708659	H	0.348652	5.415712	0.800984
H	0.843688	-2.149250	1.607607	H	0.704963	5.459741	-0.919110
H	0.097026	-2.165015	1.759015	H	-0.674540	2.402406	2.810201
				H	-0.630991	4.093566	2.324970
				C	0.481684	3.680420	4.124857
				C	2.524138	2.230375	3.805969
				H	1.390414	0.912023	2.520520
				H	2.843265	1.531847	1.782675
				H	0.174078	-2.959700	-1.330636
				H	-0.742797	-4.077988	-0.332931
				C	-0.542718	-4.695693	-2.397679
				C	-1.728175	-3.213455	-4.068943
25							
Ru	-0.696740	0.369761	-0.006451				
H	-0.635341	0.457442	-1.583751				
C	4.920094	-2.070768	0.743336				
C	4.584804	-3.266363	-0.238451				
B	2.921635	-1.713651	-0.276008				
O	3.183959	-3.030885	-0.549123				
O	3.968650	-1.054282	0.322848				

H	-2.802332	-1.549838	-3.207229	O	-1.124223	-1.603183	-0.688349
H	-1.056727	-1.431171	-3.023222	C	-4.789900	-3.624781	-1.414687
H	-5.026763	-2.544385	-0.984052	H	-5.436116	-4.507955	-1.458708
H	-5.297723	-1.804082	0.590396	H	-5.399776	-2.741328	-1.628467
C	-6.406332	-0.864080	-1.005490	H	-4.031747	-3.709401	-2.199790
C	-5.346235	1.382377	-0.488978	C	-5.224990	-3.343250	1.042406
H	-4.163874	0.540409	1.117940	H	-5.939730	-2.562362	0.762142
H	-3.204633	1.301499	-0.149128	H	-5.777097	-4.284814	1.144497
H	-4.184999	-3.565666	1.248141	H	-4.800148	-3.079807	2.013566
H	-2.820089	-4.423453	0.548258	C	-2.730696	-4.704460	1.763508
C	-2.909987	-4.517813	2.710515	H	-3.552525	-5.217134	2.274840
C	-2.509610	-2.310643	3.893394	H	-1.824771	-5.307594	1.879804
H	-2.114398	-0.643315	2.559513	H	-2.554728	-3.739654	2.248337
H	-3.762098	-1.269111	2.472936	C	-3.215679	-5.883427	-0.403699
H	2.736091	1.702740	-4.394532	H	-2.368747	-6.536177	-0.168599
H	2.762298	3.358706	-3.795038	H	-4.128023	-6.368304	-0.037506
C	4.287409	2.098680	-2.921773	H	-3.279906	-5.793062	-1.490485
H	4.423423	3.950980	-1.811892	P	2.709377	-0.615108	0.161985
H	5.458638	2.673206	-1.180223	P	-1.247233	2.097058	-0.277254
H	-2.827524	4.669717	-2.986825	C	2.746552	-2.488164	-0.106866
H	-3.223994	4.587760	-1.272568	C	4.111502	0.025955	-0.945813
C	-1.869540	6.200285	-1.773737	C	3.436543	-0.454820	1.915743
H	-1.951366	6.247496	0.388830	C	-1.825152	2.289872	-2.066761
H	-0.763384	7.352043	-0.295791	C	-0.870487	3.890139	0.217039
H	1.050562	4.619064	4.046029	C	-2.807647	1.497291	0.604120
H	-0.378820	3.892108	4.773356	H	3.812548	-2.760028	-0.107136
C	1.373255	2.600190	4.750332	C	2.146873	-2.880502	-1.475692
H	3.118574	1.412428	4.232988	C	2.075669	-3.303401	1.022155
H	3.202944	3.091044	3.703801	H	4.346191	0.993672	-0.479771
H	0.372329	-5.267485	-2.198077	C	3.694245	0.346059	-2.398820
H	-1.379986	-5.407693	-2.333776	C	5.406125	-0.815962	-0.948155
C	-0.496470	-4.091105	-3.807490	H	4.011041	-1.371569	2.116255
H	-1.656054	-2.737065	-5.055490	C	4.384360	0.745582	2.126914
H	-2.627187	-3.847993	-4.093920	C	2.272271	-0.364930	2.932264
H	-6.311875	-0.726833	-2.092877	H	-2.687509	2.971378	-2.050978
H	-7.291404	-1.493439	-0.845721	C	-2.292886	0.943620	-2.662310
C	-6.597959	0.504807	-0.335865	C	-0.743924	2.925500	-2.967867
H	-5.481335	2.334700	0.040126	H	-0.030863	4.117837	-0.457791
H	-5.205519	1.630699	-1.551351	C	-1.953149	4.962458	-0.027280
H	-3.504672	-5.440862	2.715113	C	-0.316011	4.026312	1.652495
H	-1.856478	-4.823018	2.792039	H	-2.873756	0.466423	0.231809
C	-3.277549	-3.640515	3.916445	C	-4.156906	2.173407	0.278912
H	-1.436815	-2.503255	4.035045	C	-2.628672	1.391314	2.135439
H	-2.827897	-1.672682	4.728466	H	1.095658	-2.572219	-1.505708
H	4.446230	1.026858	-2.732815	H	2.653937	-2.344852	-2.285496
H	5.046261	2.406538	-3.653248	C	2.251531	-4.394939	-1.729933
H	-2.681178	6.931640	-1.879568	H	2.192345	-4.815796	0.758716
H	-1.137550	6.428796	-2.562785	C	2.539970	-3.076258	1.988351
H	1.760255	2.940445	5.719772	H	1.018790	-3.029899	1.107003
H	0.769505	1.702631	4.949203	H	3.460678	-0.581522	-2.937171
H	-0.425567	-4.884350	-4.563286	H	2.777701	0.943638	-2.405474
H	0.411452	-3.478775	-3.905887	C	4.823400	1.080880	-3.142551
H	-7.472987	1.015669	-0.757525	C	6.542228	-0.087480	-1.689267
H	-6.807784	0.357235	0.734063	H	5.724798	-1.058699	0.073240
H	-4.358685	-3.434838	3.896907	H	5.216904	-1.773935	-1.450936
H	-3.080088	-4.178865	4.852443	H	3.853566	1.677706	1.882025
				H	5.248461	0.689639	1.457268
				C	4.891107	0.819455	3.579485
				C	2.774619	-0.303648	4.383265
				H	1.697872	0.550639	2.715839
				H	1.564752	-1.188239	2.808432
				H	-1.463176	0.228567	-2.624543
				H	-3.095339	0.509085	-2.055804
				C	-2.778489	1.104015	-4.113066
				C	-1.231919	3.079020	-4.419130
				H	-0.445751	3.909072	-2.584561
				H	0.152097	2.291278	-2.947551
25'							
Ru	0.691743	0.680392	0.008099				
H	0.673797	0.448296	-1.545644				
C	-3.016805	-4.525654	0.266158				
C	-4.144968	-3.459493	-0.031550				
B	-2.079422	-2.540415	-0.326773				
O	-3.391403	-2.215691	-0.069366				
O	-1.839118	-3.892734	-0.308386				
C	-0.498421	-0.891566	0.337699				
O	-0.754435	-1.249593	1.490644				

H	-2.355426	4.894802	-1.044471	O	-0.202825	-2.372167	0.582943
H	-2.795885	4.796579	0.655855	O	-1.911181	-0.913672	0.465856
C	-1.392754	6.377500	0.211914	C	-5.920922	-1.878277	-0.426826
C	0.254981	5.434449	1.893938	H	-6.721809	-2.508575	-0.827964
H	-1.116798	3.840941	2.378897	H	-6.378261	-1.030040	0.092719
H	0.455143	3.268904	1.837322	H	-5.335313	-1.486121	-1.264510
H	-4.173734	3.194652	0.681104	C	-5.874818	-3.177766	1.719988
H	-4.311821	2.257799	-0.802575	H	-6.458507	-2.359387	2.154512
C	-5.317189	1.369996	0.897217	H	-6.575482	-3.947682	1.376078
C	-3.782200	0.587793	2.759085	H	-5.250578	-3.601365	2.510048
H	-1.675690	0.910658	2.374857	C	-3.619817	-4.818752	0.816102
H	-2.617476	2.397120	2.576900	H	-4.429343	-5.506768	1.083428
H	1.783960	-4.636066	-2.693536	H	-2.826574	-5.389334	0.323917
H	3.311967	-4.678272	-1.817391	H	-3.203434	-4.393427	1.734445
C	1.599531	-5.205430	-0.601978	C	-4.666222	-4.337247	-1.414447
H	3.252711	-5.110575	0.793873	H	-3.933511	-5.030726	-1.839718
H	1.689710	-5.364495	1.566150	H	-5.582965	-4.900136	-1.203089
H	4.516864	1.282587	-4.177176	H	-4.888092	-3.579074	-2.169134
H	4.989394	2.060812	-2.669541	P	2.636808	-0.986557	0.143861
C	6.134279	0.280713	-3.123235	P	-1.022317	2.030229	-0.320969
H	6.804391	0.828324	-1.138534	C	2.857343	-2.672707	-0.710808
H	7.443333	-0.714583	-1.697933	C	4.062656	0.011393	-0.622812
H	5.514413	-0.063821	3.783986	C	3.228026	-1.206724	1.936298
H	5.543982	1.694471	3.696159	C	-2.056354	2.098776	-1.904019
C	3.740450	0.869564	4.593644	C	-0.004591	3.628273	-0.449893
H	1.919583	-0.224394	5.066650	C	-2.316019	2.210107	1.046030
H	3.285567	-1.246434	4.630756	H	3.896225	-2.668698	-1.072528
H	-3.072746	0.124324	-4.511417	C	1.927440	-2.795684	-1.940148
H	-3.682177	1.732415	-4.131837	C	2.698661	-3.918484	0.185669
C	-1.703424	1.740992	-5.003763	H	3.995013	0.982864	-0.109543
H	-0.428243	3.504411	-5.034515	C	3.834118	0.291364	-2.125384
H	-2.062537	3.800493	-4.449121	C	5.492936	-0.529722	-0.404827
H	-0.616014	6.588849	-0.538046	H	4.099797	-1.877845	1.933576
H	-2.184969	7.121654	0.057229	C	3.660633	0.142966	2.556580
C	-0.793830	6.522286	1.618590	C	2.128725	-1.832862	2.826523
H	0.624875	5.515156	2.924396	H	-2.615201	3.046474	-1.875339
H	1.123425	5.590155	1.236335	C	-3.078811	0.943072	-1.975998
H	-6.272484	1.862826	0.671950	C	-1.190321	2.100599	-3.183241
H	-5.351169	0.378492	0.423219	H	0.440528	3.537581	-1.451590
C	-5.148224	1.199384	2.414399	C	-0.738818	4.982946	-0.402356
H	-3.729844	-0.442165	2.382018	C	1.181815	3.626379	0.541865
H	-3.652498	0.535478	3.848123	H	-2.744916	1.200183	1.036203
H	0.519351	-5.009751	-0.593679	C	-3.480696	3.209650	0.877662
H	1.732121	-6.281047	-0.780672	C	-1.659921	2.381875	2.433171
H	6.936488	0.847403	-3.613306	H	0.890694	-2.796210	-1.588770
H	6.001278	-0.641927	-3.707658	H	2.033287	-1.925827	-2.597018
H	4.135661	0.866861	5.617705	C	2.214361	-4.083293	-2.731154
H	3.191635	1.815390	4.471720	C	2.991680	-5.207539	-0.603070
H	-2.083786	1.883099	-6.023767	H	3.373474	-3.866314	1.048438
H	-0.845216	1.057246	-5.079244	H	1.673179	-3.949893	0.567472
H	-0.352834	7.519547	1.743980	H	3.894826	-0.650913	-2.687244
H	-1.599287	6.440826	2.363564	H	2.823974	0.685020	-2.287031
H	-5.238755	2.183268	2.899914	C	4.886029	1.265828	-2.682096
H	-5.958970	0.578443	2.817937	C	6.551660	0.441423	-0.959972
H	1.669269	2.081825	-0.637704	H	5.689161	-0.715185	0.657174
H	1.790149	2.175350	0.174366	H	5.602091	-1.497552	-0.913247
				H	2.808492	0.839962	2.520673
				H	4.464943	0.608889	1.978779
				C	4.125363	-0.014106	4.015624
				C	2.605747	-2.014959	4.276563
				H	1.248733	-1.174796	2.816494
				H	1.785178	-2.785087	2.420379
				H	-2.535519	-0.009142	-1.977033
				H	-3.720319	0.931689	-1.088057
				C	-3.949895	1.038140	-3.240124
				C	-2.053706	2.183256	-4.454873
				H	-0.485868	2.940635	-3.180606

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Ru	0.633754	0.326889	-0.002282
H	0.550973	-0.004572	-1.539170
C	-4.100238	-3.716703	-0.138333
C	-5.032076	-2.646852	0.560959
B	-2.904968	-1.852565	0.365491
O	-4.069106	-1.698756	1.090841
O	-2.933757	-2.927680	-0.488878
C	-0.525280	-1.215010	0.359285

H	-0.586369	1.184047	-3.203655	O	-1.859988	-1.058217	-0.103224
H	-1.565227	5.002791	-1.122974	C	-4.504504	-3.742888	1.913868
H	-1.183334	5.124549	0.591417	H	-5.471372	-4.241307	2.043206
C	0.225451	6.150795	-0.681399	H	-3.803060	-4.153221	2.646872
C	2.143906	4.797826	0.277054	H	-4.632229	-2.677351	2.131410
H	0.809967	3.688812	1.572916	C	-3.761501	-5.456643	0.239289
H	1.735623	2.675564	0.473575	H	-3.185634	-5.909335	1.052841
H	-3.108901	4.241315	0.904247	H	-4.734367	-5.959820	0.190132
H	-3.973549	3.079137	-0.092435	H	-3.223628	-5.640210	-0.693459
C	-4.516956	3.024167	2.002637	C	-4.520561	-3.757064	-2.020296
C	-2.691616	2.207140	3.560658	H	-5.063866	-4.700861	-2.137532
H	-0.847579	1.653634	2.558651	H	-4.902529	-3.045045	-2.758802
H	-1.208699	3.381345	2.515719	H	-3.462916	-3.935906	-2.238991
H	1.523212	-4.154545	-3.581317	C	-6.188160	-2.921556	-0.340683
H	3.228879	-4.036480	-3.157084	H	-6.622524	-2.333248	-1.155820
C	2.095769	-5.329976	-1.843671	H	-6.734233	-3.870118	-0.279928
H	4.047501	-5.213119	-0.915224	H	-6.341248	-2.370613	0.590190
H	2.856588	-6.077848	0.052813	P	-1.200996	2.080905	-0.129392
H	4.713214	1.427179	-3.754183	P	2.716747	-0.747166	0.246779
H	4.764917	2.245594	-2.195389	C	-2.788329	2.017658	0.927099
C	6.314060	0.753973	-2.444208	C	-0.610376	3.839161	0.305126
H	6.519462	1.377540	-0.382513	C	-1.752258	2.300161	-1.934848
H	7.555097	0.020413	-0.814165	C	3.145916	-1.430501	1.956574
H	5.043174	-0.620734	4.033265	C	4.212893	0.376078	-0.114092
H	4.395324	0.969076	4.423382	C	2.825158	-2.263528	-0.873993
C	3.059645	-0.684900	4.891613	H	-2.954627	3.065544	1.213179
H	1.799429	-2.456837	4.876073	C	-2.568996	1.222225	2.233080
H	3.440513	-2.731873	4.300319	C	-4.081667	1.553837	0.226746
H	-4.654476	0.196245	-3.266916	H	0.308572	3.955509	-0.285765
H	-4.559851	1.953337	-3.196988	C	-0.204064	3.964156	1.790783
C	-3.094667	1.057107	-4.513572	C	-1.550155	5.005737	-0.073846
H	-1.405993	2.152453	-5.340786	H	-2.610234	2.987816	-1.944716
H	-2.570221	3.154808	-4.479672	C	-0.623901	2.929943	-2.787979
H	0.603137	6.070445	-1.711526	C	-2.188823	0.969938	-2.589858
H	-0.315267	7.104151	-0.620457	H	4.140667	-1.892259	1.868548
C	1.409801	6.147205	0.295974	C	2.168635	-2.520377	2.447713
H	2.953001	4.792690	1.018872	C	3.236238	-0.296233	3.002706
H	2.617575	4.657289	-0.705922	H	3.980314	1.262599	0.494934
H	-5.331482	3.750585	1.881210	C	5.623481	-0.090620	0.310575
H	-4.968470	2.025632	1.911966	C	4.238364	0.846564	-1.585238
C	-3.878679	3.167395	3.392015	H	2.111984	-2.928694	-0.374828
H	-3.056675	1.170526	3.550380	C	4.174994	-2.997616	-0.983493
H	-2.210367	2.363472	4.535193	C	2.234021	-2.010424	-2.278811
H	1.050532	-5.444144	-1.522649	H	-2.393852	0.171860	1.981458
H	2.352814	-6.233083	-2.413140	H	-1.665828	1.568829	2.747372
H	7.048788	1.486975	-2.801671	C	-3.782993	1.346025	3.169992
H	6.471901	-0.160589	-3.035195	C	-5.292193	1.695885	1.167436
H	3.443380	-0.838092	5.908605	H	-4.264080	2.141987	-0.680637
H	2.190966	-0.015520	4.981327	H	-3.990338	0.507765	-0.077640
H	-3.729407	1.169729	-5.402109	H	-1.096007	3.870753	2.426062
H	-2.578046	0.091554	-4.615028	H	0.465376	3.144671	2.074623
H	2.105951	6.960824	0.055643	C	0.464060	5.320362	2.076809
H	1.038840	6.342957	1.313125	C	-0.888977	6.368475	0.209009
H	-3.529055	4.202825	3.523675	H	-1.838242	4.955432	-1.129526
H	-4.626865	2.989039	4.175097	H	-2.481547	4.940712	0.505068

TS25_26'

Ru	0.655823	0.539648	0.044352
H	0.518210	0.563463	1.609077
C	-4.704621	-3.162625	-0.616254
C	-3.931878	-3.961453	0.506066
B	-2.759262	-2.094705	-0.069999
O	-2.619794	-3.342511	0.486178
O	-4.018600	-1.884812	-0.610092
C	-0.442784	-1.190083	0.084399
O	-0.029135	-2.329611	0.190990

O	-1.859988	-1.058217	-0.103224
C	-4.504504	-3.742888	1.913868
H	-5.471372	-4.241307	2.043206
H	-3.803060	-4.153221	2.646872
H	-4.632229	-2.677351	2.131410
C	-3.761501	-5.456643	0.239289
H	-3.185634	-5.909335	1.052841
H	-4.734367	-5.959820	0.190132
H	-3.223628	-5.640210	-0.693459
C	-4.520561	-3.757064	-2.020296
H	-5.063866	-4.700861	-2.137532
H	-4.902529	-3.045045	-2.758802
H	-3.462916	-3.935906	-2.238991
C	-6.188160	-2.921556	-0.340683
H	-6.622524	-2.333248	-1.155820
H	-6.734233	-3.870118	-0.279928
H	-6.341248	-2.370613	0.590190
P	-1.200996	2.080905	-0.129392
P	2.716747	-0.747166	0.246779
C	-2.788329	2.017658	0.927099
C	-0.610376	3.839161	0.305126
C	-1.752258	2.300161	-1.934848
C	3.145916	-1.430501	1.956574
C	4.212893	0.376078	-0.114092
C	2.825158	-2.263528	-0.873993
H	-2.954627	3.065544	1.213179
C	-2.568996	1.222225	2.233080
C	-4.081667	1.553837	0.226746
H	0.308572	3.955509	-0.285765
C	-0.204064	3.964156	1.790783
C	-1.550155	5.005737	-0.073846
H	-2.610234	2.987816	-1.944716
C	-0.623901	2.929943	-2.787979
C	-2.188823	0.969938	-2.589858
H	4.140667	-1.892259	1.868548
C	2.168635	-2.520377	2.447713
C	3.236238	-0.296233	3.002706
H	3.980314	1.262599	0.494934
C	5.623481	-0.090620	0.310575
C	4.238364	0.846564	-1.585238
H	2.111984	-2.928694	-0.374828
C	4.174994	-2.997616	-0.983493
C	2.234021	-2.010424	-2.278811
H	-2.393852	0.171860	1.981458
H	-1.665828	1.568829	2.747372
C	-3.782993	1.346025	3.169992
C	-5.292193	1.695885	1.167436
H	-4.264080	2.141987	-0.680637
H	-3.990338	0.507765	-0.077640
H	-1.096007	3.870753	2.426062
H	0.465376	3.144671	2.074623
C	0.464060	5.320362	2.076809
C	-0.888977	6.368475	0.209009
H	-1.838242	4.955432	-1.129526
H	-2.481547	4.940712	0.505068
H	0.256055	2.269063	-2.758119
H	-0.300731	3.892175	-2.378407
C	-1.056456	3.133121	-4.250981
C	-2.640366	1.176447	-4.045476
H	-1.339868	0.272368	-2.573676
H	-2.981297	0.484411	-2.018711
H	1.154674	-2.108057	2.489860
H	2.124658	-3.352389	1.738220
C	2.575490	-3.052866	3.832725
C	3.635658	-0.828066	4.390189
H	3.953043	0.472789	2.689918
H	2.257597	0.196708	3.067482

H	5.636001	-0.390535	1.363307	O	1.182193	-1.199412	1.622711
H	5.922058	-0.971525	-0.269395	O	1.660344	-0.963658	-0.589194
C	6.662577	1.026060	0.094884	C	4.725617	-3.537049	-2.079947
C	5.273748	1.962704	-1.804451	H	5.757678	-3.895590	-2.157020
H	4.489907	-0.001700	-2.235624	H	4.079206	-4.226705	-2.631903
H	3.242893	1.191037	-1.893687	H	4.661916	-2.556373	-2.562444
H	4.900391	-2.373316	-1.522261	C	4.347768	-4.853357	0.025524
H	4.599543	-3.190902	0.008947	H	3.841857	-5.592138	-0.605006
C	4.013572	-4.325627	-1.746483	H	5.393893	-5.162439	0.134404
C	2.075455	-3.333350	-3.048678	H	3.873990	-4.868077	1.009529
H	1.258624	-1.520018	-2.183991	C	4.869430	-2.523540	1.722820
H	2.882072	-1.336066	-2.854533	H	5.543961	-3.328112	2.034915
H	-3.616481	0.743027	4.072267	H	5.179557	-1.601464	2.224794
H	-3.879487	2.389779	3.506735	H	3.854170	-2.757599	2.056583
C	-5.084689	0.920315	2.475706	C	6.326724	-1.915942	-0.232460
H	-5.455658	2.759731	1.398726	H	6.680652	-1.073401	0.370539
H	-6.197737	1.344669	0.655711	H	7.020960	-2.751541	-0.085634
H	0.724963	5.389858	3.140862	H	6.358713	-1.615631	-1.282396
H	1.410139	5.380716	1.518037	P	-2.316036	-1.429331	-0.045477
C	-0.440507	6.492944	1.671895	P	0.640889	2.347578	0.064078
H	-0.015754	6.487023	-0.449851	C	-3.073922	-1.825467	1.647460
H	-1.584295	7.178490	-0.047279	C	-3.799694	-0.923677	-1.117024
H	-1.867879	3.875705	-4.282806	C	-1.946872	-3.199758	-0.671359
H	-0.223078	3.558894	-4.825306	C	1.811457	2.596147	1.528286
C	-1.540027	1.827087	-4.893692	C	-0.474517	3.869630	0.247099
H	-2.935352	0.211542	-4.477635	C	1.752899	2.532027	-1.454008
H	-3.538300	1.812564	-4.063213	H	-3.879910	-2.549747	1.453156
H	1.849991	-3.808531	4.160542	C	-3.693064	-0.589046	2.334269
H	3.547043	-3.565308	3.757772	C	-2.047899	-2.499945	2.587388
C	2.678775	-1.927460	4.870331	H	-3.470583	-1.196854	-2.128791
H	3.659725	0.001402	5.109277	C	-4.013016	0.603546	-1.149985
H	4.658741	-1.231463	4.345188	C	-5.127289	-1.662401	-0.847855
H	6.430578	1.868038	0.764331	H	-2.598558	-3.861337	-0.079574
H	7.658558	0.665202	0.383022	C	-2.256624	-3.459412	-2.163092
C	6.675386	1.523494	-1.357226	C	-0.475833	-3.581956	-0.397606
H	5.285376	2.259023	-2.861481	H	2.092716	3.661093	1.515828
H	4.971529	2.852865	-1.232585	C	3.107568	1.760211	1.445260
H	4.986577	-4.827167	-1.833385	C	1.104568	2.301365	2.872037
H	3.363909	-4.996949	-1.166481	H	-0.712470	3.836838	1.320553
C	3.402029	-4.102805	-3.137749	C	0.127776	5.258623	-0.045612
H	1.326824	-3.952183	-2.534368	C	-1.815176	3.706762	-0.496309
H	1.683556	-3.135218	-4.055128	H	2.323802	1.593228	-1.393777
H	-5.037567	-0.154949	2.248470	C	2.772789	3.689574	-1.525867
H	-5.941584	1.063437	3.147090	C	0.938581	2.465005	-2.765515
H	0.075628	7.448348	1.832012	H	-2.913060	0.171383	2.463588
H	-1.328121	6.504684	2.321950	H	-4.466031	-0.139195	1.700704
H	-1.896653	2.013570	-5.914993	C	-4.302594	-0.934575	3.704106
H	-0.691827	1.131529	-4.979346	C	-2.655239	-2.824531	-2.823847
H	3.009595	-2.325640	5.838531	H	-1.680295	-3.430372	2.142116
H	1.681525	-1.492758	5.032559	H	-1.175427	-1.845618	2.706422
H	7.389543	2.349074	-1.471892	H	-4.284934	0.976571	-0.154493
H	7.025863	0.713292	-2.013995	H	-3.069484	1.094407	-1.424069
H	4.111568	-3.530752	-3.754861	C	-5.105861	0.999198	-2.158693
H	3.251836	-5.064167	-3.645875	C	-6.212484	-1.259973	-1.862944
H	1.703944	1.961672	0.554238	H	-4.978390	-2.749061	-0.875588
H	1.712345	2.072530	-0.249865	H	-5.485838	-1.424508	0.161761
				H	-1.653557	-2.780131	-2.784605
				H	-3.306525	-3.253906	-2.395059
				C	-1.949923	-4.917171	-2.558885
				C	-0.176737	-5.042425	-0.765686
				H	0.170225	-2.931534	-0.995664
				H	-0.200034	-3.399298	0.643790
				H	2.858338	0.696112	1.462267
				H	3.642329	1.939012	0.507622
				C	4.040070	2.070121	2.629747
				C	2.027268	2.604781	4.066013
				H	0.180551	2.884124	2.970747

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Ru	-0.666324	0.349717	-0.056201
H	-1.204179	0.727417	1.376215
C	4.914437	-2.299011	0.204759
C	4.251388	-3.472941	-0.621313
B	2.803440	-1.722221	-0.416862
O	2.853984	-3.075795	-0.654702
O	4.023549	-1.185469	-0.076434
C	0.823687	-0.719162	0.560451

H	0.813416	1.244633	2.887331
H	1.079943	5.396171	0.479847
H	0.343438	5.343557	-1.118601
C	-0.852481	6.380242	0.343386
C	-2.801324	4.832009	-0.135556
H	-1.644953	3.707396	-1.582293
H	-2.257419	2.737270	-0.240889
H	2.250388	4.646885	-1.630827
H	3.362868	3.755633	-0.605783
C	3.710836	3.509113	-2.733807
C	1.860842	2.308193	-3.987252
H	0.225773	1.630428	-2.728326
H	0.342969	3.382732	-2.879316
H	-4.711350	-0.024678	4.163118
H	-5.150472	-1.622852	3.565755
C	-3.268131	-1.586788	4.629893
H	-3.435656	-3.592059	3.846099
H	-1.881807	-3.263014	4.607532
H	-5.262582	2.085446	-2.131613
H	-4.761229	0.757615	-3.175294
C	-6.424578	0.260689	-1.885856
H	-5.916467	-1.600450	-2.866419
H	-7.153219	-1.773098	-1.624558
H	-2.638915	-5.581879	-2.016222
H	-2.161155	-5.056962	-3.627443
C	-0.505045	-5.319306	-2.237747
H	0.880686	-5.249363	-0.564586
H	-0.764258	-5.717758	-0.124552
H	4.946212	1.455285	2.549909
H	4.368295	3.119863	2.576444
C	3.344440	1.821578	3.974992
H	1.506291	2.366721	5.002646
H	2.245853	3.683429	4.095294
H	-1.017381	6.357246	1.430721
H	-0.408915	7.358141	0.115135
C	-2.197964	6.222845	-0.380392
H	-3.730088	4.712708	-0.708744
H	-3.074688	4.738496	0.925945
H	4.426127	4.340933	-2.777123
H	4.303143	2.592379	-2.598278
C	2.921667	3.417736	-4.048225
H	2.360973	1.330509	-3.930099
H	1.262984	2.301310	-4.908116
H	-2.472333	-0.860802	4.851500
H	-3.727350	-1.855137	5.590374
H	-7.174877	0.530418	-2.640027
H	-6.826611	0.584299	-0.914163
H	-0.343575	-6.377497	-2.482453
H	0.182538	-4.740458	-2.871712
H	4.008315	2.092797	4.806585
H	3.131022	0.748081	4.074952
H	-2.898685	7.003631	-0.057932
H	-2.045008	6.367100	-1.460479
H	2.426277	4.381938	-4.238019
H	3.602639	3.246159	-4.891811

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Ru	-0.317486	0.946212	-0.010728
H	-0.453355	1.589518	1.411927
C	1.932424	-4.765695	0.350771
C	0.798342	-5.283342	-0.621709
B	0.587604	-3.039730	-0.271728
O	-0.120189	-4.158130	-0.651403
O	1.864888	-3.326809	0.160291
C	-0.033281	-0.889182	0.747744
O	0.009195	-1.427934	1.836401

O	0.078211	-1.771495	-0.407394
C	1.281704	-5.500720	-2.062178
H	1.931662	-6.378429	-2.145275
H	0.411156	-5.654630	-2.707631
H	1.826964	-4.627965	-2.435625
C	0.036868	-6.514340	-0.132413
H	-0.742387	-6.775737	-0.855896
H	0.707746	-7.375417	-0.031227
H	-0.445192	-6.331692	0.830609
C	1.630524	-5.029678	1.832590
H	1.704555	-6.094720	2.078053
H	2.355161	-4.482328	2.443127
H	0.633122	-4.671122	2.103578
C	3.344730	-5.237689	0.009961
H	4.057988	-4.795482	0.713299
H	3.422773	-6.328108	0.091747
H	3.640045	-4.942522	-0.999832
P	-2.676710	0.503185	0.022810
P	2.045268	1.431144	0.082944
C	-3.868306	1.920326	-0.403521
C	-3.119739	-0.869141	-1.198724
C	-3.431198	-0.088493	1.670951
C	2.868145	1.425423	1.783535
C	2.431590	3.192101	-0.535042
C	3.086441	0.191184	-0.890128
H	-4.873051	1.472673	-0.368951
C	-3.661015	2.496605	-1.820660
C	-3.831737	3.057634	0.641597
H	-2.761449	-1.765813	-0.675989
C	-2.294712	-0.798678	-2.503203
C	-4.616288	-1.067560	-1.516137
H	-4.467114	0.286743	1.666153
C	-3.496258	-1.623345	1.853175
C	-2.694726	0.526530	2.885880
H	3.894205	1.787525	1.627560
C	2.967934	0.026471	2.431602
C	2.160723	2.400214	2.751672
H	1.636430	3.771408	-0.041682
C	3.774855	3.843203	-0.131214
C	2.220060	3.354557	-2.057056
H	2.962674	-0.717693	-0.284423
C	4.598372	0.469379	-1.013571
C	2.485240	-0.146486	-2.273269
H	-2.642853	2.898015	-1.907715
H	-3.749260	1.708010	-2.573829
C	-4.668603	3.614622	-2.143157
C	-4.833722	4.178023	0.310227
H	-4.053219	2.668463	1.640049
H	-2.816753	3.476702	0.687592
H	-2.577701	0.082907	-3.092794
H	-1.232072	-0.699568	-2.259532
C	-2.508022	-2.065051	-3.350886
C	-4.833637	-2.332305	-2.368284
H	-5.209732	-1.132892	-0.595875
H	-4.997664	-0.198084	-2.069620
H	-2.479350	-2.033415	1.845318
H	-4.044259	-2.097326	1.032899
C	-4.185756	-1.997116	3.179192
C	-3.395900	0.170636	4.207453
H	-1.670676	0.138156	2.898249
H	-2.612240	1.613705	2.788929
H	1.964833	-0.387794	2.575660
H	3.502815	-0.670534	1.776589
C	3.696665	0.100490	3.785545
C	2.879549	2.471908	4.109715
H	2.093738	3.407072	2.320642
H	1.129325	2.056828	2.899360

H	3.935909	3.778990	0.949301	O	0.306550	0.031015	3.057625
H	4.609031	3.310530	-0.604967	O	0.300415	2.023663	2.029641
C	3.818072	5.325094	-0.551218	C	-0.652084	3.600999	-1.870245
C	2.249841	4.834405	-2.475948	H	-0.703756	4.422518	-2.592372
H	3.017440	2.823022	-2.593352	H	-0.866933	2.667141	-2.395621
H	1.274311	2.897439	-2.370156	H	-1.428120	3.754671	-1.114600
H	4.758331	1.359316	-1.637430	C	1.788969	3.291875	-2.316763
H	5.040096	0.686890	-0.033673	H	1.512852	2.433303	-2.938346
C	5.331513	-0.723302	-1.654863	H	1.852898	4.171357	-2.967830
C	3.216882	-1.343002	-2.906503	H	2.777817	3.101454	-1.895184
H	1.420716	-0.379860	-2.166655	C	2.535325	4.942507	-0.011821
H	2.562185	0.717001	-2.945556	H	3.002959	5.393300	-0.893657
H	-4.468055	4.011106	-3.146992	H	2.656938	5.628527	0.831895
H	-5.683691	3.191010	-2.171951	H	3.068772	4.018080	0.230565
C	-4.620542	4.739170	-1.101171	C	0.331524	6.004406	-0.552085
H	-5.856843	3.781117	0.389822	H	0.581444	6.747807	0.211477
H	-4.750726	4.977097	1.058227	H	0.655200	6.394675	-1.523979
H	-1.938436	-1.986636	-4.286404	H	-0.754625	5.889611	-0.563817
H	-2.099709	-2.926994	-2.804310	P	2.292743	-0.920648	-0.018034
C	-3.995619	-2.299449	-3.654958	P	-2.411211	-0.194380	0.191309
H	-4.554988	-3.215886	-1.775640	C	2.589931	-2.703402	0.563628
H	-5.899351	-2.440552	-2.609733	C	2.709945	-0.949448	-1.868101
H	-5.237751	-1.674632	3.141410	C	3.838271	-0.089228	0.751085
H	-4.199152	-3.089706	3.286785	C	-3.272936	-0.083203	1.871073
C	-3.501199	-1.349250	4.389524	C	-2.908048	-1.935400	-0.382926
H	-2.846519	0.617437	5.046512	C	-3.412227	1.057377	-0.850206
H	-4.404371	0.612761	4.223639	H	3.618344	-2.947190	0.255408
H	3.739483	-0.901229	4.232211	C	1.638568	-3.727445	-0.090018
H	4.739165	0.416519	3.624889	C	2.513688	-2.810962	2.104084
C	3.014591	1.082695	4.747863	H	3.000312	0.092553	-2.060574
H	2.334860	3.150191	4.779577	C	1.457033	-1.202602	-2.735772
H	3.880973	2.907685	3.971500	C	3.875558	-1.851985	-2.320984
H	3.055873	5.879310	0.016681	H	4.547215	-0.914303	0.921470
H	4.787788	5.758358	-0.273587	C	4.549853	0.948519	-0.143802
C	3.561858	5.509650	-2.053151	C	3.524099	0.564915	2.116644
H	2.110310	4.916264	-3.561769	H	-4.344755	-0.237854	1.680112
H	1.401905	5.358628	-2.010309	C	-3.104769	1.319670	2.500128
H	6.399514	-0.490677	-1.759680	C	-2.814794	-1.182450	2.857028
H	5.263152	-1.589931	-0.981455	H	-2.518207	-2.536805	0.449598
C	4.727933	-1.091416	-3.018352	C	-4.408358	-2.263079	-0.524356
H	3.041971	-2.230863	-2.282803	C	-2.136699	-2.408732	-1.633472
H	2.792243	-1.558339	-3.895895	H	-2.935829	2.011047	-0.578620
H	-3.641143	5.238204	-1.150160	C	-4.924717	1.213742	-0.566343
H	-5.373912	5.504643	-1.327370	C	-3.189639	0.857325	-2.366052
H	-4.128398	-3.233434	-4.216271	H	0.604989	-3.439421	0.137419
H	-4.364423	-1.490472	-4.303862	H	1.738543	-3.709354	-1.181045
H	-4.047302	-1.591096	5.310981	C	1.890121	-5.160264	0.412213
H	-2.490746	-1.767626	4.499238	C	2.744166	-4.249638	2.599339
H	3.574486	1.147705	5.690088	H	3.264306	-2.162445	2.566529
H	2.014059	0.702835	5.000238	H	1.535942	-2.446159	2.443458
H	3.543726	6.576941	-2.308613	H	1.082915	-2.221142	-2.577669
H	4.394129	5.066642	-2.620388	H	0.648472	-0.518995	-2.430712
H	4.907267	-0.268578	-3.726943	C	1.762438	-1.009084	-4.231492
H	5.233155	-1.974015	-3.431808	C	4.180494	-1.658553	-3.817836
H	-0.555011	2.442405	-1.074397	H	4.776654	-1.651735	-1.728288
H	-0.639830	2.718852	-0.303292	H	3.618616	-2.904930	-2.145253
				H	3.856388	1.774442	-0.355129
				H	4.831626	0.518568	-1.110043
				C	5.820494	1.501398	0.530181
				C	4.798007	1.084242	2.802894
				H	2.839632	1.405709	1.958312
				H	2.993257	-0.120287	2.780530
				H	-2.042734	1.530796	2.653536
				H	-3.481703	2.096061	1.822379
				C	-3.830933	1.426055	3.852355
				C	-3.536346	-1.054911	4.211373
				H	-3.018335	-2.176964	2.442105
27							
Ru	0.030422	-0.152352	0.160740				
H	-0.238671	-1.594531	0.757521				
C	1.036375	4.687393	-0.225974				
C	0.735064	3.503776	-1.232225				
B	0.494643	2.808784	0.949072				
O	0.728457	2.342875	-0.343993				
O	0.508997	4.183453	1.023432				
C	0.233982	0.548189	1.966564				

H	-1.733464	-1.110560	3.008052	O	0.164756	2.040562	1.945700
H	-4.965909	-1.950840	0.366297	C	-0.710875	3.327727	-2.099968
H	-4.831748	-1.709112	-1.372418	H	-0.755396	4.099685	-2.875367
C	-4.623918	-3.768826	-0.766553	H	-0.865934	2.354589	-2.574711
C	-2.354277	-3.911248	-1.885446	H	-1.528587	3.499488	-1.393643
H	-2.461420	-1.848761	-2.519284	C	1.757050	3.068778	-2.410727
H	-1.067826	-2.207414	-1.498657	H	1.532903	2.162334	-2.982759
H	-5.450861	0.283833	-0.811919	H	1.831521	3.903424	-3.117255
H	-5.107582	1.404851	0.495101	H	2.728017	2.935119	-1.929359
C	-5.533987	2.362840	-1.391646	C	2.348014	4.946090	-0.249884
C	-3.801343	1.999751	-3.196159	H	2.807103	5.347657	-1.159482
H	-2.119302	0.757305	-2.587953	H	2.414045	5.706568	0.534210
H	-3.660474	-0.083257	-2.679417	H	2.928310	4.078872	0.079200
H	1.174914	-5.844478	-0.063328	C	0.098180	5.840230	-0.885207
H	2.892510	-5.489675	0.098531	H	0.290420	6.642308	-0.165611
C	1.785357	-5.247347	1.939349	H	0.419714	6.188052	-1.873759
H	3.780341	-4.548600	2.377904	H	-0.979461	5.663937	-0.908269
H	2.637927	-4.279005	3.691309	P	2.370067	-0.845428	0.070437
H	0.866976	-1.226589	-4.828109	P	-2.476937	-0.259753	0.040674
H	2.013748	0.046403	-4.415778	C	2.617211	-2.620318	0.710512
C	2.933956	-1.894146	-4.684047	C	3.269210	-0.874327	-1.625482
H	4.548079	-0.634679	-3.982728	C	3.716559	0.053888	1.116669
H	4.989944	-2.333506	-4.124799	C	-3.481309	0.590923	1.406927
H	6.550852	0.684511	0.629097	C	-3.099049	-2.051848	0.215244
H	6.283922	2.253295	-0.122525	C	-3.281040	0.494423	-1.526720
C	5.537330	2.094460	1.916419	H	3.695928	-2.818074	0.632005
H	4.534788	1.541024	3.765054	C	1.879784	-3.666896	-0.151894
H	5.465675	0.239076	3.029654	C	2.227170	-2.774737	2.198340
H	-3.663336	2.423522	4.278559	H	3.525895	0.183380	-1.766069
H	-4.916904	1.327900	3.698332	C	2.423866	-1.247539	-2.862856
C	-3.354314	0.339456	4.825067	C	4.590873	-1.678178	-1.624516
H	-3.159747	-1.825513	4.896426	H	4.451729	-0.734787	1.339186
H	-4.611132	-1.254017	4.076408	C	4.469352	1.194458	0.394000
H	-4.291838	-4.326906	0.121272	C	3.190010	0.602554	2.462061
H	-5.695278	-3.977708	-0.884299	H	-4.533183	0.454963	1.122250
C	-3.845989	-4.259778	-1.996240	C	-3.211214	2.110903	1.462646
H	-1.823053	-4.217642	-2.796328	C	-3.313507	-0.039581	2.808600
H	-1.908855	-4.481374	-1.056829	H	-2.725094	-2.293543	1.220642
H	-6.608584	2.438771	-1.180492	C	-4.629492	-2.263473	0.220250
H	-5.085361	3.314728	-1.070325	C	-2.446010	-3.080118	-0.734853
C	-5.296554	2.173782	-2.895697	H	-2.729380	1.439959	-1.611127
H	-3.276916	2.938491	-2.969432	C	-4.784002	0.861126	-1.489891
H	-3.646164	1.804726	-4.265596	C	-2.989974	-0.308400	-2.814470
H	0.754269	-5.019213	2.246920	H	0.809036	-3.431550	-0.151459
H	1.998254	-6.268637	2.281233	H	2.214401	-3.613171	-1.193488
H	3.164395	-1.708737	-5.740944	C	2.082757	-5.101314	0.367273
H	2.636936	-2.950946	-4.609895	C	2.411288	-4.218115	2.701171
H	6.473752	2.416295	2.390218	H	2.840300	-2.115566	2.819332
H	4.916560	2.995854	1.805701	H	1.187268	-2.457434	2.341571
H	-3.897946	0.412234	5.776254	H	2.067600	-2.283673	-2.795518
H	-2.290575	0.498330	5.048983	H	1.534707	-0.614252	-2.910279
H	-3.976876	-5.342142	-2.123289	C	3.225816	-1.071314	-4.166797
H	-4.262131	-3.786772	-2.898642	C	5.385690	-1.481651	-2.927573
H	-5.842206	1.282279	-3.239417	H	5.217823	-1.402476	-0.768792
H	-5.702564	3.024395	-3.458117	H	4.369136	-2.747785	-1.512721
				H	3.752156	1.987888	0.141523
				H	4.913625	0.859289	-0.547031
				C	5.599822	1.778479	1.264133
				C	4.332144	1.131289	3.344983
				H	2.494405	1.423388	2.264081
				H	2.612692	-0.144218	3.007069
				H	-2.166684	2.283618	1.737099
				H	-3.364327	2.571270	0.477652
				C	-4.115067	2.805062	2.496420
				C	-4.209074	0.668321	3.842508
				H	-3.577163	-1.103223	2.785810
				H	-2.268661	0.018902	3.125132
27'							
Ru	-0.007192	-0.217190	0.044967				
H	-0.222246	-1.629283	0.709704				
C	0.869561	4.588812	-0.461991				
C	0.646849	3.323231	-1.392812				
B	0.372153	2.770824	0.834475				
O	0.637207	2.229221	-0.425791				
O	0.354560	4.147857	0.814560				
C	0.061397	0.533006	1.913704				
O	0.014418	0.067991	3.022804				

H	-5.130402	-1.557327	0.890234
H	-5.026970	-2.078703	-0.786930
C	-4.991480	-3.700991	0.639244
C	-2.797713	-4.519839	-0.318597
H	-2.788220	-2.917901	-1.764783
H	-1.361010	-2.953369	-0.731575
H	-5.391563	-0.049523	-1.421668
H	-5.024150	1.464939	-0.610309
C	-5.194296	1.646753	-2.750762
C	-3.389293	0.475655	-4.077003
H	-1.933475	-0.587144	-2.873296
H	-3.561849	-1.245107	-2.794437
H	1.518274	-5.801079	-0.263107
H	3.143162	-5.380388	0.270734
C	1.657943	-5.233037	1.834150
H	3.482505	-4.472116	2.699315
H	2.078629	-4.281433	3.745129
H	2.606729	-1.376193	-5.020759
H	3.445769	-0.002169	-4.308438
C	4.544009	-1.854986	-4.154057
H	5.701655	-0.430671	-3.008594
H	6.304538	-2.081554	-2.894669
H	6.370822	1.005615	1.403023
H	6.084270	2.603367	0.724498
C	5.106466	2.249164	2.637307
H	3.918766	1.493743	4.294312
H	5.020580	0.309372	3.594986
H	-3.879645	3.876694	2.527588
H	-5.167149	2.722767	2.182217
C	-3.947895	2.179963	3.887817
H	-4.043069	0.222657	4.831613
H	-5.267096	0.492075	3.592888
H	-4.677748	-3.859785	1.681426
H	-6.081804	-3.828474	0.619337
C	-4.314860	-4.743973	-0.260311
H	-2.334311	-5.229553	-1.016542
H	-2.360480	-4.723126	0.670238
H	-6.265934	1.880623	-2.705484
H	-4.665198	2.611392	-2.758291
C	-4.868335	0.881754	-4.040007
H	-2.764435	1.377511	-4.157568
H	-3.180731	-0.129223	-4.969237
H	0.576087	-5.051845	1.916666
H	1.835354	-6.254511	2.195159
H	5.107411	-1.670324	-5.077726
H	4.326949	-2.933318	-4.129620
H	5.952810	2.587404	3.249263
H	4.444462	3.118389	2.509368
H	-4.622532	2.662571	4.607107
H	-2.923160	2.359623	4.241559
H	-4.540009	-5.757957	0.094571
H	-4.730858	-4.668678	-1.276330
H	-5.492054	-0.023135	-4.091513
H	-5.123299	1.487232	-4.919286
H	-0.108449	-0.569600	-1.743752
H	-0.123812	-1.314260	-1.378355

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Ru	0.549781	-0.366177	0.202025
H	1.217802	-1.341348	1.265620
C	-4.108977	2.949943	0.180341
C	-3.482407	3.934564	-0.885198
B	-1.918160	2.400217	-0.204813
O	-2.068185	3.670206	-0.753798
O	-3.142123	1.873257	0.205963
C	-0.345155	0.855798	1.295791

O	-0.737741	1.299915	2.320967
O	-0.722877	1.791546	-0.106741
C	-3.875937	3.591646	-2.330057
H	-4.924637	3.830772	-2.538109
H	-3.247283	4.170337	-3.014255
H	-3.714241	2.529321	-2.541200
C	-3.726815	5.419889	-0.618211
H	-3.230371	6.017904	-1.389805
H	-4.797564	5.654808	-0.644545
H	-3.325455	5.723769	0.351357
C	-4.156191	3.545246	1.595704
H	-4.906800	4.338801	1.679494
H	-4.410312	2.752084	2.305823
H	-3.182409	3.952201	1.885104
C	-5.476618	2.376311	-0.188747
H	-5.803451	1.677237	0.588447
H	-6.227875	3.171231	-0.264376
H	-5.446935	1.835857	-1.138252
P	2.643362	0.857906	0.046173
P	-1.256393	-1.946929	0.194984
C	4.087602	0.278461	1.128323
C	3.236857	0.583207	-1.733665
C	2.753512	2.753225	0.232518
C	-2.237066	-2.225677	1.782738
C	-0.547358	-3.678098	-0.109027
C	-2.567112	-1.541403	-1.103204
H	4.970223	0.834933	0.777735
C	4.370626	-1.231214	0.968618
C	3.871373	0.621827	2.619492
H	2.627307	1.304757	-2.293155
C	2.835107	-0.801311	-2.286541
C	4.717266	0.893153	-2.034046
H	3.813196	2.962017	0.453101
C	2.367456	3.539340	-1.042798
C	1.891277	3.273862	1.407675
H	-2.812825	-3.151087	1.626083
C	-3.239946	-1.091496	2.096195
C	-1.301059	-2.441586	2.994275
H	-0.113449	-3.900991	0.876686
C	-1.518750	-4.826468	-0.451071
C	0.633654	-3.671368	-1.101336
H	-2.859068	-0.526149	-0.795524
C	-3.852543	-2.396240	-1.170407
C	-1.941832	-1.417853	-2.511041
H	3.462201	-1.789491	1.230355
H	4.599578	-1.471559	-0.074864
C	5.535709	-1.703175	1.856144
C	5.031862	0.133620	3.504496
H	3.766557	1.702524	2.749960
H	2.930924	0.167126	2.959343
H	3.361257	-1.602594	-1.753933
H	1.758725	-0.963180	-2.122175
C	3.140184	-0.912093	-3.790289
C	5.019330	0.771692	-3.539039
H	4.977176	1.899257	-1.682465
H	5.363236	0.194710	-1.485350
H	1.327071	3.303284	-1.302006
H	2.993398	3.249737	-1.893236
C	2.517028	5.059423	-0.839570
C	2.086644	4.782604	1.628284
H	0.841993	3.090589	1.166242
H	2.098363	2.731318	2.333733
H	-2.700533	-0.149309	2.227290
H	-3.930656	-0.933445	1.262746
C	-4.041925	-1.402095	3.372514
C	-2.099180	-2.746593	4.273452
H	-0.593671	-3.258049	2.805894

H	-0.699840	-1.536540	3.139617	C	-3.372940	4.555929	-1.858447
H	-2.364748	-4.853167	0.245614	H	-4.331316	5.086288	-1.882177
H	-1.937999	-4.666934	-1.452765	H	-2.693237	5.043106	-2.565043
C	-0.791269	-6.183712	-0.441247	H	-3.534703	3.529389	-2.201578
C	1.359536	-5.028537	-1.120941	C	-2.517045	6.032061	-0.021437
H	0.275243	-3.438115	-2.113495	H	-1.965707	6.571427	-0.798954
H	1.343271	-2.884200	-0.819763	H	-3.472501	6.546939	0.134276
H	-3.611290	-3.414958	-1.494019	H	-1.935889	6.087753	0.901920
H	-4.319701	-2.484907	-0.183805	C	-3.220455	4.082540	2.046499
C	-4.858936	-1.789141	-2.165631	H	-3.707744	5.029724	2.302705
C	-2.942952	-0.827921	-3.518851	H	-3.607809	3.302767	2.709593
H	-1.041306	-0.791862	-2.470773	H	-2.146916	4.175732	2.236466
H	-1.624915	-2.410108	-2.863205	C	-4.996496	3.531785	0.362810
H	5.679498	-2.783803	1.725965	H	-5.418082	2.853695	1.112520
H	6.467677	-1.221967	1.522786	H	-5.501688	4.499772	0.462461
C	5.294583	-1.366793	3.332709	H	-5.222222	3.124125	-0.625662
H	5.944222	0.691395	3.244569	P	2.735199	0.446447	-0.151523
H	4.812030	0.368409	4.553892	P	-1.496227	-1.900616	0.072903
H	2.877967	-1.914897	-4.151550	C	3.633724	0.851121	1.470162
H	2.502958	-0.203656	-4.339838	C	3.990248	-0.580811	-1.163637
C	4.615155	-0.604560	-4.089155	C	2.813236	2.053425	-1.165660
H	4.468885	1.554105	-4.082023	C	-2.095822	-2.370064	1.804104
H	6.085834	0.957034	-3.720939	C	-1.190974	-3.612715	-0.717999
H	3.581910	5.297813	-0.693804	C	-3.025068	-1.123069	-0.710930
H	2.204573	5.577726	-1.755540	H	4.450506	1.534792	1.189800
C	1.715833	5.569010	0.364547	C	4.258452	-0.383705	2.158208
H	1.471204	5.108677	2.476520	C	2.719257	1.561929	2.493174
H	3.133023	4.991137	1.900618	H	3.577741	-0.476477	-2.179196
H	-4.732149	-0.574218	3.580692	C	4.033771	-2.098740	-0.869307
H	-4.665280	-2.294466	3.206494	C	5.436671	-0.030248	-1.208454
C	-3.122191	-1.643480	4.577077	H	3.861754	2.170950	-1.473376
H	-1.407439	-2.868909	5.117048	C	1.951984	1.904352	-2.442358
H	-2.623011	-3.707770	4.156806	C	2.422845	3.342017	-0.410919
H	-0.431684	-6.395735	0.576434	H	-2.858442	-3.146232	1.652522
H	-1.496479	-6.985077	-0.697113	C	-2.772360	-1.220073	2.582149
C	0.396297	-6.188393	-1.414334	C	-0.953912	-2.982396	2.645439
H	2.169016	-5.007741	-1.862238	H	-0.168156	-3.827207	-0.374622
H	1.835119	-5.191198	-0.142453	C	-2.074357	-4.798319	-0.262731
H	-5.760573	-2.414076	-2.209703	C	-1.153171	-3.573633	-2.262750
H	-5.178268	-0.802767	-1.798700	H	-3.228643	-0.289849	-0.023547
C	-4.246555	-1.638238	-3.565969	C	-4.293463	-1.998539	-0.782634
H	-3.168926	0.208646	-3.229923	C	-2.732340	-0.466567	-2.079515
H	-2.485563	-0.782149	-4.515845	H	3.458761	-1.095715	2.406378
H	4.425421	-1.933413	3.697694	H	4.946581	-0.903513	1.488601
H	6.152568	-1.678475	3.942330	C	5.026327	0.002891	3.436424
H	4.801806	-0.651843	-5.169530	C	3.499715	1.987852	3.748007
H	5.246572	-1.378993	-3.628377	H	2.220372	2.428748	2.055767
H	1.889825	6.643388	0.509801	H	1.922594	0.871826	2.787620
H	0.642700	5.441328	0.164270	H	4.477377	-2.282362	0.115907
H	-3.713857	-1.904968	5.464239	H	3.025866	-2.518248	-0.825332
H	-2.588335	-0.712463	4.814404	C	4.864819	-2.842354	-1.930144
H	0.928101	-7.147077	-1.363949	C	6.282705	-0.771350	-2.260761
H	0.018483	-6.093756	-2.443402	H	5.449827	1.041588	-1.430809
H	-4.036701	-2.637206	-3.977298	H	5.910571	-0.148031	-0.225207
H	-4.964718	-1.165220	-4.248119	H	0.908318	1.767746	-2.137906
TS26 28'				H	2.246216	1.011534	-3.009782
Ru	0.515838	-0.563396	-0.067790	C	2.060020	3.142513	-3.348744
H	1.123989	-1.573525	0.987938	C	2.526928	4.576795	-1.325275
C	-3.491736	3.674702	0.590457	H	1.396043	3.252842	-0.040973
C	-2.737410	4.583862	-0.460710	H	3.079928	3.490256	0.453074
B	-1.593742	2.614790	-0.137474	H	-2.065522	-0.397361	2.724653
O	-1.450546	3.934098	-0.561912	H	-3.617993	-0.814039	2.016412
O	-2.862628	2.386471	0.390992	C	-3.273731	-1.703921	3.955451
C	-0.200943	0.771942	1.161473	C	-1.456212	-3.460597	4.018303
O	-0.495802	1.272712	2.188993	H	-0.479399	-3.817429	2.114920
O	-0.606070	1.705913	-0.236895	H	-0.172191	-2.225682	2.782883
				H	-2.086703	-4.884440	0.827604

H	-3.113090	-4.635890	-0.577770	C	-3.008484	0.412265	1.741737
C	-1.564906	-6.128367	-0.851548	C	-3.392557	-0.464815	-1.210975
C	-0.624314	-4.894755	-2.847367	O	1.020222	-3.828066	-1.424905
H	-2.167827	-3.405175	-2.646767	O	-0.130442	-2.584064	0.139539
H	-0.543212	-2.738742	-2.622160	H	4.032187	2.548730	0.080976
H	-4.127807	-2.833785	-1.476508	C	2.274601	3.490846	0.899402
H	-4.520524	-2.442058	0.194172	C	2.760029	3.132925	-1.556192
C	-5.503823	-1.183804	-1.274523	H	3.017163	-0.847355	1.670715
C	-3.948361	0.341224	-2.565790	C	1.799422	0.487659	2.785921
H	-1.861385	0.190285	-1.987071	C	4.276376	0.785272	2.260142
H	-2.488113	-1.230078	-2.828581	H	4.574793	0.573550	-1.087477
H	5.430198	-0.903466	3.906567	C	4.160169	-1.487380	-0.626400
H	5.893376	0.620500	3.157125	C	3.214800	-0.219846	-2.579823
C	4.153879	0.779506	4.429778	H	-4.089929	2.333141	-0.433418
H	4.275011	2.719191	3.472752	C	-2.563652	2.764450	-1.895645
H	2.821427	2.497894	4.443664	C	-2.543535	3.451551	0.542032
H	4.887333	-3.914850	-1.697036	H	-2.545774	1.274195	2.246462
H	4.373012	-2.745082	-2.909941	C	-4.530972	0.509675	1.977382
C	6.292997	-2.287355	-2.021400	C	-2.437314	-0.844689	2.432323
H	5.873698	-0.563485	-3.260681	H	-2.784934	-0.406070	-2.125472
H	7.307119	-0.376778	-2.255238	C	-4.825928	-0.026784	-1.585666
H	3.090241	3.233701	-3.726537	C	-3.393824	-1.946547	-0.776721
H	1.415976	3.009069	-4.227975	C	0.617061	-4.758019	-0.407273
C	1.676898	4.422116	-2.593560	C	0.254065	-3.810959	0.807334
H	2.216575	5.467987	-0.764850	H	1.188085	3.454196	0.750025
H	3.579983	4.733725	-1.606900	H	2.463136	3.140614	1.918610
H	-3.726067	-0.862053	4.495104	C	2.755627	4.947531	0.779984
H	-4.071653	-2.448881	3.812883	C	3.226872	4.595356	-1.667273
C	-2.144708	-2.326212	4.788644	H	3.314940	2.536710	-2.285190
H	-0.615257	-3.862257	4.598567	H	1.699221	3.061126	-1.830760
H	-2.165936	-4.290886	3.881747	H	1.591667	1.558798	2.889067
H	-0.570823	-6.344495	-0.432475	H	0.866864	0.020322	2.430723
H	-2.221973	-6.947028	-0.530511	C	2.168207	-0.086375	4.166310
C	-1.468999	-6.088376	-2.382175	C	4.631170	0.205070	3.641323
H	-0.614537	-4.836740	-3.943515	H	5.074114	0.554118	1.543453
H	0.419593	-5.039116	-2.531314	H	4.236544	1.879524	2.337467
H	-6.385613	-1.834381	-1.344560	H	3.302475	-2.172795	-0.626358
H	-5.742077	-0.409928	-0.530545	H	4.545564	-1.445461	0.398045
C	-5.220420	-0.516690	-2.628142	C	5.257165	-2.069872	-1.537494
H	-4.107752	1.177629	-1.872386	C	4.319709	-0.779861	-3.491206
H	-3.734432	0.777644	-3.550423	H	2.348223	-0.888274	-2.610786
H	3.365911	0.116431	4.815774	H	2.871618	0.741617	-2.970807
H	4.750642	1.096411	5.294956	H	-1.469331	2.761143	-1.951705
H	6.852158	-2.795093	-2.817743	H	-2.905916	2.022221	-2.625341
H	6.823415	-2.501149	-1.081487	C	-3.093640	4.154263	-2.285762
H	1.799560	5.298932	-3.243383	C	-3.064117	4.845037	0.144640
H	0.618004	4.375594	-2.307138	H	-2.899788	3.217011	1.551956
H	-2.534307	-2.695108	5.746383	H	-1.446830	3.468705	0.587511
H	-1.403027	-1.550031	5.026248	H	-4.942014	1.412567	1.511010
H	-1.049175	-7.028219	-2.762913	H	-5.030045	-0.345002	1.502077
H	-2.479975	-6.002012	-2.807539	C	-4.860291	0.505131	3.481386
H	-5.098331	-1.294973	-3.396757	C	-2.765024	-0.849087	3.934837
H	-6.078702	0.093975	-2.937298	H	-2.851896	-1.746492	1.968335
H	1.194689	-1.915289	-1.061026	H	-1.352876	-0.902027	2.281069
H	0.936660	-1.383853	-1.641758	H	-5.479192	-0.081515	-0.704994
				H	-4.848071	1.011992	-1.930041
				C	-5.397083	-0.929035	-2.696898
				C	-3.953473	-2.846823	-1.891428
				H	-2.384731	-2.263464	-0.500494
				H	-4.025783	-2.061799	0.115791
				C	1.768073	-5.731668	-0.144868
				C	-0.595227	-5.531186	-0.953834
				C	1.454857	-3.501570	1.711194
				C	-0.910680	-4.302063	1.670304
				H	2.229179	5.566457	1.518342
				H	3.825174	5.001831	1.033764
				C	2.544367	5.499352	-0.634682

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Ru	0.007825	0.378209	-0.151687
P	2.401983	0.748643	0.004318
P	-2.387202	0.629955	-0.032385
B	0.384565	-2.602554	-1.183453
H	-0.032745	1.952456	-0.190598
C	2.952713	2.563422	-0.132266
C	2.924770	0.243145	1.753566
C	3.699057	-0.095150	-1.113582
C	-2.991591	2.369627	-0.464298

H	4.316523	4.639356	-1.519419	C	-3.431282	-0.415753	-1.263746
H	3.036171	4.959935	-2.684696	O	1.038864	-3.854374	-1.342977
H	1.372650	0.139638	4.887991	O	-0.010638	-2.626512	0.304768
H	2.229071	-1.182315	4.098584	H	3.887621	2.709200	-0.063075
C	3.514225	0.462135	4.663496	C	2.211080	3.466848	1.058806
H	4.795157	-0.878738	3.548467	C	2.378269	3.306836	-1.462779
H	5.577586	0.634917	3.993869	H	3.450006	-0.834933	1.344146
H	6.155722	-1.438031	-1.466386	C	2.589572	0.325490	2.886061
H	5.544785	-3.063261	-1.168643	C	4.746044	0.849480	1.657308
C	4.803427	-2.149936	-3.000086	H	4.340574	0.823383	-1.438089
H	3.937190	-0.856191	-4.516669	C	4.091069	-1.293398	-1.126767
H	5.169770	-0.080198	-3.523494	C	2.826104	0.080067	-2.791293
H	-2.747677	4.407620	-3.295866	H	-4.245617	2.249078	-0.127841
H	-4.193314	4.131736	-2.328088	C	-2.759140	2.881502	-1.548574
C	-2.648674	5.226329	-1.282193	C	-2.703652	3.279951	0.952181
H	-2.699575	5.590787	0.863219	H	-2.681006	0.862480	2.410107
H	-4.162236	4.854776	0.215974	C	-4.698990	0.255287	2.027369
H	-4.450957	1.416143	3.942797	C	-2.699395	-1.265270	2.304798
H	-5.947980	0.545855	3.623609	H	-2.853546	-0.149395	-2.159203
C	-4.275686	-0.728004	4.185801	C	-4.904311	-0.049409	-1.549342
H	-2.375164	-1.764825	4.398526	C	-3.293298	-1.943961	-1.092072
H	-2.247968	-0.008083	4.421418	C	0.758979	-4.778318	-0.280903
H	-6.422677	-0.616851	-2.933898	C	0.493623	-3.820203	0.948394
H	-4.805591	-0.782101	-3.612240	H	1.118006	3.368379	1.052097
C	-5.365908	-2.413852	-2.308683	H	2.557365	3.058499	2.013638
H	-3.280740	-2.801192	-2.759429	C	2.588683	4.956960	0.988650
H	-3.961365	-3.892436	-1.555474	C	2.751163	4.799234	-1.520660
H	1.957029	-6.322274	-1.047257	H	2.862750	2.794836	-2.298113
H	1.524245	-6.424915	0.668886	H	1.295932	3.191900	-1.604911
H	2.691615	-5.205410	0.108533	H	2.369545	1.368146	3.148559
H	-1.436318	-4.859525	-1.154322	H	1.627975	-0.189435	2.816445
H	-0.931533	-6.316426	-0.267593	C	3.412409	-0.315651	4.019604
H	-0.310706	-5.998868	-1.901473	C	5.557081	0.191893	2.787957
H	2.315085	-3.160765	1.129310	H	5.294625	0.757998	0.712710
H	1.758865	-4.377053	2.295443	H	4.665865	1.924044	1.869001
H	1.177826	-2.705898	2.410521	H	3.275051	-2.027170	-1.083202
H	-1.097727	-3.593997	2.484305	H	4.618010	-1.332524	-0.168524
H	-0.677788	-5.274697	2.119743	C	5.083980	-1.711771	-2.229230
H	-1.831041	-4.401614	1.090597	C	3.831134	-0.292517	-3.894249
H	1.466321	5.548857	-0.848958	H	2.029530	-0.668913	-2.770255
H	2.927273	6.525335	-0.708633	H	2.353854	1.034437	-3.033823
H	3.771752	0.011688	5.630406	H	-1.665877	2.912617	-1.626230
H	3.423570	1.544819	4.837108	H	-3.103890	2.223129	-2.353618
H	5.620708	-2.522052	-3.631712	C	-3.330770	4.293983	-1.760003
H	3.979838	-2.872792	-3.082538	C	-3.269909	4.694489	0.735401
H	-3.067135	6.204467	-1.552267	H	-3.024133	2.916205	1.935772
H	-1.554098	5.329298	-1.325402	H	-1.606855	3.323844	0.971519
H	-4.481868	-0.684417	5.262831	H	5.064691	1.225199	1.720088
H	-4.777220	-1.631153	3.807408	H	-5.237874	-0.513454	1.458262
H	-6.058830	-2.583201	-1.470486	C	-5.030761	0.093920	3.522899
H	-5.726662	-3.031039	-3.141494	C	-3.016850	-1.424577	3.801152
C	-0.059586	0.183649	-2.005212	H	-3.199025	-2.068325	1.750246
O	-0.206080	0.549110	-3.112099	H	-1.629267	-1.392318	2.116983
O	0.281349	-1.631992	-2.074600	H	-5.533561	-0.319962	-0.691645
				H	-5.026894	1.028051	-1.702249
				C	-5.412352	-0.790368	-2.801782
				C	-3.787151	-2.681425	-2.347753
				H	-2.255427	-2.209048	-0.879599
				H	-3.897362	-2.269005	-0.233729
				C	1.952542	-5.722157	-0.120944
				C	-0.484822	-5.585801	-0.690746
				C	1.777750	-3.443028	1.700447
				C	-0.545991	-4.336709	1.944611
				H	2.130010	5.490610	1.831374
				H	3.677533	5.063269	1.107828
				C	2.163921	5.586330	-0.343421
				H	3.846967	4.899871	-1.509819

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Ru	-0.082230	0.421555	-0.017460
P	2.365847	0.807367	-0.016675
P	-2.507784	0.550838	0.075079
B	0.397192	-2.639062	-1.056204
H	-0.156542	1.978931	-0.202975
C	2.791062	2.658968	-0.122909
C	3.331017	0.238588	1.533685
C	3.501344	0.110736	-1.400816
C	-3.149118	2.312383	-0.165704
C	-3.181565	0.106306	1.786037

H	2.409938	5.221596	-2.474485
H	2.873338	-0.205407	4.969599
H	3.496234	-1.396388	3.832481
C	4.819583	0.284342	4.129873
H	5.735401	-0.865320	2.541693
H	6.544365	0.666706	2.857848
H	5.954777	-1.038734	-2.198377
H	5.461848	-2.718993	-2.009984
C	4.455723	-1.667078	-3.626920
H	3.319392	-0.288943	-4.864824
H	4.625012	0.468755	-3.953885
H	-3.011797	4.675421	-2.738330
H	-4.429885	4.244418	-1.787867
C	-2.896707	5.253715	-0.644038
H	-2.908609	5.360293	1.530014
H	-4.365857	4.663759	0.829293
H	-4.573489	0.923267	4.082961
H	-6.114878	0.177421	3.673500
C	-4.516178	-1.241154	4.081157
H	-2.683921	-2.410875	4.149777
H	-2.445361	-0.679934	4.376093
H	-6.466461	-0.537394	-2.976110
H	-4.854724	-0.430055	-3.678496
C	-5.239177	-2.311151	-2.682195
H	-3.131486	-2.425910	-3.191526
H	-3.696201	-3.765497	-2.199675
H	2.064927	-6.323170	-1.029354
H	1.808785	-6.407417	0.722974
H	2.883660	-5.170646	0.030787
H	-1.357818	-4.935253	-0.808501
H	-0.729015	-6.368036	0.036579
H	-0.290110	-6.060545	-1.657443
H	2.549161	-3.088422	1.010772
H	2.182029	-4.289680	2.266411
H	1.552696	-2.637534	2.407012
H	-0.662264	-3.625033	2.769044
H	-0.232233	-5.295914	2.373337
H	-1.522556	-4.469848	1.473680
H	1.065785	5.582069	-0.413745
H	2.477334	6.637255	-0.389018
H	5.390575	-0.224072	4.917186
H	4.744021	1.340385	4.429552
H	5.207975	-1.908023	-4.389535
H	3.673115	-2.435236	-3.695758
H	-3.349856	6.242656	-0.790148
H	-1.806855	5.397154	-0.694092
H	-4.715840	-1.303958	5.158539
H	-5.072572	-2.066002	3.611758
H	-5.901054	-2.687789	-1.887377
H	-5.556794	-2.802136	-3.610979
C	-0.205209	0.161580	-1.926312
O	-0.444029	0.458680	-3.030926
O	0.198757	-1.677285	-1.936761
H	-0.067928	0.250505	1.819627
H	-0.127909	1.055500	1.686116

C	-3.472285	-2.095921	-0.276623
C	-2.899557	0.856078	-1.114169
O	0.777920	3.232458	0.992655
O	0.077114	3.285181	-1.205981
H	4.235614	-2.527364	-0.421358
C	2.603608	-3.505958	-1.436531
C	3.117533	-3.624715	1.042451
H	2.926935	1.025619	-1.001828
C	2.199094	-0.026700	-2.697450
C	4.537939	-0.209021	-1.725468
H	4.142753	-0.976667	1.665973
C	3.616538	1.101935	1.516667
C	2.324983	-0.652784	2.793614
H	-4.209564	0.179276	1.628153
C	-2.516118	1.402013	2.153106
C	-2.879733	-1.013515	2.833658
H	-3.118452	-2.763128	0.523232
C	-5.006406	-1.991781	-0.135841
C	-3.108439	-2.792354	-1.607103
H	-2.214055	1.636256	-0.758638
C	-4.335800	1.419368	-1.061994
C	-2.491039	0.580293	-2.578344
C	0.576749	4.620225	0.668687
C	0.576166	4.602997	-0.910806
H	1.531161	-3.678027	-1.279369
H	2.690496	-2.904273	-2.347334
C	3.313895	-4.854818	-1.646564
C	3.834241	-4.969045	0.821552
H	3.579889	-3.112561	1.893105
H	2.073907	-3.819268	1.315494
H	2.231951	-1.028483	-3.146304
H	1.155313	0.183275	-2.451985
C	2.714744	1.001364	-3.719521
C	5.046366	0.832022	-2.738636
H	5.148093	-0.172769	-0.814086
H	4.676899	-1.210483	-2.155228
H	2.726396	1.723129	1.362218
H	4.297650	1.296723	0.681111
C	4.308880	1.528443	2.824627
C	3.014247	-0.226669	4.100184
H	1.394118	-0.080103	2.675062
H	2.034930	-1.707622	2.850166
H	-1.422454	1.323840	2.183615
H	-2.742815	2.170157	1.405374
C	-3.043106	1.859377	3.523946
C	-3.404471	-0.547739	4.202025
H	-3.352947	-1.966704	2.570543
H	-1.801233	-1.211811	2.907268
H	-5.285569	-1.520711	0.813321
H	-5.408762	-1.354366	-0.933468
C	-5.661840	-3.382626	-0.226620
C	-3.758446	-4.183783	-1.694438
H	-3.458586	-2.184264	-2.450750
H	-2.021837	-2.877193	-1.707246
H	-5.042672	0.679173	-1.460181
H	-4.647539	1.627689	-0.031867
C	-4.440180	2.707934	-1.899998
C	-2.582972	1.869450	-3.412975
H	-1.473060	0.180482	-2.616489
H	-3.154872	-0.177568	-3.016246
C	1.693739	5.445572	1.309907
C	-0.778870	5.038760	1.261282
C	1.988561	4.704422	-1.509734
C	-0.336293	5.637512	-1.571960
H	2.856916	-5.380990	-2.494597
H	4.364336	-4.674146	-1.920494
C	3.262939	-5.725750	-0.384730

28

Ru	-0.061843	-0.912160	0.114651
P	2.355852	-1.048860	-0.003436
P	-2.458072	-0.539862	0.066066
B	0.338781	2.451445	-0.098193
H	-0.150844	-1.562724	-1.311941
C	3.174402	-2.738867	-0.223377
C	3.044505	0.012071	-1.404948
C	3.218049	-0.389635	1.557474
C	-3.123515	0.044448	1.733785

H	4.907481	-4.786404	0.660573	C	-3.312916	-0.359345	1.555790
H	3.753756	-5.579182	1.730303	O	0.639581	3.764135	1.210529
H	2.126028	0.928860	-4.643221	O	0.178985	2.945913	-0.898490
H	2.544130	2.011417	-3.320832	H	4.108032	-2.542414	-0.165014
C	4.208227	0.815265	-4.025151	C	2.309692	-3.639975	-0.615557
H	4.997726	1.832696	-2.284421	C	3.202173	-3.116820	1.684036
H	6.103500	0.642941	-2.967182	H	2.959223	0.836626	-1.552658
H	5.262509	0.987657	2.925420	C	2.642561	-0.823560	-2.863670
H	4.559614	2.595759	2.771067	C	4.761104	-0.348171	-1.610837
C	3.435090	1.248243	4.054135	H	4.287398	-0.409420	1.526290
H	2.341414	-0.408218	4.948470	C	3.642731	1.589735	1.050660
H	3.901955	-0.856044	4.265753	C	2.547362	0.077203	2.734603
H	-2.566051	2.808633	3.799128	H	-4.236653	-2.266627	-0.617573
H	-4.122626	2.061062	3.450773	C	-2.783492	-3.474515	0.393588
C	-2.800694	0.802803	4.609994	C	-2.692704	-2.770675	-2.031833
H	-3.184558	-1.311851	4.958700	H	-2.611534	0.275368	-2.306695
H	-4.500285	-0.457047	4.158592	C	-4.711349	0.140566	-1.880848
H	-5.339848	-3.987428	0.634077	C	-3.142616	1.964174	-1.102881
H	-6.752343	-3.283346	-0.147820	H	-2.902848	-1.196362	2.140574
C	-5.282791	-4.107665	-1.525596	C	-4.850086	-0.469619	1.626907
H	-3.504380	-4.650793	-2.654736	C	-2.838417	0.929833	2.264657
H	-3.334565	-4.827991	-0.910342	C	0.477306	4.910507	0.363383
H	-5.471147	3.085063	-1.873023	C	0.640129	4.297849	-1.085340
H	-3.809291	3.483935	-1.442253	H	1.286822	-3.718822	-0.229276
C	-3.990873	2.480675	-3.351038	H	2.212194	-3.308824	-1.653653
H	-1.844645	2.586452	-3.030420	C	2.982703	-5.022679	-0.572492
H	-2.310599	1.654802	-4.454898	C	3.869110	-4.504242	1.734857
H	1.627774	5.367368	2.400605	H	3.787627	-2.423953	2.295824
H	1.607699	6.505433	1.041913	H	2.205760	-3.180169	2.138468
H	2.681877	5.089348	1.008337	H	2.938639	-1.876862	-2.952159
H	-1.598107	4.471053	0.807946	H	1.549193	-0.809791	-2.858303
H	-0.978665	6.106928	1.120584	C	3.177523	-0.060099	-4.088632
H	-0.775721	4.827326	2.335664	C	5.325887	0.414813	-2.823725
H	2.665756	3.980007	-1.045073	H	5.227656	0.019309	-0.691579
H	2.417701	5.705535	-1.389890	H	5.042715	-1.406111	-1.701647
H	1.934468	4.479763	-2.580055	H	2.702891	2.130952	0.914837
H	-0.277571	5.537389	-2.661266	H	4.208083	1.673958	0.117369
H	-0.033677	6.658356	-1.309803	C	4.440122	2.269192	2.178850
H	-1.379751	5.497402	-1.279056	C	3.334040	0.757094	3.868162
H	2.219363	-6.003113	-0.176710	C	1.595955	0.598491	2.579706
H	3.812570	-6.662390	-0.544166	H	2.309393	-0.949940	3.025522
H	4.557403	1.593570	-4.716027	H	-1.693129	-3.574094	0.447414
H	4.356895	-0.147199	-4.537793	H	-3.128290	-3.219647	1.401901
H	3.968477	1.523532	4.973310	C	-3.395874	-4.823740	-0.023582
H	2.536102	1.879291	4.006832	C	-3.302031	-4.120265	-2.450761
H	-3.219996	1.135081	5.568405	H	-2.964949	-2.005152	-2.767975
H	-1.717973	0.684004	4.764466	H	-1.598277	-2.843908	-2.046128
H	-5.721128	-5.113782	-1.540470	H	-4.822889	-0.913029	-2.153801
H	-5.714431	-3.565394	-2.380255	H	-5.402117	0.324191	-1.048822
H	-4.703808	1.802927	-3.845273	C	-5.128733	1.013824	-3.078734
H	-4.022681	3.425911	-3.908333	C	-3.563154	2.838469	-2.296548
C	-0.302265	-2.631075	0.710867	H	-3.796189	2.194955	-0.251697
O	-0.490386	-3.714245	1.115525	H	-2.120895	2.213256	-0.806001
O	0.189005	1.149093	-0.072955	H	-5.301527	0.381814	1.100549
				H	-5.213963	-1.377886	1.131768
				C	-5.327639	-0.457785	3.091986
				C	-3.303687	0.934404	3.730920
				H	-1.752289	1.038790	2.191962
				H	-3.268726	1.804813	1.760188
				C	1.526017	5.958360	0.743112
				C	-0.930249	5.476001	0.620120
				C	2.104742	4.233489	-1.549048
				C	-0.201910	4.970883	-2.171000
				H	2.399020	-5.733734	-1.171543
				H	3.976621	-4.961931	-1.041274
				C	3.130347	-5.531163	0.867463
				H	4.909390	-4.416786	1.386602
28'							
Ru	-0.034051	-0.591531	0.038236				
P	2.399881	-0.838249	0.042381				
P	-2.484739	-0.655225	-0.117086				
B	0.292930	2.606404	0.482182				
H	-0.070382	-1.961798	-0.810871				
C	3.083727	-2.603933	0.230220				
C	3.219534	-0.231860	-1.557712				
C	3.328110	0.116437	1.396734				
C	-3.141881	-2.359414	-0.611626				
C	-3.263615	0.462566	-1.439499				

H	3.917650	-4.846593	2.776511	C	-3.425073	-0.398344	-1.089924
H	2.760131	-0.492528	-5.007184	C	-3.376116	0.451653	1.744394
H	2.826945	0.981664	-4.044814	C	3.514050	-0.211236	1.499600
C	4.712366	-0.082539	-4.140837	C	2.945619	2.324768	0.124860
H	5.116054	1.487687	-2.703206	C	3.273714	-0.334848	-1.434240
H	6.418401	0.311763	-2.850582	O	-1.335029	-2.690003	-0.116738
H	5.420393	1.778158	2.282134	O	0.935952	-2.664065	-0.433925
H	4.641228	3.312453	1.901798	H	-3.936340	2.178567	-1.052610
C	3.689360	2.207038	3.514653	C	-2.061754	3.092144	-1.514833
H	2.740616	0.723928	4.790985	C	-3.424698	3.467311	0.559123
H	4.258122	0.192688	4.070620	H	-3.121450	-1.412620	-0.809203
H	-3.104070	-5.597117	0.698450	C	-2.989142	-0.179931	-2.556129
H	-4.493258	-4.754494	0.019427	C	-4.965191	-0.302652	-0.983389
C	-2.968807	-5.226904	-1.441071	H	-4.387377	0.850241	1.570909
H	-2.939588	-4.392603	-3.450504	C	-3.523964	-1.039709	2.132818
H	-4.394938	-4.019851	-2.531993	C	-2.750423	1.218514	2.935107
H	-4.502392	0.757280	-3.946286	H	4.537277	0.123717	1.280816
H	-6.162971	0.777915	-3.361558	C	3.559269	-1.753984	1.567642
C	-4.984172	2.510385	-2.773306	C	3.119718	0.384361	2.871974
H	-3.491610	3.897758	-2.018553	H	2.276927	2.688055	0.919717
H	-2.853818	2.685606	-3.123071	C	4.386472	2.706452	0.543168
H	-6.423902	-0.510507	3.124497	C	2.585381	3.110177	-1.157412
H	-4.956629	-1.362662	3.595834	H	3.040783	-1.393614	-1.256063
C	-4.828233	0.784442	3.845089	C	4.807824	-0.182917	-1.537731
H	-2.813351	0.109392	4.269027	C	2.612172	0.031515	-2.781955
H	-2.975282	1.861222	4.217990	C	-0.997409	-4.036309	-0.566892
H	1.343678	6.303863	1.766305	C	0.452474	-3.833304	-1.157317
H	1.478292	6.829149	0.078120	H	-1.170450	3.450386	-0.985007
H	2.537164	5.545343	0.706108	H	-1.710318	2.377743	-2.265486
H	-1.702871	4.748707	0.349797	C	-2.732900	4.295722	-2.199157
H	-1.114234	6.402152	0.063807	C	-4.088373	4.692119	-0.099196
H	-1.031372	5.689236	1.689053	H	-4.122034	3.042453	1.287132
H	2.740473	3.766817	-0.791220	H	-2.537710	3.795009	1.118768
H	2.507335	5.227734	-1.772732	H	-3.243671	0.841379	-2.872726
H	2.161632	3.628744	-2.461010	H	-1.901530	-0.276581	-2.640923
H	-0.046939	4.461305	-3.128709	C	-3.685700	-1.161857	-3.514560
H	0.086895	6.020988	-2.299112	C	-5.654448	-1.296875	-1.937125
H	-1.268277	4.930313	-1.939216	H	-5.304678	-0.493541	0.039354
H	2.131541	-5.711262	1.291262	H	-5.303608	0.711685	-1.238361
H	3.656582	-6.494296	0.883385	H	-2.535655	-1.471005	2.321180
H	5.075612	0.521250	-4.982186	H	-3.961382	-1.625426	1.318743
H	5.049725	-1.113030	-4.327190	C	-4.390216	-1.194669	3.396048
H	4.290863	2.661620	4.312901	C	-3.618944	1.077943	4.197818
H	2.766298	2.796649	3.429792	H	-1.753844	0.811937	3.128360
H	-3.451131	-6.168785	-1.732492	H	-2.615765	2.277746	2.702854
H	-1.884506	-5.411593	-1.452410	H	2.559183	-2.157750	1.746037
H	-5.241074	3.106556	-3.658399	H	3.895785	-2.172380	0.612681
H	-5.702996	2.789371	-1.988361	C	4.503018	-2.228541	2.687796
H	-5.310782	1.678659	3.422550	C	4.069706	-0.101099	3.980995
H	-5.133167	0.734712	4.898479	H	3.131026	1.480516	2.838106
C	-0.149031	-1.604431	1.565623	H	2.093716	0.095969	3.117373
O	-0.248318	-2.248060	2.531953	H	4.691027	2.188072	1.455976
O	0.126715	1.414677	0.998760	H	5.095994	2.408229	-0.239040
H	0.038229	0.743940	-1.441911	C	4.506275	4.225143	0.777218
H	-0.012177	0.046383	-1.784426	C	2.679605	4.628549	-0.926142
				H	3.287224	2.837843	-1.956464
				H	1.585726	2.850808	-1.519834
				H	5.060531	0.871987	-1.707664
				H	5.298591	-0.476666	-0.604059
				C	5.384204	-1.016350	-2.696363
				C	3.200987	-0.789623	-3.943411
				H	1.532192	-0.126989	-2.716167
				H	2.762205	1.095331	-3.000755
				C	-2.047695	-4.489353	-1.580021
				C	-1.046321	-4.954943	0.662311
				C	0.455151	-3.474613	-2.648460
				C	1.422663	-4.984948	-0.893597

TS19

Ru	-0.010319	0.340056	0.186039
P	-2.438354	0.694086	0.116286
P	2.460605	0.472667	0.077802
B	-0.149371	-2.026112	0.132695
H	0.093839	1.688073	-0.724408
H	-0.086169	0.030092	-1.384543
H	0.022191	1.999691	0.260387
C	-3.018183	2.422133	-0.501962

H	-2.035175	4.751300	-2.913803
H	-3.597677	3.949215	-2.784676
C	-3.194334	5.334946	-1.167758
H	-5.036007	4.377609	-0.561360
H	-4.348826	5.427379	0.673170
H	-3.374230	-0.952850	-4.546519
H	-3.355889	-2.185456	-3.289177
C	-5.213271	-1.088673	-3.391621
H	-5.408112	-2.322801	-1.626077
H	-6.744226	-1.196884	-1.848870
H	-5.413272	-0.850310	3.178976
H	-4.467935	-2.257817	3.658008
C	-3.824623	-0.394729	4.577649
H	-3.149726	1.622404	5.027639
H	-4.598443	1.551698	4.027814
H	4.491401	-3.325232	2.733337
H	5.536475	-1.936493	2.444666
C	4.116230	-1.633583	4.048344
H	3.749462	0.314847	4.945051
H	5.084036	0.285195	3.794624
H	3.873344	4.504837	1.632503
H	5.537708	4.472621	1.060149
C	4.082019	5.035734	-0.454394
H	2.418378	5.161085	-1.849954
H	1.936933	4.926361	-0.171054
H	6.471192	-0.871391	-2.750037
H	5.221310	-2.084405	-2.488883
C	4.726594	-0.651852	-4.033196
H	2.947407	-1.850107	-3.804982
H	2.732026	-0.479213	-4.886383
H	-3.027202	-4.538730	-1.092826
H	-1.811865	-5.490252	-1.960097
H	-2.124309	-3.806763	-2.428484
H	-0.340870	-4.632089	1.429023
H	-0.839174	-5.995093	0.387655
H	-2.051498	-4.909999	1.094074
H	-0.196405	-2.619823	-2.852077
H	0.133094	-4.319424	-3.266794
H	1.471068	-3.203262	-2.948600
H	2.406331	-4.737429	-1.306559
H	1.077145	-5.907185	-1.375383
H	1.541498	-5.170901	0.175803
H	-2.310500	5.775220	-0.682754
H	-3.723079	6.160194	-1.661867
H	-5.687087	-1.832355	-4.045338
H	-5.558842	-0.102656	-3.737345
H	-4.488931	-0.478390	5.447821
H	-2.858503	-0.827104	4.874108
H	4.821708	-1.961427	4.823113
H	3.125982	-2.012248	4.338699
H	4.117425	6.110664	-0.235631
H	4.799983	4.858095	-1.269000
H	4.984969	0.385937	-4.292688
H	5.121849	-1.283053	-4.839635
C	0.038757	-1.352063	1.837871
O	0.142021	-2.479946	2.316932
O	0.014957	-0.214580	2.358399

TS20

Ru	0.006138	0.349344	0.080548
P	-2.434143	0.636303	-0.061736
P	2.448483	0.265619	0.052478
B	-0.193382	-1.688813	-0.103824
H	0.047528	0.026442	-1.629038
H	-0.023039	0.116694	1.753559
H	0.071315	0.888786	-1.607785
C	-2.950467	2.439711	-0.410144

C	-3.300304	-0.313676	-1.476437
C	-3.598006	0.224255	1.403260
C	3.382425	-0.522710	1.503701
C	3.156708	2.025314	0.057068
C	3.159739	-0.673608	-1.446055
O	0.695993	-2.569782	-0.738816
O	-1.264679	-2.432348	0.408171
H	-3.997021	2.383998	-0.739906
C	-2.121025	3.060101	-1.556086
C	-2.925438	3.379800	0.816205
H	-3.337664	-1.328791	-1.062319
C	-2.518916	-0.433536	-2.802451
C	-4.747269	0.140924	-1.774327
H	-4.441046	0.923894	1.293807
C	-4.181837	-1.206957	1.421348
C	-2.917336	0.499615	2.760523
H	4.433968	-0.566340	1.191268
C	2.902873	-1.965582	1.764915
C	3.338915	0.283653	2.818779
H	2.867514	2.376280	1.056928
C	4.690409	2.159073	-0.057757
C	2.461543	2.988293	-0.932259
H	2.494225	-1.544444	-1.476930
C	4.610254	-1.202685	-1.350668
C	2.979680	0.084441	-2.780647
C	0.124622	-3.898203	-0.811196
C	-0.983861	-3.850190	0.308482
H	-1.068459	3.104592	-1.246569
H	-2.153471	2.425948	-2.448572
C	-2.604269	4.475006	-1.919432
C	-3.415273	4.792980	0.449435
H	-3.561221	2.987963	1.616543
H	-1.906279	3.442771	1.213272
H	-2.410571	0.550518	-3.277693
H	-1.509191	-0.805840	-2.611658
C	-3.228107	-1.384080	-3.785864
C	-5.458519	-0.825971	-2.737645
H	-5.331791	0.241884	-0.852783
H	-4.728139	1.134994	-2.241276
H	-3.356879	-1.923575	1.487191
H	-4.721751	-1.428709	0.496000
C	-5.151732	-1.404831	2.601655
C	-3.884862	0.313963	3.941379
H	-2.069844	-0.185643	2.872843
H	-2.500812	1.509612	2.796264
H	1.849160	-1.928797	2.069838
H	2.933455	-2.559902	0.846233
C	3.733637	-2.651344	2.863137
C	4.181366	-0.396427	3.914099
H	3.711077	1.303342	2.670112
H	2.305743	0.367951	3.170430
H	5.199366	1.500484	0.655532
H	5.011672	1.843890	-1.059372
C	5.142210	3.612749	0.174507
C	2.911985	4.440245	-0.695203
H	2.698347	2.706512	-1.965440
H	1.375834	2.913716	-0.821836
H	5.321696	-0.367377	-1.303893
H	4.755421	-1.790537	-0.439343
C	4.956479	-2.091808	-2.560753
C	3.308732	-0.812976	-3.986091
H	1.959410	0.468389	-2.877416
H	3.647174	0.956289	-2.805193
C	1.233307	-4.927278	-0.580206
C	-0.437356	-4.069353	-2.230668
C	-0.488857	-4.310048	1.688206
C	-2.279543	-4.587244	-0.037583

H	-1.972145	4.886720	-2.717115
H	-3.624506	4.417001	-2.328114
C	-2.599750	5.402624	-0.697786
H	-4.474677	4.744928	0.154519
H	-3.368077	5.437452	1.336807
H	-2.663458	-1.428704	-4.726278
H	-3.218513	-2.402344	-3.368984
C	-4.681059	-0.969421	-4.052526
H	-5.555655	-1.812100	-2.259660
H	-6.478995	-0.471260	-2.932717
H	-6.024868	-0.748387	2.466095
H	-5.533963	-2.434394	2.589675
C	-4.493224	-1.093415	3.950924
H	-3.352992	0.510286	4.880862
H	-4.692323	1.059288	3.876063
H	3.347241	-3.663726	3.042024
H	4.770464	-2.771985	2.513984
C	3.728106	-1.840602	4.166038
H	4.118717	0.189992	4.839629
H	5.239914	-0.395030	3.612673
H	4.916154	3.897622	1.212837
H	6.231905	3.685740	0.061272
C	4.438144	4.585490	-0.782169
H	2.424866	5.102610	-1.422824
H	2.570688	4.762845	0.299280
H	5.996260	-2.434972	-2.478857
H	4.327071	-2.993644	-2.531398
C	4.736046	-1.368075	-3.895173
H	2.592786	-1.647264	-4.021638
H	3.177386	-0.245897	-4.917079
H	1.975858	-4.854097	-1.382353
H	0.829906	-5.946865	-0.589364
H	1.747096	-4.767599	0.370197
H	-1.223385	-3.338133	-2.439294
H	-0.845019	-5.073452	-2.391405
H	0.369794	-3.909030	-2.953080
H	0.431699	-3.793607	1.973658
H	-0.307826	-5.390270	1.717925
H	-1.252024	-4.069438	2.435160
H	-2.996549	-4.481242	0.783237
H	-2.094160	-5.657941	-0.184552
H	-2.743774	-4.189264	-0.943131
H	-1.563298	5.556409	-0.363524
H	-2.994222	6.391420	-0.965553
H	-5.171372	-1.697370	-4.711599
H	-4.692886	-0.006857	-4.585412
H	-5.221714	-1.194943	4.766016
H	-3.698316	-1.828458	4.144640
H	4.370536	-2.317722	4.917525
H	2.710088	-1.830867	4.581728
H	4.737975	5.618386	-0.562858
H	4.764048	4.377561	-1.812677
H	5.452767	-0.537371	-3.980612
H	4.940686	-2.044652	-4.735012
C	0.153383	1.661715	2.421298
O	0.124675	1.414440	3.583411
O	0.250951	2.452705	1.512907

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Ru	0.003878	0.309156	-0.182236
P	-2.352564	0.640739	0.161735
P	2.369554	0.231552	0.196478
B	-0.186778	-1.692027	-0.405588
H	-0.019759	0.334902	1.399366
C	-2.710741	2.469209	0.567529
C	-3.660008	0.230032	-1.168318

C	-3.162537	-0.157439	1.721656
C	2.895296	-0.640349	1.800341
C	3.034595	1.982889	0.522406
C	3.475294	-0.615830	-1.106638
O	0.651142	-2.436959	-1.249734
O	-1.185202	-2.534959	0.104852
H	-3.790670	2.534138	0.767397
C	-2.381767	3.416621	-0.603958
C	-1.978772	2.946920	1.841779
H	-3.802178	-0.848841	-1.021874
C	-3.162617	0.383885	-2.621448
C	-5.033492	0.916018	-1.000065
H	-3.828653	0.629858	2.109022
C	-4.036158	-1.407122	1.465668
C	-2.132193	-0.491183	2.824130
H	3.994046	-0.648864	1.803330
C	2.400116	-2.100689	1.822136
C	2.444038	0.071870	3.094177
H	2.543006	2.227469	1.474752
C	4.554085	2.133961	0.743189
C	2.521522	3.032687	-0.486495
H	2.843384	-1.470930	-1.382075
C	4.848300	-1.168759	-0.660285
C	3.647653	0.241501	-2.380916
C	0.032264	-3.711727	-1.540414
C	-0.943989	-3.901955	-0.316087
H	-1.315374	3.333771	-0.847409
H	-2.925058	3.122163	-1.508124
C	-2.708339	4.883464	-0.273867
C	-2.301636	4.414812	2.173159
H	-2.246964	2.321517	2.698943
H	-0.894922	2.831532	1.701582
H	-2.960058	1.439739	-2.850233
H	-2.221844	-0.157690	-2.750361
C	-4.198744	-0.151494	-3.627206
C	-6.066509	0.370066	-2.002449
H	-5.412614	0.797246	0.022035
H	-4.925572	1.996118	-1.166607
H	-3.404028	-2.198702	1.049487
H	-4.821848	-1.199800	0.733792
C	-4.712192	-1.903430	2.757842
C	-2.808261	-0.972733	4.118887
H	-1.462889	-1.269829	2.442541
H	-1.498589	0.372431	3.043093
H	1.303402	-2.085648	1.817509
H	2.704106	-2.632015	0.912969
C	2.893652	-2.857936	3.066037
C	2.923271	-0.681380	4.349363
H	2.831307	1.095919	3.135495
H	1.349326	0.146345	3.101212
H	4.909524	1.418504	1.494128
H	5.086201	1.900593	-0.188052
C	4.919543	3.564772	1.179419
C	2.893077	4.460008	-0.047988
H	2.940587	2.844701	-1.482995
H	1.433063	2.952513	-0.587136
H	5.506737	-0.347337	-0.348193
H	4.741016	-1.829548	0.205445
C	5.531172	-1.955983	-1.794818
C	4.325857	-0.549816	-3.512518
H	2.678147	0.607596	-2.730499
H	4.260404	1.124852	-2.155522
C	1.128236	-4.771269	-1.667729
C	-0.696024	-3.562062	-2.885454
C	-0.313251	-4.646628	0.869451
C	-2.285845	-4.552179	-0.662371
H	-2.436837	5.521709	-1.124717

H	-3.794738	4.991744	-0.135360
C	-1.988230	5.349617	0.997991
H	-3.368715	4.500684	2.428217
H	-1.742931	4.721545	3.067205
H	-3.832606	-0.003038	-4.651537
H	-4.302521	-1.238165	-3.487588
C	-5.571322	0.511232	-3.448693
H	-6.257176	-0.691597	-1.785376
H	-7.023682	0.892170	-1.872785
H	-5.421173	-1.138644	3.110413
H	-5.308224	-2.799007	2.536267
C	-3.697432	-2.196239	3.868996
H	-2.040258	-1.204306	4.869056
H	-3.419576	-0.159767	4.540639
H	2.508141	-3.886141	3.052649
H	3.991107	-2.936851	3.038246
C	2.465737	-2.145975	4.355869
H	2.560843	-0.164151	5.247465
H	4.022478	-0.646930	4.392801
H	4.481242	3.762736	2.169007
H	6.007632	3.651866	1.297438
C	4.404124	4.610225	0.180000
H	2.545737	5.181213	-0.798944
H	2.361839	4.698868	0.885817
H	6.511500	-2.316053	-1.455530
H	4.930820	-2.849688	-2.020749
C	5.681336	-1.115219	-3.069154
H	3.667025	-1.375621	-3.817734
H	4.449610	0.094979	-4.392639
H	1.775322	-4.527494	-2.517158
H	0.699372	-5.764644	-1.846033
H	1.751956	-4.819406	-0.771915
H	-1.471856	-2.792064	-2.831968
H	-1.157770	-4.501504	-3.209264
H	0.027760	-3.253386	-3.646304
H	0.656256	-4.221522	1.139804
H	-0.177774	-5.712452	0.653591
H	-0.975458	-4.554927	1.736709
H	-2.899963	-4.640573	0.240212
H	-2.138840	-5.560583	-1.067369
H	-2.844657	-3.963014	-1.393223
H	-0.902688	5.354771	0.817672
H	-2.269912	6.381952	1.242831
H	-6.299290	0.077404	-4.146394
H	-5.493976	1.579433	-3.701217
H	-4.213375	-2.496468	4.790622
H	-3.066153	-3.045876	3.569501
H	2.866229	-2.667096	5.235200
H	1.369574	-2.182645	4.439919
H	4.638048	5.622753	0.533325
H	4.929397	4.484559	-0.778718
H	6.374997	-0.282949	-2.875337
H	6.129197	-1.714571	-3.872388
C	0.081178	1.387123	-2.664992
O	0.027677	2.550335	-2.829710
O	0.158571	0.209812	-2.740806

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Ru	0.023038	0.357748	-0.238357
P	-2.384208	0.682842	0.122617
P	2.427254	0.296563	0.123654
B	-0.162121	-1.694949	-0.338207
H	0.040929	0.831271	1.295147
C	-2.844479	2.516040	0.357929
C	-3.669073	0.050556	-1.124542
C	-3.074416	0.001574	1.787608
C	2.918863	-0.524168	1.761929

C	3.161553	2.032222	0.373071
C	3.449028	-0.665687	-1.150913
O	0.636614	-2.480881	-1.152700
O	-1.138148	-2.466491	0.281605
H	-3.900982	2.499682	0.666418
C	-2.734991	3.371733	-0.921560
C	-2.040166	3.180555	1.498086
H	-3.715857	-1.020296	-0.882446
C	-3.213069	0.132513	-2.597747
C	-5.092420	0.633837	-0.972996
H	-3.750933	0.795813	2.139176
C	-3.906673	-1.298587	1.691405
C	-1.974569	-0.190656	2.856260
H	4.016990	-0.535707	1.773673
C	2.434676	-1.985743	1.841650
C	2.457417	0.243437	3.020113
H	2.617501	2.360135	1.271126
C	4.671372	2.099711	0.693967
C	2.812713	3.058176	-0.727329
H	2.811838	-1.547321	-1.298383
C	4.855796	-1.162370	-0.747970
C	3.514664	0.057125	-2.515328
C	-0.014191	-3.764237	-1.347071
C	-0.943404	-3.867943	-0.075929
H	-1.698649	3.375324	-1.273085
H	-3.333077	2.940001	-1.730349
C	-3.198075	4.818602	-0.673230
C	-2.489555	4.632239	1.742468
H	-2.143033	2.614571	2.429643
H	-0.972202	3.167101	1.240982
H	-3.121938	1.180709	-2.910789
H	-2.220580	-0.309148	-2.713172
C	-4.214951	-0.581365	-3.523192
C	-6.091532	-0.089020	-1.894340
H	-5.438733	0.577758	0.065734
H	-5.081629	1.699155	-1.236496
H	-3.261895	-2.101450	1.320716
H	-4.732297	-1.192831	0.982512
C	-4.496396	-1.697072	3.057712
C	-2.559462	-0.586405	4.223086
H	-1.289506	-0.971978	2.507259
H	-1.373056	0.715689	2.965978
H	1.337524	-1.990969	1.834200
H	2.752653	-2.552190	0.959170
C	2.929647	-2.680634	3.121428
C	2.937133	-0.449054	4.309186
H	2.834783	1.271641	3.013144
H	1.362092	0.310720	3.021841
H	4.945928	1.389236	1.481675
H	5.244165	1.816589	-0.199070
C	5.088809	3.519894	1.118466
C	3.229650	4.478561	-0.305402
H	3.328652	2.800473	-1.660898
H	1.744952	3.042258	-0.952920
H	5.528984	-0.309227	-0.596907
H	4.828704	-1.712287	0.198807
C	5.446533	-2.079219	-1.836407
C	4.101517	-0.862039	-3.600407
H	2.517450	0.385245	-2.818832
H	4.146560	0.951635	-2.431732
C	1.062900	-4.843710	-1.454373
C	-0.788771	-3.671039	-2.669709
C	-0.285956	-4.562841	1.123374
C	-2.315115	-4.494164	-0.334156
H	-3.091219	5.399447	-1.598262
H	-4.269812	4.824082	-0.421586
C	-2.408646	5.477573	0.465031

H	-3.526331	4.631194	2.111704
H	-1.876660	5.076644	2.537695
H	-3.885771	-0.486193	-4.565768
H	-4.212759	-1.658112	-3.293087
C	-5.640794	-0.036357	-3.361318
H	-6.182339	-1.139116	-1.577966
H	-7.088676	0.357131	-1.783840
H	-5.213502	-0.927532	3.381741
H	-5.069441	-2.627625	2.949036
C	-3.411907	-1.857187	4.128886
H	-1.742810	-0.724957	4.944148
H	-3.178222	0.238036	4.609244
H	2.555203	-3.712434	3.153212
H	4.027693	-2.748846	3.099593
C	2.490060	-1.915267	4.376630
H	2.566246	0.103926	5.181920
H	4.035654	-0.403953	4.356054
H	4.587913	3.774705	2.064476
H	6.167675	3.543336	1.321078
C	4.720084	4.559751	0.051391
H	2.990182	5.184545	-1.110669
H	2.631546	4.785289	0.566231
H	6.453070	-2.402685	-1.539520
H	4.833512	-2.989939	-1.907073
C	5.487890	-1.389781	-3.207079
H	3.417470	-1.708149	-3.757771
H	4.154462	-0.320725	-4.553799
H	1.677818	-4.657759	-2.340961
H	0.613099	-5.837998	-1.559255
H	1.721044	-4.851133	-0.582232
H	-1.549120	-2.885499	-2.631151
H	-1.274220	-4.619348	-2.925244
H	-0.089044	-3.412072	-3.469728
H	0.703103	-4.151611	1.337436
H	-0.183780	-5.640456	0.954524
H	-0.913117	-4.414288	2.008502
H	-2.895492	-4.513882	0.594174
H	-2.211095	-5.527683	-0.685016
H	-2.884795	-3.931886	-1.077452
H	-1.356018	5.578577	0.162775
H	-2.780634	6.492911	0.654352
H	-6.340208	-0.596893	-3.995061
H	-5.670640	1.006931	-3.709247
H	-3.863433	-2.093183	5.101388
H	-2.765749	-2.707956	3.866307
H	2.889666	-2.395366	5.279186
H	1.393680	-1.956400	4.457433
H	4.978786	5.568868	0.397437
H	5.319210	4.375949	-0.853026
H	6.197535	-0.549587	-3.167702
H	5.866977	-2.082391	-3.969841
C	0.051050	1.210167	-2.111520
O	0.043677	2.402302	-2.333566
O	0.080705	0.092185	-2.629683

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Ru	-0.016927	0.286645	-0.129204
P	-2.411260	0.713690	0.143328
P	2.386126	0.333168	0.152128
B	-0.181679	-1.787992	-0.513428
H	0.081137	1.247485	1.172701
C	-2.792020	2.573373	0.127489
C	-3.719782	-0.022418	-1.019812
C	-3.074077	0.220055	1.869708
C	2.931427	-0.253061	1.869673
C	2.986830	2.127271	0.146308
C	3.454721	-0.702136	-1.023093

O	0.884729	-2.686204	-0.528286
O	-1.399601	-2.466401	-0.462939
H	-3.877811	2.653126	0.282485
C	-2.448670	3.217647	-1.233599
C	-2.111002	3.355233	1.272024
H	-3.785964	-1.055934	-0.659729
C	-3.284184	-0.133285	-2.498060
C	-5.121083	0.619675	-0.914360
H	-3.780533	1.014922	2.154385
C	-3.839202	-1.121735	1.913268
C	-1.935352	0.186625	2.915414
H	4.029303	-0.214293	1.869010
C	2.506968	-1.714411	2.132334
C	2.444263	0.645488	3.027429
H	2.453279	2.530466	1.018975
C	4.494804	2.362778	0.375017
C	2.494027	2.950044	-1.065007
H	2.861127	-1.622650	-1.081116
C	4.875725	-1.096552	-0.561441
C	3.511836	-0.112182	-2.450570
C	0.353136	-3.988000	-0.892995
C	-1.128572	-3.890960	-0.364278
H	-1.380146	3.084527	-1.443535
H	-2.979386	2.709057	-2.044219
C	-2.797672	4.715708	-1.266154
C	-2.469579	4.851478	1.232324
H	-2.400313	2.946293	2.246484
H	-1.022381	3.239988	1.192601
H	-3.145918	0.861082	-2.940208
H	-2.323084	-0.645985	-2.559909
C	-4.331617	-0.905665	-3.320928
C	-6.159448	-0.166251	-1.734761
H	-5.451284	0.689340	0.129920
H	-5.083383	1.648552	-1.296798
H	-3.175302	-1.922742	1.565827
H	-4.696332	-1.105934	1.234288
C	-4.349374	-1.445603	3.329648
C	-2.446931	-0.130684	4.330029
H	-1.209719	-0.580585	2.609178
H	-1.386982	1.132155	2.924767
H	1.410688	-1.771271	2.116501
H	2.846975	-2.373874	1.328437
C	3.027659	-2.221654	3.487199
C	2.958733	0.138264	4.387117
H	2.776277	1.680074	2.888415
H	1.346975	0.667428	3.033998
H	4.857645	1.803461	1.245839
H	5.058585	1.995048	-0.492485
C	4.798165	3.860751	0.567250
C	2.792675	4.446084	-0.867206
H	2.987951	2.607801	-1.982056
H	1.423293	2.795557	-1.223344
H	5.513309	-0.206354	-0.482302
H	4.854492	-1.556996	0.431853
C	5.517024	-2.088518	-1.551078
C	4.142541	-1.110064	-3.437010
H	2.515005	0.170481	-2.799901
H	4.118551	0.803667	-2.447409
C	1.211062	-5.065060	-0.230113
C	0.442698	-4.116724	-2.420996
C	-1.264168	-4.294220	1.110946
C	-2.167632	-4.635219	-1.203448
H	-2.505479	5.137443	-2.236219
H	-3.888764	4.837385	-1.187688
C	-2.122788	5.482647	-0.122123
H	-3.546551	4.972734	1.423317
H	-1.948524	5.374093	2.045239

H	-4.017219	-0.941768	-4.371874
H	-4.364996	-1.947770	-2.968955
C	-5.732590	-0.289603	-3.204105
H	-6.276292	-1.171955	-1.304060
H	-7.139823	0.322447	-1.658861
H	-5.100515	-0.696029	3.621041
H	-4.866844	-2.413947	3.317745
C	-3.219569	-1.454252	4.366388
H	-1.600203	-0.159765	5.028482
H	-3.103632	0.683995	4.670916
H	2.693173	-3.254908	3.648805
H	4.127690	-2.250514	3.467046
C	2.565798	-1.323144	4.641929
H	2.574549	0.783264	5.188106
H	4.055139	0.227511	4.414725
H	4.320052	4.207415	1.495689
H	5.878252	4.006349	0.700233
C	4.285455	4.700445	-0.611508
H	2.455826	5.008762	-1.747158
H	2.209112	4.821863	-0.012843
H	6.532677	-2.338528	-1.216831
H	4.942903	-3.026895	-1.535513
C	5.544604	-1.538842	-2.983718
H	3.494109	-1.994776	-3.516352
H	4.184231	-0.662636	-4.438355
H	2.223745	-5.036382	-0.646419
H	0.799667	-6.063699	-0.418735
H	1.285850	-4.916864	0.849782
H	-0.148091	-3.345134	-2.921284
H	0.103554	-5.101090	-2.762287
H	1.486347	-3.990256	-2.726867
H	-0.544767	-3.756936	1.736702
H	-1.110606	-5.369854	1.250187
H	-2.271303	-4.048450	1.461759
H	-3.163818	-4.484372	-0.773801
H	-1.966187	-5.713083	-1.214220
H	-2.186124	-4.272613	-2.233641
H	-1.032111	5.459995	-0.264309
H	-2.419967	6.539222	-0.139661
H	-6.463494	-0.887584	-3.763907
H	-5.728797	0.710347	-3.663217
H	-3.622175	-1.639639	5.370571
H	-2.530005	-2.282422	4.145733
H	2.986979	-1.671966	5.593667
H	1.471881	-1.392469	4.738476
H	4.467408	5.766864	-0.425785
H	4.855574	4.438460	-1.515227
H	6.219257	-0.670337	-3.025325
H	5.958923	-2.288398	-3.670454
C	0.011347	0.507771	-2.075600
O	0.075873	1.338527	-2.948805
O	-0.086449	-0.805028	-2.094715

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Ru	-0.017352	0.221147	-0.229201
P	2.288763	0.988298	-0.102258
P	-2.479226	0.148935	-0.180232
B	0.524642	-1.977099	-0.208726
H	-0.262208	1.742303	0.285121
C	2.499297	2.846344	-0.426222
C	2.899337	0.721677	1.666069
C	3.739976	0.353257	-1.184706
C	-3.447863	-0.756429	-1.532808
C	-3.178288	1.918668	-0.309768
C	-3.138219	-0.652474	1.400366
O	1.825674	-2.394416	0.049222
O	-0.406476	-2.836107	0.354991

H	3.569535	3.041807	-0.257617
C	1.698610	3.776349	0.507648
C	2.175482	3.187091	-1.899113
H	3.239686	-0.322181	1.637746
C	1.737695	0.767893	2.681532
C	4.075131	1.593632	2.154783
H	4.334148	1.257545	-1.387523
C	4.687337	-0.675035	-0.525858
C	3.257897	-0.212636	-2.539748
H	-4.510077	-0.556897	-1.328495
C	-3.260360	-2.289846	-1.504101
C	-3.121483	-0.192653	-2.937011
H	-2.557602	2.325783	-1.122072
C	-4.657686	2.096935	-0.726975
C	-2.898611	2.784805	0.938287
H	-2.916980	-1.713739	1.220484
C	-4.651178	-0.523164	1.675397
C	-2.319786	-0.253452	2.647377
C	1.764564	-3.772042	0.517532
C	0.301443	-3.861711	1.103752
H	0.628911	3.570319	0.383322
H	1.933114	3.575198	1.558490
C	1.970734	5.259861	0.199791
C	2.423377	4.672711	-2.214106
H	2.774840	2.575057	-2.580700
H	1.124215	2.936412	-2.096286
H	1.311334	1.777443	2.731515
H	0.927289	0.105174	2.341047
C	2.200770	0.337030	4.083826
C	4.544047	1.153760	3.553481
H	4.914427	1.553817	1.450786
H	3.763199	2.644547	2.203809
H	4.122083	-1.587058	-0.305902
H	5.083408	-0.302653	0.424123
C	5.874740	-1.006759	-1.450671
C	4.441564	-0.517156	-3.473039
H	2.707462	-1.141130	-2.358030
H	2.555873	0.466223	-3.031531
H	-2.203776	-2.544752	-1.628221
H	-3.565627	-2.695722	-0.532728
C	-4.081436	-2.974494	-2.611828
C	-3.948075	-0.890314	-4.030449
H	-3.306458	0.887793	-2.973710
H	-2.055498	-0.326351	-3.143817
H	-4.893379	1.516571	-1.622981
H	-5.318601	1.728825	0.067881
C	-4.976879	3.579559	-0.998929
C	-3.204934	4.268265	0.670410
H	-3.529978	2.443036	1.769900
H	-1.857172	2.671955	1.254490
H	-4.905900	0.529959	1.851591
H	-5.233887	-0.847035	0.804982
C	-5.069913	-1.337423	2.912667
C	-2.755883	-1.048123	3.891106
H	-1.254890	-0.430370	2.452128
H	-2.429826	0.818454	2.850550
C	2.882120	-3.989898	1.537442
C	1.989468	-4.667623	-0.709438
C	0.215974	-3.488389	2.589665
C	-0.407703	-5.195103	0.863619
H	1.377390	5.889665	0.875542
H	3.027100	5.490524	0.404953
C	1.653136	5.597149	-1.262767
H	3.500028	4.884659	-2.130029
H	2.146417	4.877738	-3.256252
H	1.366593	0.410717	4.793515
H	2.496638	-0.722433	4.055412

C	3.391008	1.179889	4.568137
H	4.954026	0.134608	3.494339
H	5.363462	1.800532	3.892968
H	6.491416	-0.104397	-1.580804
H	6.517573	-1.753233	-0.965082
C	5.417935	-1.508368	-2.826641
H	4.064992	-0.916622	-4.423188
H	4.972774	0.416644	-3.713452
H	-3.897578	-4.056287	-2.583479
H	-5.155133	-2.833953	-2.412325
C	-3.746644	-2.411060	-3.999094
H	-3.668453	-0.487203	-5.012371
H	-5.015921	-0.661050	-3.889945
H	-4.390649	3.917517	-1.866321
H	-6.033491	3.683179	-1.278449
C	-4.654554	4.470013	0.208471
H	-3.007023	4.856934	1.575866
H	-2.518210	4.642821	-0.103164
H	-6.145023	-1.210431	3.094517
H	-4.909603	-2.407538	2.714689
C	-4.263915	-0.923736	4.151787
H	-2.506077	-2.109011	3.746770
H	-2.186162	-0.709523	4.766372
H	3.854752	-3.886296	1.045609
H	2.829234	-4.998158	1.964473
H	2.836643	-3.264350	2.353396
H	1.238506	-4.473455	-1.478924
H	1.973379	-5.729678	-0.441220
H	2.971057	-4.438448	-1.137294
H	0.689153	-2.522053	2.789942
H	0.690778	-4.244867	3.223781
H	-0.836535	-3.415130	2.879353
H	-1.420672	-5.152166	1.277486
H	0.124007	-6.017257	1.357123
H	-0.487719	-5.418429	-0.202215
H	0.573242	5.476470	-1.434716
H	1.889381	6.647959	-1.474756
H	3.736023	0.822447	5.546743
H	3.061799	2.219637	4.713178
H	6.285520	-1.678617	-3.477465
H	4.916025	-2.479833	-2.709323
H	-4.363873	-2.895279	-4.767192
H	-2.698936	-2.641421	-4.238077
H	-4.837388	5.524534	-0.035282
H	-5.334981	4.217830	1.035721
H	-4.505183	0.118429	4.409606
H	-4.551772	-1.534101	5.017366
C	0.201878	-1.361504	-1.855424
O	0.248530	-2.395452	-2.519214
O	0.053697	-0.150078	-2.259576

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Ru	-0.066427	-0.129047	-0.158879
P	-2.525541	-0.375658	0.020541
P	2.350516	-0.528868	-0.130871
B	0.117852	1.955693	0.521565
H	-0.078762	0.929266	1.325468
C	-3.272784	-1.967679	-0.708093
C	-2.985841	-0.477867	1.858234
C	-3.754014	0.906584	-0.664130
C	3.479287	0.008939	-1.549442
C	2.488781	-2.411324	-0.171111
C	3.248166	0.140714	1.400280
O	-0.912030	2.889229	0.396965
O	1.349945	2.611242	0.591490
H	-4.271272	-2.036656	-0.251350
C	-2.476639	-3.232862	-0.319639

C	-3.482880	-1.933078	-2.240270
H	-2.925992	0.576692	2.163724
C	-1.955423	-1.232890	2.727560
C	-4.405480	-0.988302	2.183058
H	-4.663522	0.332629	-0.899924
C	-4.160348	2.034996	0.309163
C	-3.210650	1.525561	-1.972557
H	4.489893	-0.325557	-1.272929
C	3.503665	1.546043	-1.687850
C	3.137966	-0.636074	-2.910652
H	2.153090	-2.628515	-1.193840
C	3.880652	-3.046226	0.015286
C	1.456095	-3.099392	0.750236
H	2.945396	1.194598	1.374824
C	4.792509	0.098221	1.420254
C	2.690469	-0.448861	2.714107
C	-0.328423	4.188432	0.114180
C	1.121725	4.036208	0.707428
H	-1.474994	-3.167860	-0.759033
H	-2.354012	-3.296449	0.766861
C	-3.161726	-4.515754	-0.823662
C	-4.166852	-3.219234	-2.739634
H	-4.097656	-1.074679	-2.528174
H	-2.516568	-1.826259	-2.744516
H	-1.968340	-2.303817	2.488824
H	-0.941068	-0.872009	2.514617
C	-2.263536	-1.055411	4.225152
C	-4.729430	-0.808964	3.677390
H	-5.159778	-0.477323	1.573509
H	-4.475982	-2.056037	1.934193
H	-3.267199	2.601869	0.593525
H	-4.593997	1.627759	1.228468
C	-5.196013	2.974278	-0.338298
C	-4.245938	2.456589	-2.625566
H	-2.301945	2.085978	-1.732266
H	-2.905377	0.751726	-2.682286
H	2.489315	1.890013	-1.923233
H	3.771296	2.019417	-0.737797
C	4.480795	1.999980	-2.785699
C	4.130799	-0.189362	-3.998530
H	3.147775	-1.728820	-2.842746
H	2.125390	-0.344662	-3.207177
H	4.619375	-2.575594	-0.644604
H	4.227324	-2.882917	1.044395
C	3.831198	-4.561206	-0.257495
C	1.401017	-4.611819	0.474215
H	1.710651	-2.935212	1.804743
H	0.460631	-2.661077	0.588611
H	5.144571	-0.940783	1.438596
H	5.209713	0.555155	0.517065
C	5.345943	0.841224	2.651831
C	3.233893	0.305937	3.939290
H	1.594502	-0.414323	2.712490
H	2.977670	-1.505490	2.799833
C	-1.186168	5.263912	0.781780
C	-0.339455	4.382644	-1.409315
C	1.209797	4.384650	2.201488
C	2.217429	4.776967	-0.059849
H	-2.554103	-5.387327	-0.547261
H	-4.131878	-4.636661	-0.317375
C	-3.381578	-4.475128	-2.341088
H	-5.183644	-3.277708	-2.321447
H	-4.280410	-3.169100	-3.830222
H	-1.533355	-1.614473	4.824570
H	-2.143591	0.004719	4.493310
C	-3.691185	-1.509038	4.566758
H	-4.750348	0.264672	3.916135

H	-5.734578	-1.195738	3.889808
H	-6.125503	2.413583	-0.520823
H	-5.452358	3.777532	0.365303
C	-4.697071	3.564145	-1.663945
H	-3.823930	2.893403	-3.540088
H	-5.122716	1.868985	-2.938537
H	4.448344	3.093748	-2.878850
H	5.508419	1.744587	-2.484744
C	4.170849	1.338431	-4.135073
H	3.855128	-0.651318	-4.955053
H	5.137606	-0.559231	-3.750502
H	3.582588	-4.726892	-1.315825
H	4.823379	-5.002308	-0.095201
C	2.785886	-5.260397	0.624683
H	0.682162	-5.089949	1.152480
H	1.028526	-4.771416	-0.547199
H	6.441889	0.776498	2.660279
H	5.096970	1.909304	2.565553
C	4.768687	0.294648	3.964877
H	2.875725	1.345361	3.909468
H	2.832782	-0.138932	4.859407
H	-2.180997	5.281184	0.324783
H	-0.739091	6.256377	0.649572
H	-1.309646	5.077360	1.851194
H	0.233603	3.599293	-1.914086
H	0.068646	5.358573	-1.693816
H	-1.370645	4.328169	-1.770318
H	0.438508	3.863786	2.777551
H	1.106342	5.461346	2.374684
H	2.186967	4.069652	2.582232
H	3.188875	4.586611	0.408822
H	2.043020	5.859170	-0.043209
H	2.275494	4.448966	-1.099680
H	-2.406335	-4.466426	-2.847039
H	-3.908166	-5.378282	-2.676311
H	-3.907705	-1.320325	5.626037
H	-3.768109	-2.596869	4.421265
H	-5.480033	4.179978	-2.125686
H	-3.849098	4.235336	-1.462905
H	4.912838	1.637464	-4.886884
H	3.194578	1.692938	-4.496602
H	2.734083	-6.328484	0.377454
H	3.102176	-5.198119	1.676999
H	5.119677	-0.737576	4.113627
H	5.142644	0.876949	4.816906
C	-0.068359	-1.051308	-1.966721
O	-0.019081	-2.137788	-2.515993
O	-0.132687	0.171875	-2.300166

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Ru	-0.088555	-0.840537	-0.127743
P	2.430890	-1.075709	-0.035797
P	-2.528077	-0.887650	0.087928
H	-0.069144	-1.210351	1.399760
C	3.721431	0.220451	-0.525975
C	2.836203	-1.368644	1.806326
C	2.982547	-2.653316	-0.930500
C	-3.132882	-1.765058	1.656500
C	-3.310004	0.849594	0.197024
C	-3.453608	-1.686843	-1.361357
H	4.661975	-0.184324	-0.125649
C	3.938918	0.441096	-2.038132
C	3.455163	1.580038	0.151467
H	2.178512	-0.632197	2.288298
C	4.273521	-1.103480	2.311429
C	2.375895	-2.766022	2.278811
H	2.452251	-3.437640	-0.374690

C	4.486476	-3.003463	-0.880197
C	2.466293	-2.733996	-2.388664
H	-2.837585	-1.051526	2.437725
C	-4.664469	-1.957189	1.753884
C	-2.399242	-3.083759	1.992938
H	-2.597882	1.451578	-0.378263
C	-4.707638	1.029724	-0.441692
C	-3.303635	1.392435	1.644048
H	-4.503119	-1.394091	-1.229089
C	-3.431498	-3.230188	-1.430349
C	-2.955185	-1.105396	-2.703939
H	3.026128	0.846350	-2.487683
H	4.166258	-0.500865	-2.543579
C	5.113260	1.411357	-2.276246
C	4.632402	2.545675	-0.063667
H	3.276662	1.453497	1.224657
H	2.543666	2.014034	-0.266985
H	4.620178	-0.106610	2.023874
H	4.974389	-1.820161	1.863404
C	4.347487	-1.227022	3.845517
C	2.444097	-2.891533	3.810343
H	3.022431	-3.535644	1.833744
H	1.356753	-2.968470	1.936914
H	4.852055	-2.996621	0.151729
H	5.069105	-2.247219	-1.422952
C	4.754334	-4.388738	-1.500470
C	2.722961	-4.126108	-2.988489
H	2.968797	-1.984258	-3.009854
H	1.398882	-2.501026	-2.431644
H	-5.186355	-1.012642	1.573827
H	-5.003737	-2.652577	0.975268
C	-5.081434	-2.510923	3.128999
C	-2.829242	-3.625703	3.367648
H	-2.600458	-3.845233	1.230182
H	-1.319611	-2.915726	1.991496
H	-4.693698	0.730691	-1.493944
H	-5.445799	0.388537	0.058246
C	-5.193396	2.488766	-0.356509
C	-3.776933	2.855263	1.694009
H	-3.981159	0.799235	2.272925
H	-2.302749	1.310628	2.079018
H	-2.405120	-3.591438	-1.549751
H	-3.812402	-3.670128	-0.504255
C	-4.283801	-3.736721	-2.609766
C	-3.798559	-1.609478	-3.887047
H	-2.943598	-0.011458	-2.688195
H	-1.911219	-1.414088	-2.848968
H	6.043530	0.942861	-1.919840
H	5.241297	1.572730	-3.354854
C	4.917302	2.752961	-1.557138
H	4.411861	3.507939	0.416152
H	5.532605	2.147134	0.429603
H	3.732358	-0.434807	4.296590
H	5.378391	-1.049181	4.178805
C	3.854258	-2.593210	4.338426
H	1.727839	-2.188095	4.259282
H	2.127444	-3.898189	4.112975
H	5.831834	-4.598712	-1.482078
H	4.275371	-5.157392	-0.875979
C	4.212098	-4.494928	-2.932635
H	2.136988	-4.870840	-2.431239
H	2.362354	-4.154072	-4.024948
H	-4.855663	-1.761458	3.902170
H	-6.168600	-2.662741	3.149804
C	-4.348587	-3.816492	3.462088
H	-2.504557	-2.922665	4.149362
H	-2.311203	-4.573048	3.565360

H	-4.546458	3.119147	-0.982969
H	-6.203591	2.561169	-0.780795
C	-5.172835	3.020565	1.081568
H	-3.066854	3.484916	1.141469
H	-3.770911	3.208253	2.733978
H	-5.337096	-3.468022	-2.437337
H	-4.243460	-4.833125	-2.644709
C	-3.823033	-3.142599	-3.947557
H	-3.403773	-1.195208	-4.823856
H	-4.827927	-1.232499	-3.788767
H	4.068296	3.281900	-2.009505
H	5.799777	3.391547	-1.695435
H	4.544618	-3.375518	3.988636
H	3.869647	-2.631288	5.435351
H	4.778505	-3.814189	-3.585788
H	4.372098	-5.508017	-3.323537
H	-4.662311	-4.600066	2.756075
H	-4.630270	-4.167119	4.463371
H	-5.905622	2.466132	1.687162
H	-5.481385	4.073848	1.103418
H	-2.811971	-3.510917	-4.175958
H	-4.473645	-3.485773	-4.762429
C	0.686527	4.091224	2.306378
C	0.602490	2.878937	3.338191
B	0.241194	2.104001	1.170022
O	0.113958	1.790030	2.534396
O	0.675324	3.436371	1.025750
O	-0.015328	1.297572	0.153356
C	-0.370681	3.093032	4.502536
H	-0.395103	2.191579	5.124189
H	-0.057300	3.931452	5.135728
H	-1.387505	3.284097	4.151648
C	1.965511	2.456639	3.908583
H	2.383768	3.216934	4.577484
H	1.835386	1.531829	4.480482
H	2.690214	2.260880	3.114069
C	1.963182	4.933567	2.406039
H	1.952562	5.698586	1.622341
H	2.029378	5.443684	3.374269
H	2.862340	4.328433	2.269438
C	-0.527764	5.030709	2.358238
H	-0.564210	5.600208	3.293454
H	-0.460870	5.741698	1.528022
H	-1.465286	4.480340	2.252071
C	0.496797	3.224677	-3.213017
C	-1.051844	3.246964	-2.864545
B	-0.103118	1.293300	-2.130298
H	-0.013007	0.090375	-2.011576
O	-1.308649	1.875045	-2.449510
O	0.981535	2.050373	-2.504784
C	-1.403788	4.166970	-1.689714
H	-1.276864	5.220902	-1.961315
H	-2.455432	4.014430	-1.426369
H	-0.793414	3.953800	-0.809889
C	-1.973558	3.550312	-4.047806
H	-3.016365	3.496989	-3.717799
H	-1.795064	4.559783	-4.435796
H	-1.842324	2.834522	-4.862668
C	0.792881	2.980950	-4.699461
H	0.500524	3.836331	-5.318070
H	1.868267	2.819425	-4.824722
H	0.274948	2.090384	-5.068852
C	1.273794	4.444558	-2.715798
H	2.325129	4.353714	-3.007761
H	0.882933	5.366734	-3.161577
H	1.227517	4.525731	-1.627673
C	-0.144379	-2.649663	-0.453541

O	-0.159004	-3.811413	-0.599807
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Ru	-0.078580	-0.837770	0.002161
P	2.441789	-1.080653	0.081794
P	-2.528419	-0.897733	0.160911
H	-0.060793	-1.184033	1.566727
C	3.737586	0.206823	-0.423230
C	2.881573	-1.396836	1.913844
C	2.966102	-2.654715	-0.836657
C	-3.179961	-1.804969	1.694267
C	-3.325882	0.832192	0.278181
C	-3.400928	-1.666880	-1.332792
H	4.682023	-0.219142	-0.055604
C	3.903444	0.445276	-1.939026
C	3.518558	1.561828	0.281482
H	2.239945	-0.660615	2.417925
C	4.330136	-1.149271	2.394928
C	2.415469	-2.791954	2.386255
H	2.447078	-3.440954	-0.273303
C	4.469977	-3.007102	-0.817304
C	2.420932	-2.728440	-2.284368
H	-2.923468	-1.098065	2.495198
C	-4.711891	-2.014479	1.729077
C	-2.446133	-3.119628	2.043968
H	-2.632114	1.445207	-0.306552
C	-4.721432	1.015225	-0.364772
C	-3.322613	1.371312	1.726130
H	-4.459284	-1.403366	-1.206498
C	-3.340758	-3.205449	-1.454194
C	-2.894918	-1.027835	-2.646405
H	2.972505	0.858275	-2.339995
H	4.107883	-0.492382	-2.461895
C	5.069444	1.416024	-2.212901
C	4.701938	2.512849	0.034471
H	3.373330	1.423619	1.358909
H	2.612168	2.026013	-0.115659
H	4.685472	-0.156984	2.102552
H	5.014277	-1.874643	1.935462
C	4.425986	-1.276082	3.927484
C	2.508084	-2.925278	3.915954
H	3.046775	-3.565299	1.926240
H	1.388033	-2.980303	2.062395
H	4.857515	-3.000542	0.206523
H	5.042041	-2.252740	-1.373595
C	4.719885	-4.393353	-1.442269
C	2.660168	-4.121138	-2.890122
H	2.915827	-1.980145	-2.913001
H	1.355449	-2.485406	-2.306437
H	-5.236749	-1.073123	1.542009
H	-5.011515	-2.702482	0.927754
C	-5.177171	-2.591487	3.078827
C	-2.924278	-3.684017	3.393507
H	-2.609678	-3.873343	1.264477
H	-1.369571	-2.938766	2.088211
H	-4.705049	0.708868	-1.414458
H	-5.470878	0.388910	0.136780
C	-5.179671	2.484000	-0.293738
C	-3.785699	2.837563	1.773326
H	-4.004669	0.780107	2.352383
H	-2.323085	1.288664	2.165749
H	-2.304808	-3.535593	-1.582275
H	-3.714031	-3.688626	-0.546171
C	-4.173595	-3.687171	-2.657800
C	-3.720203	-1.503610	-3.853385
H	-2.894951	0.064408	-2.588731
H	-1.843932	-1.311662	-2.789087

H	6.014522	0.941936	-1.905463
H	5.149042	1.592455	-3.293747
C	4.908834	2.747999	-1.467444
H	4.523040	3.467563	0.546534
H	5.618199	2.087986	0.472833
H	3.824107	-0.479297	4.389350
H	5.462989	-1.107782	4.246326
C	3.928081	-2.639290	4.424238
H	1.803441	-2.219220	4.379297
H	2.188931	-3.930944	4.218994
H	5.796701	-4.607514	-1.445524
H	4.250548	-5.160069	-0.808118
C	4.148718	-4.497059	-2.863275
H	2.081898	-4.864396	-2.322797
H	2.279781	-4.146146	-3.919479
H	-4.991460	-1.850040	3.870285
H	-6.262504	-2.755142	3.053570
C	-4.443723	-3.893217	3.424820
H	-2.639410	-2.987669	4.196621
H	-2.403099	-4.627784	3.599868
H	-4.506639	3.096549	-0.910690
H	-6.181251	2.576142	-0.734078
C	-5.171797	3.018015	1.143694
H	-3.065131	3.459415	1.224867
H	-3.786383	3.191363	2.813060
H	-5.233613	-3.447857	-2.483038
H	-4.109137	-4.780448	-2.732872
C	-3.716754	-3.033943	-3.969650
H	-3.325453	-1.049963	-4.771866
H	-4.757117	-1.148408	-3.751965
H	4.036297	3.282441	-1.866115
H	5.783827	3.388552	-1.639645
H	4.607209	-3.425859	4.062436
H	3.959237	-2.680555	5.520693
H	4.705283	-3.818881	-3.527358
H	4.296337	-5.510857	-3.257169
H	-4.719725	-4.670893	2.696940
H	-4.761259	-4.259895	4.409509
H	-5.918470	2.473610	1.741411
H	-5.466975	4.075214	1.160811
H	-2.697791	-3.374941	-4.205268
H	-4.356395	-3.359345	-4.800411
C	0.641629	4.445930	1.910315
C	0.525908	3.329853	3.040597
B	0.224908	2.393553	0.960004
O	0.044313	2.173274	2.312367
O	0.667312	3.671211	0.684575
O	-0.012730	1.427509	0.039240
C	-0.475424	3.643539	4.154796
H	-0.517307	2.800027	4.851585
H	-0.170744	4.532728	4.718553
H	-1.481776	3.806909	3.763723
C	1.869806	2.939631	3.671009
H	2.272599	3.743973	4.295884
H	1.719264	2.057723	4.301950
H	2.613761	2.686585	2.912084
C	1.917329	5.289716	1.965821
H	1.927377	5.985609	1.120854
H	1.958963	5.878179	2.889516
H	2.817678	4.674740	1.903238
C	-0.573884	5.379531	1.830640
H	-0.639933	6.031057	2.708521
H	-0.478597	6.011010	0.941843
H	-1.508277	4.819866	1.744047
C	0.497597	2.663981	-3.321835
C	-0.998588	2.988152	-2.938849
B	-0.093686	1.397835	-1.467306

H	-0.068634	0.089205	-1.684844
O	-1.316416	1.931865	-2.017395
O	0.998895	2.056826	-2.122668
C	-1.150955	4.333195	-2.207740
H	-1.000785	5.184681	-2.882155
H	-2.167775	4.399186	-1.803527
H	-0.447536	4.411238	-1.375191
C	-1.988261	2.931301	-4.106509
H	-2.998846	3.149631	-3.743171
H	-1.740820	3.675398	-4.873464
H	-2.005721	1.943098	-4.572991
C	0.608231	1.641788	-4.468314
H	0.299676	2.066893	-5.430148
H	1.651190	1.319843	-4.557789
H	-0.002227	0.756098	-4.267560
C	1.355324	3.890035	-3.642996
H	2.373576	3.574947	-3.897215
H	0.951550	4.441912	-4.500419
H	1.414572	4.565323	-2.786345
C	-0.130523	-2.637457	-0.266857
O	-0.143859	-3.799548	-0.407517

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Ru	0.039516	-0.833763	-0.047760
P	-2.451452	-0.925654	-0.006353
P	2.457735	-1.121863	-0.186394
H	-0.068993	-0.968720	-1.688868
C	-3.637467	0.417391	0.614491
C	-3.050998	-1.155830	-1.810268
C	-3.023406	-2.492034	0.903511
C	3.113610	-2.295706	-1.551726
C	3.496885	0.424972	-0.539254
C	3.245524	-1.780868	1.413225
H	-4.634081	0.048569	0.333627
C	-3.647189	0.639310	2.140543
C	-3.417225	1.765662	-0.102705
H	-2.431948	-0.409921	-2.328703
C	-4.526261	-0.865880	-2.172033
C	-2.645596	-2.534825	-2.376307
H	-2.609287	-3.289104	0.272655
C	-4.546041	-2.736451	0.993515
C	-2.376240	-2.664922	2.298945
H	4.080931	-1.851619	-1.825591
C	3.409207	-3.757585	-1.147691
C	2.231118	-2.288626	-2.819972
H	3.144101	1.140985	0.213056
C	5.026134	0.258014	-0.373508
C	3.198738	1.024150	-1.930287
H	4.263196	-2.098333	1.141131
C	2.499737	-2.997823	2.005736
C	3.351193	-0.698920	2.510401
H	-2.655129	0.971243	2.459904
H	-3.864739	-0.294943	2.664531
C	-4.708050	1.683009	2.541578
C	-4.502641	2.787147	0.276694
H	-3.396704	1.629300	-1.189518
H	-2.445815	2.170549	0.193767
H	-4.844368	0.116339	-1.809591
H	-5.188367	-1.602406	-1.698943
C	-4.738157	-0.923963	-3.697500
C	-2.858061	-2.603104	-3.897898
H	-3.249213	-3.320703	-1.899598
H	-1.597987	-2.743250	-2.145806
H	-5.013412	-2.661550	0.006854
H	-5.015203	-1.967169	1.621951
C	-4.851048	-4.125231	1.588843
C	-2.673987	-4.058561	2.876509

H	-2.764047	-1.906956	2.989844	O	0.126726	1.523366	-0.072427
H	-1.298604	-2.496779	2.241810	C	0.334013	3.616146	-4.284617
H	4.055977	-3.799891	-0.265157	H	0.121935	2.783118	-4.962215
H	2.473219	-4.267506	-0.887974	H	0.108931	4.549317	-4.813488
C	4.091525	-4.519460	-2.299749	H	1.400547	3.595498	-4.050645
C	2.910234	-3.042277	-3.976571	C	-1.998497	3.325118	-3.433331
H	1.270389	-2.761123	-2.588048	H	-2.347674	4.188033	-4.010287
H	1.988660	-1.267199	-3.126728	H	-2.102144	2.430848	-4.055860
H	5.280965	-0.151888	0.607838	H	-2.647526	3.205779	-2.562420
H	5.407584	-0.455445	-1.117348	C	-1.366807	5.659259	-1.817560
C	5.759436	1.598614	-0.564553	H	-1.125393	6.347018	-1.000805
C	3.923028	2.368361	-2.119146	H	-1.430173	6.242689	-2.743023
H	3.544279	0.333096	-2.711431	H	-2.346902	5.223778	-1.610730
H	2.122782	1.148870	-2.076386	C	1.096466	5.263683	-2.012477
H	1.491740	-2.673808	2.289807	H	1.170723	5.904370	-2.897485
H	2.374443	-3.793812	1.270048	H	1.247725	5.886426	-1.125163
C	3.222802	-3.553765	3.244620	H	1.904890	4.528940	-2.048280
C	4.068341	-1.233050	3.763830	C	-0.074156	2.674946	3.364708
H	3.874354	0.191354	2.151759	C	1.414167	2.969196	2.925001
H	2.337392	-0.372548	2.766581	B	0.327505	1.762903	1.309877
H	-5.710015	1.279531	2.329142	H	0.175062	-0.269707	1.629124
H	-4.666338	1.848614	3.626567	O	1.589487	2.069452	1.796865
C	-4.533203	3.012526	1.794173	O	-0.682567	2.256099	2.115106
H	-4.320037	3.736563	-0.245155	C	1.615755	4.393646	2.385429
H	-5.485307	2.426738	-0.063754	H	1.558602	5.141821	3.183669
H	-4.155137	-0.119330	-4.170347	H	2.608639	4.458654	1.928004
H	-5.792340	-0.724137	-3.931278	H	0.873479	4.633188	1.618806
C	-4.305782	-2.274092	-4.284789	C	2.472266	2.659562	3.982358
H	-2.176698	-1.890223	-4.384955	H	3.469177	2.857428	3.574493
H	-2.582341	-3.600412	-4.264875	H	2.336842	3.298061	4.863283
H	-5.937775	-4.261473	1.668684	H	2.437856	1.615881	4.300015
H	-4.489555	-4.897953	0.894306	C	-0.197446	1.513271	4.360627
C	-4.183782	-4.325578	2.955902	H	0.219769	1.777432	5.338309
H	-2.198497	-4.820234	2.241635	H	-1.256336	1.271957	4.497090
H	-2.218106	-4.151084	3.871080	H	0.301933	0.615469	3.987001
H	5.076289	-4.068816	-2.496140	C	-0.838803	3.892496	3.883928
H	4.279422	-5.556647	-1.992543	H	-1.861244	3.601372	4.146211
C	3.253869	-4.485633	-3.584728	H	-0.363660	4.297144	4.785330
H	3.831893	-2.515120	-4.267844	H	-0.894342	4.683012	3.132132
H	2.254774	-3.031977	-4.857311	C	-0.016565	-2.641491	0.011798
H	5.460731	2.289561	0.237534	O	-0.056037	-3.815356	0.001877
H	6.841671	1.446168	-0.458815				
C	5.439164	2.232054	-1.924812				
H	3.533112	3.092508	-1.388791	32			
H	3.702898	2.772489	-3.116658	Ru	-0.140828	0.121431	0.157914
H	4.215827	-3.928869	2.953031	P	-2.501766	-0.015431	-0.094851
H	2.667335	-4.415747	3.636426	P	2.267034	0.144832	0.128117
C	3.381629	-2.482361	4.330088	C	-2.759327	-1.093347	-1.629465
H	4.113452	-0.443263	4.525959	C	-3.544067	-0.678170	1.340287
H	5.111361	-1.477194	3.509761	C	-3.446222	1.578439	-0.491976
H	-3.587180	3.478292	2.101915	C	3.073472	1.842637	-0.064564
H	-5.337015	3.710198	2.063835	C	2.927017	-0.804067	-1.371434
H	-4.970766	-3.062836	-3.901867	C	3.043520	-0.506110	1.732488
H	-4.422359	-2.270268	-5.376462	H	-3.693114	-0.780136	-2.120391
H	-4.635653	-3.634798	3.683793	C	-2.846132	-2.607176	-1.339159
H	-4.377199	-5.340578	3.326786	C	-1.571661	-0.824655	-2.590073
H	2.321815	-5.046310	-3.421833	H	-3.496973	0.167024	2.043716
H	3.786271	-4.991140	-4.401113	C	-2.919387	-1.881696	2.079680
H	5.850847	1.599171	-2.725187	C	-5.040491	-0.936254	1.048106
H	5.928813	3.210400	-2.016267	H	-4.511351	1.306803	-0.526619
H	2.386952	-2.206601	4.710022	C	-3.242898	2.623169	0.628574
H	3.946943	-2.877475	5.184420	C	-3.085489	2.198603	-1.857664
C	-0.278298	4.589785	-1.918041	H	4.160269	1.691546	-0.001251
C	-0.527022	3.477660	-3.028476	C	2.651256	2.783976	1.085195
B	-0.098402	2.498370	-1.008014	C	2.766845	2.499357	-1.427345
O	-0.140984	2.248142	-2.353402	H	2.490102	-0.223943	-2.199503
O	-0.288133	3.821225	-0.682978	C	4.456400	-0.820491	-1.583892
				C	2.363357	-2.236607	-1.501191

H	2.470141	0.061937	2.480526
C	4.538636	-0.216611	1.993305
C	2.743759	-1.996869	1.997765
H	-1.955432	-2.914657	-0.775864
H	-3.711254	-2.828387	-0.707812
C	-2.947130	-3.432530	-2.634108
C	-1.652085	-1.658692	-3.879693
H	-1.496508	0.236160	-2.839370
H	-0.636944	-1.096295	-2.061709
H	-2.933853	-2.768707	1.434361
H	-1.867368	-1.679576	2.295785
C	-3.692296	-2.191453	3.372579
C	-5.810071	-1.263373	2.341452
H	-5.506359	-0.070875	0.563854
H	-5.145082	-1.777023	0.349764
H	-2.172131	2.854211	0.694768
H	-3.539284	2.217166	1.603099
C	-4.033442	3.915471	0.363019
C	-3.874597	3.494332	-2.120401
H	-2.008500	2.411205	-1.876561
H	-3.293589	1.490764	-2.668558
H	1.560447	2.896814	1.060211
H	2.902101	2.346542	2.059146
C	3.311712	4.167534	0.960735
C	3.419515	3.888117	-1.548679
H	3.121597	1.867918	-2.251028
H	1.678503	2.588222	-1.536550
H	4.877363	0.188521	-1.511303
H	4.927299	-1.416399	-0.790992
C	4.816640	-1.432543	-2.951284
C	2.711081	-2.842416	-2.871494
H	2.786380	-2.874050	-0.715455
H	1.280548	-2.239396	-1.339714
H	5.158970	-0.782238	1.285638
H	4.772768	0.841849	1.840709
C	4.927707	-0.610749	3.430926
C	3.120067	-2.385081	3.437337
H	1.687252	-2.204526	1.802929
H	3.331247	-2.616276	1.305974
H	-2.993574	-4.500129	-2.383358
H	-3.890648	-3.191474	-3.146712
C	-1.772400	-3.158465	-3.582027
H	-2.527357	-1.329663	-4.459757
H	-0.771989	-1.457830	-4.504050
H	-3.244767	-3.061787	3.869623
H	-3.586827	-1.346412	4.069264
C	-5.182545	-2.441424	3.099846
H	-5.812238	-0.375144	2.990499
H	-6.860070	-1.476484	2.101604
H	-5.111964	3.698206	0.393095
H	-3.837886	4.636377	1.167259
C	-3.677340	4.523104	-0.999912
H	-3.570412	3.917106	-3.086869
H	-4.945519	3.255797	-2.207767
H	2.966816	4.813561	1.778388
H	4.401336	4.067280	1.080122
C	3.007781	4.814757	-0.396975
H	3.150907	4.335653	-2.514547
H	4.514688	3.777959	-1.549832
H	4.432718	-0.778766	-3.748530
H	5.907715	-1.459363	-3.069331
C	4.226571	-2.840043	-3.120289
H	2.316588	-3.864814	-2.936805
H	2.211726	-2.262844	-3.662845
H	5.997356	-0.420099	3.588844
H	4.387451	0.038051	4.136025
C	4.594480	-2.077600	3.737147

H	2.479839	-1.830901	4.139175
H	2.912465	-3.450740	3.599658
H	-0.840607	-3.511279	-3.115982
H	-1.891212	-3.724659	-4.514587
H	-5.721633	-2.617110	4.039731
H	-5.292432	-3.357842	2.500436
H	-4.283583	5.417903	-1.191801
H	-2.627279	4.849353	-0.987522
H	3.519224	5.782284	-0.483487
H	1.929605	5.019868	-0.465370
H	4.451725	-3.228405	-4.121812
H	4.709351	-3.521915	-2.404507
H	5.231525	-2.728931	3.119753
H	4.831518	-2.310071	4.783378
C	-0.214542	0.738205	1.844066
O	-0.264010	1.133946	2.946201
H	-0.121652	-1.515712	0.635827
H	-0.154816	1.675562	-0.537097

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Ru	0.044490	0.175220	-0.107950
P	2.401840	0.686319	0.057520
P	-2.341780	0.436501	-0.032420
B	0.098029	-1.959030	0.716740
H	-0.037219	1.188630	1.086500
H	0.172800	-0.858290	1.354850
H	-0.052879	1.335180	-1.275960
C	2.855121	2.435529	-0.535870
C	3.085600	0.655129	1.840230
C	3.766060	-0.312062	-0.858560
C	-3.423530	-0.253528	-1.433100
C	-2.834069	2.275931	-0.090620
C	-3.148250	-0.370418	1.492170
O	1.239559	-2.728621	0.529170
O	-1.025731	-2.767369	0.846980
H	3.904091	2.583978	-0.241170
C	2.001152	3.523609	0.146890
C	2.781971	2.599009	-2.068990
H	3.240980	-0.420302	2.002200
C	2.109521	1.103119	2.950420
C	4.445141	1.364368	2.033260
H	4.557470	0.416378	-1.093490
C	4.412479	-1.462712	-0.053580
C	3.226520	-0.879992	-2.188760
H	-4.467170	-0.093558	-1.131600
C	-3.215791	-1.773718	-1.601370
C	-3.231100	0.476302	-2.779760
H	-2.429969	2.562261	-1.072400
C	-4.343829	2.602692	-0.088980
C	-2.117128	3.176921	0.937440
H	-2.732301	-1.382619	1.419680
C	-4.685450	-0.517598	1.553750
C	-2.631750	0.220501	2.822890
C	0.840058	-4.110190	0.315010
C	-0.594212	-4.147740	0.966780
H	0.948342	3.341190	-0.098620
H	2.085082	3.453499	1.236550
C	2.396963	4.941489	-0.301110
C	3.169042	4.020388	-2.516940
H	3.450251	1.886638	-2.564170
H	1.762321	2.373009	-2.406140
H	1.897951	2.176919	2.863470
H	1.151440	0.589819	2.837460
C	2.696351	0.820709	4.346190
C	5.039511	1.077838	3.423910
H	5.162891	1.071167	1.258000
H	4.305541	2.449028	1.931820

H	3.633439	-2.179112	0.232860
H	4.862820	-1.092592	0.872000
C	5.509599	-2.177743	-0.865340
C	4.322679	-1.580232	-3.010190
H	2.429279	-1.594751	-1.955460
H	2.777990	-0.085691	-2.793650
H	-2.164911	-1.965009	-1.846050
H	-3.405351	-2.292958	-0.656250
C	-4.112691	-2.357108	-2.706220
C	-4.115600	-0.124358	-3.887430
H	-3.463549	1.541782	-2.679010
H	-2.179160	0.425341	-3.083240
H	-4.891769	1.984362	-0.808180
H	-4.763729	2.379172	0.900190
C	-4.591958	4.089722	-0.405160
C	-2.353688	4.665821	0.628500
H	-2.489308	2.962681	1.947450
H	-1.046718	2.959161	0.941130
H	-5.162030	0.466143	1.651930
H	-5.079510	-0.966867	0.635860
C	-5.102751	-1.394337	2.750920
C	-3.038690	-0.657508	4.018600
H	-1.543220	0.334751	2.790940
H	-3.052109	1.224412	2.971200
C	1.874478	-5.019271	0.979940
C	0.828688	-4.356890	-1.200260
C	-0.575602	-4.473250	2.468420
C	-1.606502	-5.044649	0.254950
H	1.747403	5.677069	0.191460
H	3.423383	5.159048	0.031810
C	2.318113	5.092239	-1.825250
H	4.230222	4.197778	-2.284700
H	3.071892	4.098009	-3.607780
H	1.995251	1.164569	5.118060
H	2.797510	-0.267111	4.479600
C	4.067751	1.482468	4.540800
H	5.264890	0.004107	3.507800
H	5.994901	1.607137	3.537160
H	6.336429	-1.474963	-1.048760
H	5.928809	-2.999253	-0.269120
C	4.991769	-2.703932	-2.209430
H	3.895139	-1.975422	-3.941440
H	5.083370	-0.842042	-3.305390
H	-3.915232	-3.431878	-2.815840
H	-5.168361	-2.263437	-2.409470
C	-3.899631	-1.635538	-4.043610
H	-3.919780	0.392362	-4.836160
H	-5.172240	0.062873	-3.643850
H	-4.252298	4.300582	-1.430260
H	-5.669638	4.299603	-0.384340
C	-3.849357	5.008062	0.575120
H	-1.848977	5.285381	1.381600
H	-1.889797	4.910361	-0.338830
H	-6.197491	-1.472997	2.789150
H	-4.721321	-2.414578	2.596050
C	-4.560480	-0.849908	4.079890
H	-2.548841	-1.638229	3.928580
H	-2.673920	-0.208929	4.952250
H	2.839748	-4.912191	0.474340
H	1.573087	-6.071061	0.909350
H	2.016818	-4.767671	2.033360
H	0.117918	-3.699530	-1.708060
H	0.578597	-5.396750	-1.436930
H	1.824858	-4.146421	-1.601890
H	0.136178	-3.837640	3.004580
H	-0.316253	-5.520920	2.655410
H	-1.571612	-4.287289	2.882780

H	-2.575602	-4.978949	0.760620
H	-1.284503	-6.092309	0.278990
H	-1.748642	-4.747499	-0.786340
H	1.271143	4.986949	-2.145620
H	2.642053	6.095739	-2.131010
H	4.483611	1.222028	5.522820
H	3.945771	2.575978	4.532680
H	5.810059	-3.154303	-2.786370
H	4.258858	-3.504342	-2.028220
H	-4.572561	-2.039438	-4.811130
H	-2.874191	-1.823529	-4.395660
H	-3.993857	6.060232	0.296940
H	-4.283327	4.887802	1.579220
H	-5.037490	0.118313	4.294540
H	-4.831501	-1.520838	4.905650
C	0.234360	-0.340140	-3.563620
O	0.002900	-1.239710	-2.848720
O	0.461260	0.525560	-4.313490

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Ru	0.042863	0.174869	-0.148544
P	2.396698	0.687092	0.033128
P	-2.343769	0.432182	-0.033096
B	0.109579	-1.984969	0.662311
H	-0.023223	1.183446	1.054376
H	0.169339	-0.882196	1.293312
H	-0.057377	1.381994	-1.265334
C	2.847131	2.443424	-0.541978
C	3.065880	0.645874	1.822255
C	3.781153	-0.295155	-0.873965
C	-3.458565	-0.257224	-1.409635
C	-2.827418	2.276133	-0.084401
C	-3.122331	-0.375020	1.505080
O	1.254768	-2.754810	0.513790
O	-1.020995	-2.787636	0.747703
H	3.894160	2.592726	-0.240940
C	1.987068	3.523726	0.145927
C	2.781905	2.619114	-2.074056
H	3.227133	-0.429671	1.977068
C	2.079773	1.078153	2.929602
C	4.419439	1.362708	2.030032
H	4.569334	0.441869	-1.092698
C	4.427843	-1.447150	-0.070572
C	3.268271	-0.859585	-2.216436
H	-4.493461	-0.054568	-1.103272
C	-3.315919	-1.786789	-1.562738
C	-3.249422	0.440778	-2.770604
H	-2.360285	2.576899	-1.033372
C	-4.329403	2.630771	-0.168902
C	-2.166062	3.144819	1.007379
H	-2.790975	-1.412424	1.370569
C	-4.660567	-0.397944	1.646440
C	-2.491321	0.109944	2.829602
C	0.858887	-4.133664	0.275806
C	-0.597444	-4.170488	0.876662
H	0.935310	3.340598	-0.103553
H	2.068077	3.445010	1.235240
C	2.381351	4.946078	-0.289270
C	3.166375	4.045320	-2.508770
H	3.455185	1.912819	-2.571411
H	1.764927	2.392708	-2.418726
H	1.859588	2.150708	2.849107
H	1.126751	0.558251	2.806192
C	2.659750	0.789796	4.327047
C	5.006768	1.069981	3.422370
H	5.144664	1.080506	1.257695
H	4.273028	2.447112	1.935765

H	3.652864	-2.175836	0.196027
H	4.859014	-1.082631	0.866142
C	5.546622	-2.140574	-0.871521
C	4.387557	-1.532985	-3.028935
H	2.481961	-1.591607	-1.999725
H	2.812366	-0.068975	-2.820883
H	-2.279413	-2.028782	-1.824454
H	-3.511215	-2.289699	-0.610299
C	-4.261780	-2.340975	-2.642322
C	-4.191035	-0.121909	-3.850281
H	-3.404892	1.521232	-2.683785
H	-2.211482	0.310477	-3.096394
H	-4.844895	2.037387	-0.931112
H	-4.815881	2.400501	0.787270
C	-4.527094	4.127567	-0.475641
C	-2.349147	4.642879	0.708472
H	-2.618853	2.923673	1.983080
H	-1.103270	2.903430	1.087442
H	-5.039959	0.617151	1.821236
H	-5.141160	-0.758554	0.730519
C	-5.091148	-1.294922	2.823402
C	-2.911476	-0.786367	4.007045
H	-1.400807	0.132189	2.743333
H	-2.812441	1.138472	3.040566
C	1.867098	-5.050899	0.968820
C	0.897361	-4.368011	-1.240844
C	-0.630715	-4.502959	2.376400
C	-1.587264	-5.061273	0.126705
H	1.727835	5.676186	0.206214
H	3.405805	5.163848	0.049550
C	2.308659	5.108765	-1.812522
H	4.225809	4.224234	-2.269926
H	3.074375	4.131469	-3.599464
H	1.951077	1.122905	5.096731
H	2.767967	-0.298229	4.453226
C	4.024983	1.459839	4.535646
H	5.238946	-0.002792	3.500019
H	5.957770	1.604938	3.545719
H	6.368318	-1.426291	-1.032307
H	5.965000	-2.964097	-0.277490
C	5.058910	-2.657053	-2.230585
H	3.981192	-1.922369	-3.972002
H	5.142108	-0.780066	-3.301844
H	-4.113651	-3.424347	-2.744633
H	-5.304857	-2.198719	-2.321602
C	-4.051687	-1.643609	-3.993107
H	-3.991539	0.373781	-4.809356
H	-5.230726	0.121232	-3.584364
H	-4.118370	4.345888	-1.473668
H	-5.599569	4.359283	-0.520150
C	-3.830919	5.017409	0.563444
H	-1.882188	5.240067	1.502838
H	-1.818167	4.890777	-0.222747
H	-6.185316	-1.284318	2.917099
H	-4.806696	-2.334872	2.603882
C	-4.438643	-0.859820	4.143187
H	-2.509984	-1.798217	3.848976
H	-2.463978	-0.413356	4.937949
H	2.849096	-4.944192	0.496429
H	1.564481	-6.101049	0.881573
H	1.975150	-4.806391	2.027991
H	0.206572	-3.702227	-1.765115
H	0.649828	-5.404479	-1.494292
H	1.907454	-4.159661	-1.607384
H	0.062876	-3.870562	2.939480
H	-0.378269	-5.551728	2.566649
H	-1.640133	-4.318439	2.757519

H	-2.572873	-4.994798	0.599238
H	-1.269382	-6.110009	0.157442
H	-1.693081	-4.759415	-0.917556
H	1.263485	5.002408	-2.138362
H	2.630548	6.115711	-2.109003
H	4.436177	1.195344	5.518564
H	3.895379	2.552516	4.534437
H	5.893115	-3.088920	-2.798827
H	4.334210	-3.469824	-2.072131
H	-4.762992	-2.024228	-4.737564
H	-3.045967	-1.882337	-4.370807
H	-3.935937	6.075804	0.291197
H	-4.331326	4.893912	1.535808
H	-4.823405	0.131738	4.425786
H	-4.721114	-1.545842	4.952566
C	0.221943	-0.298443	-3.367859
O	0.025448	-1.150012	-2.584832
O	0.413385	0.503139	-4.194115

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Ru	0.040278	0.250344	-0.232102
P	2.393567	0.734834	-0.014288
P	-2.352064	0.460161	-0.061012
B	0.162810	-2.170650	0.683915
H	0.001746	1.240325	0.996971
H	0.197577	-1.025300	1.126660
H	-0.083206	1.613141	-1.080121
C	2.858170	2.525554	-0.454110
C	3.046443	0.555659	1.774250
C	3.790418	-0.185008	-0.974614
C	-3.484528	-0.253661	-1.412149
C	-2.893652	2.287833	-0.076296
C	-3.060114	-0.392464	1.486569
O	1.304708	-2.906202	0.503475
O	-0.974583	-2.938016	0.710892
H	3.915788	2.633261	-0.172832
C	2.040861	3.563500	0.342895
C	2.752378	2.822710	-1.965515
H	3.209923	-0.528019	1.849023
C	2.046950	0.899991	2.899741
C	4.396785	1.256683	2.048053
H	4.581035	0.565339	-1.131890
C	4.427803	-1.387439	-0.241382
C	3.300855	-0.661682	-2.360095
H	-4.516532	-0.079306	-1.079192
C	-3.306553	-1.778782	-1.575725
C	-3.331711	0.453158	-2.776911
H	-2.448315	2.617652	-1.026454
C	-4.405715	2.600818	-0.138839
C	-2.243666	3.155468	1.022933
H	-2.725153	-1.424597	1.318478
C	-4.591619	-0.436293	1.683655
C	-2.386898	0.071454	2.797635
C	0.909991	-4.276167	0.184619
C	-0.567101	-4.338783	0.742032
H	0.978306	3.420206	0.115146
H	2.153499	3.400058	1.419843
C	2.452904	5.007664	0.007149
C	3.155887	4.270794	-2.298796
H	3.393338	2.143352	-2.537472
H	1.722657	2.644325	-2.297811
H	1.817648	1.973208	2.894608
H	1.098368	0.386856	2.725711
C	2.612881	0.512947	4.278537
C	4.968146	0.868697	3.423899
H	5.132184	1.027198	1.267854
H	4.252001	2.345304	2.024789

H	3.651242	-2.133570	-0.030715
H	4.847640	-1.087337	0.722635
C	5.557913	-2.028757	-1.069909
C	4.434901	-1.275949	-3.198844
H	2.521406	-1.417681	-2.207325
H	2.841217	0.159242	-2.918309
H	-2.272242	-1.992030	-1.868988
H	-3.463122	-2.290436	-0.620500
C	-4.270566	-2.352995	-2.628986
C	-4.299535	-0.125786	-3.824276
H	-3.504953	1.530251	-2.680153
H	-2.305931	0.343370	-3.145770
H	-4.912407	2.005686	-0.905462
H	-4.876251	2.342788	0.818291
C	-4.646698	4.096505	-0.419786
C	-2.470566	4.652679	0.750554
H	-2.682249	2.905998	1.998561
H	-1.174490	2.939973	1.088323
H	-4.971552	0.571469	1.894766
H	-5.102085	-0.779938	0.777316
C	-4.970413	-1.363511	2.854657
C	-2.752366	-0.857546	3.967838
H	-1.301173	0.114408	2.670813
H	-2.712889	1.090707	3.042769
C	1.897272	-5.225720	0.862082
C	0.997146	-4.425075	-1.339319
C	-0.652794	-4.779222	2.210086
C	-1.547816	-5.148801	-0.103816
H	1.830554	5.709383	0.578074
H	3.491418	5.177511	0.330262
C	2.340180	5.291277	-1.495708
H	4.225199	4.410827	-2.078316
H	3.034577	4.444375	-3.376060
H	1.893884	0.784818	5.062618
H	2.727407	-0.580838	4.326195
C	3.971479	1.173622	4.550444
H	5.205498	-0.205858	3.428302
H	5.914809	1.397649	3.596886
H	6.381864	-1.306069	-1.170482
H	5.967268	-2.890053	-0.525015
C	5.091855	-2.452460	-2.467741
H	4.042601	-1.599431	-4.172010
H	5.193205	-0.506535	-3.408301
H	-4.095293	-3.431200	-2.743302
H	-5.306227	-2.242520	-2.273227
C	-4.125140	-1.642379	-3.981533
H	-4.147248	0.379512	-4.786842
H	-5.334639	0.089420	-3.518815
H	-4.254929	4.341021	-1.418484
H	-5.725414	4.299836	-0.449437
C	-3.963387	4.988974	0.625709
H	-2.012189	5.249594	1.550090
H	-1.955400	4.929865	-0.181258
H	-6.060315	-1.365004	2.989226
H	-4.686107	-2.395636	2.600542
C	-4.272649	-0.952957	4.159084
H	-2.345874	-1.860640	3.770019
H	-2.274738	-0.501709	4.890393
H	2.893532	-5.089600	0.429445
H	1.602301	-6.269942	0.707063
H	1.968309	-5.039372	1.936040
H	0.332379	-3.723638	-1.850516
H	0.748134	-5.443596	-1.655529
H	2.021181	-4.209956	-1.660413
H	0.029618	-4.201803	2.841675
H	-0.419800	-5.842744	2.328082
H	-1.671634	-4.608704	2.571691

H	-2.546760	-5.093562	0.340846
H	-1.251953	-6.203643	-0.138591
H	-1.611966	-4.770006	-1.125982
H	1.284213	5.229641	-1.797316
H	2.673743	6.312699	-1.721407
H	4.373402	0.842294	5.516877
H	3.835093	2.262893	4.625104
H	5.934445	-2.848474	-3.049592
H	4.362322	-3.271493	-2.375677
H	-4.851775	-2.037982	-4.703100
H	-3.127057	-1.850755	-4.395004
H	-4.099488	6.048050	0.370395
H	-4.450262	4.837917	1.601020
H	-4.657110	0.026626	4.480968
H	-4.516494	-1.661875	4.961256
C	0.162534	-0.042177	-2.868861
O	-0.001818	-1.094134	-2.338734
O	0.314478	0.801066	-3.673234

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Ru	-0.042029	-0.374775	-0.234114
P	-2.430033	-0.811905	-0.029061
P	2.378653	-0.514783	-0.080201
B	-0.226507	2.416182	0.777815
H	-0.016984	-1.461340	0.934516
H	-0.281910	1.250803	1.076887
H	0.093265	-1.825113	-0.821309
C	-2.913563	-2.600139	-0.443323
C	-3.051819	-0.573894	1.756430
C	-3.777803	0.134678	-1.018044
C	3.453097	0.219217	-1.457611
C	2.973934	-2.320399	-0.056161
C	3.029137	0.399888	1.448975
O	-1.343854	3.156427	0.541084
O	0.937200	3.125308	0.776929
H	-3.979949	-2.681441	-0.184917
C	-2.142262	-3.644656	0.391376
C	-2.776520	-2.915711	-1.949966
H	-3.187727	0.514913	1.808213
C	-2.039506	-0.918973	2.870212
C	-4.416600	-1.230712	2.065545
H	-4.596186	-0.590509	-1.152050
C	-4.367502	1.375309	-0.308327
C	-3.275126	0.560518	-2.417183
H	4.496687	0.089640	-1.136751
C	3.210295	1.732848	-1.648595
C	3.295097	-0.519033	-2.807351
H	2.496737	-2.700835	-0.971785
C	4.492255	-2.583691	-0.182555
C	2.413764	-3.162161	1.111147
H	2.715718	1.428776	1.223072
C	4.552518	0.429728	1.698268
C	2.299427	0.007499	2.753007
C	-0.895384	4.481677	0.103692
C	0.580735	4.541725	0.670116
H	-1.069399	-3.535086	0.195028
H	-2.282393	-3.464756	1.462536
C	-2.577076	-5.083006	0.059770
C	-3.193927	-4.361527	-2.274947
H	-3.398708	-2.234874	-2.539335
H	-1.741522	-2.746135	-2.270293
H	-1.835020	-1.996885	2.883505
H	-1.081019	-0.432213	2.670142
C	-2.569106	-0.488057	4.249678
C	-4.949126	-0.799451	3.444104
H	-5.156968	-0.989734	1.293595
H	-4.306056	-2.323473	2.058411

H	-3.567666	2.103881	-0.122624
H	-4.790401	1.114301	0.666043
C	-5.483016	2.029251	-1.146858
C	-4.397336	1.187032	-3.261842
H	-2.470167	1.292084	-2.289393
H	-2.836020	-0.280742	-2.958666
H	2.166261	1.889818	-1.941333
H	3.357062	2.272132	-0.706386
C	4.145067	2.318096	-2.722167
C	4.235562	0.069330	-3.874195
H	3.503340	-1.588760	-2.694519
H	2.261827	-0.444717	-3.161494
H	4.936823	-2.005681	-0.998291
H	5.000345	-2.268279	0.737377
C	4.771330	-4.081023	-0.414739
C	2.678290	-4.661341	0.887592
H	2.898412	-2.857409	2.048774
H	1.342298	-2.981997	1.231324
H	4.902238	-0.572377	1.978062
H	5.099608	0.712416	0.791993
C	4.902996	1.411293	2.832718
C	2.637025	0.989223	3.888213
H	1.217753	-0.024396	2.588320
H	2.595443	-1.004408	3.058303
C	-1.853152	5.521213	0.681942
C	-0.967845	4.482319	-1.427759
C	0.675529	5.114240	2.089974
C	1.597118	5.222145	-0.243692
H	-1.989282	-5.790379	0.659514
H	-3.628932	-5.225184	0.351263
C	-2.421655	-5.386113	-1.435329
H	-4.271719	-4.481222	-2.085276
H	-3.042964	-4.550177	-3.345556
H	-1.843259	-0.762378	5.026379
H	-2.654707	0.608963	4.275662
C	-3.939443	-1.107776	4.558480
H	-5.157565	0.280863	3.429994
H	-5.905861	-1.298825	3.646008
H	-6.328074	1.328332	-1.223537
H	-5.862611	2.915574	-0.620943
C	-5.013636	2.401692	-2.558092
H	-3.999474	1.473595	-4.243772
H	-5.180846	0.436874	-3.449464
H	3.930323	3.386970	-2.855567
H	5.187531	2.251401	-2.374410
C	4.010409	1.576024	-4.059042
H	4.086426	-0.458324	-4.824905
H	5.281084	-0.107716	-3.578135
H	4.340450	-4.379769	-1.381815
H	5.853839	-4.247929	-0.490894
C	4.173802	-4.952429	0.698723
H	2.282475	-5.237810	1.734030
H	2.125584	-4.994260	-0.003336
H	5.986875	1.404971	3.007948
H	4.643196	2.432304	2.516264
C	4.151405	1.074984	4.128884
H	2.251556	1.985297	3.624970
H	2.122631	0.685619	4.809537
H	-2.853519	5.366351	0.265883
H	-1.531575	6.535078	0.417480
H	-1.925589	5.450401	1.769596
H	-0.345259	3.694607	-1.860768
H	-0.663256	5.449811	-1.840540
H	-2.001367	4.291924	-1.733790
H	-0.031487	4.624829	2.767286
H	0.481359	6.191709	2.103627
H	1.685641	4.943101	2.474946

H	2.588444	5.186936	0.219566
H	1.334892	6.274625	-0.400689
H	1.659378	4.727191	-1.214933
H	-1.355812	-5.346526	-1.704076
H	-2.766009	-6.404239	-1.659230
H	-4.314935	-0.746200	5.524542
H	-3.829806	-2.198398	4.653883
H	-5.848622	2.808329	-3.143731
H	-4.258801	3.199793	-2.491755
H	4.718086	1.980998	-4.794322
H	3.002370	1.742201	-4.465509
H	4.333530	-6.015783	0.478008
H	4.703247	-4.745978	1.641070
H	4.510185	0.108092	4.512527
H	4.375397	1.819884	4.903544
C	-0.129972	-0.152274	-2.320647
O	-0.211669	-0.886609	-3.275215
O	-0.055536	1.058750	-2.029694

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Ru	0.083625	-0.143114	-0.180451
P	2.421357	0.036595	0.083283
P	-2.280789	0.188583	-0.129180
H	0.033067	0.468722	1.274196
C	3.214787	-1.104076	1.384966
C	3.525252	-0.228796	-1.449039
C	3.035835	1.750673	0.687597
C	-2.813647	1.945152	-0.594295
C	-2.937550	0.022273	1.640818
C	-3.391634	-0.863271	-1.272113
H	4.301778	-0.949854	1.325575
C	2.914657	-2.585686	1.072215
C	2.781735	-0.774750	2.830079
H	3.383097	0.708418	-2.002487
C	3.022873	-1.336073	-2.399115
C	5.036178	-0.391581	-1.181819
H	3.964486	1.553635	1.246300
C	3.377661	2.744359	-0.446619
C	2.025731	2.423867	1.646013
H	-3.908978	1.983355	-0.507249
C	-2.434313	2.275447	-2.055936
C	-2.233509	3.016416	0.353582
H	-2.422473	0.861403	2.130026
C	-4.449354	0.200798	1.890926
C	-2.420119	-1.250689	2.347095
H	-2.804731	-0.861883	-2.203035
C	-4.806044	-0.353012	-1.630323
C	-3.488875	-2.334201	-0.809732
H	1.826202	-2.733642	1.056842
H	3.274137	-2.848271	0.071649
C	3.540227	-3.543864	2.100170
C	3.408829	-1.737413	3.854591
H	3.067256	0.249396	3.090335
H	1.686514	-0.825045	2.901497
H	3.094759	-2.321020	-1.917563
H	1.967400	-1.167299	-2.632574
C	3.836028	-1.362077	-3.706465
C	5.844611	-0.412298	-2.491979
H	5.407567	0.408542	-0.529278
H	5.214250	-1.335095	-0.648064
H	2.480549	2.912924	-1.059839
H	4.145061	2.338157	-1.112075
C	3.889885	4.091342	0.097539
C	2.558653	3.751400	2.209509
H	1.097722	2.604378	1.091752
H	1.752443	1.754508	2.465543
H	-1.345049	2.193051	-2.160056

H	-2.867589	1.543990	-2.748806	P	-2.321531	0.150140	-0.142028
C	-2.883484	3.690766	-2.457739	H	0.004993	-0.047870	1.416114
C	-2.676492	4.433571	-0.050668	C	3.360495	-1.408390	1.045890
H	-2.543891	2.829064	1.388062	C	3.459801	0.238621	-1.462367
H	-1.138796	2.949098	0.336834	C	2.958365	1.508676	1.168199
H	-4.821668	1.116164	1.415111	C	-2.802050	1.915897	-0.613073
H	-5.002389	-0.634468	1.440650	C	-3.037237	-0.029047	1.598224
C	-4.759701	0.239198	3.399133	C	-3.343575	-0.895098	-1.356977
C	-2.732165	-1.214829	3.853072	H	4.408579	-1.083285	1.134187
H	-2.883179	-2.144014	1.909333	C	3.328713	-2.741695	0.264728
H	-1.338108	-1.340315	2.190496	C	2.810277	-1.618410	2.474397
H	-5.442882	-0.353005	-0.736724	H	3.198700	1.269928	-1.734994
H	-4.775085	0.679723	-1.990301	C	3.003985	-0.628941	-2.656476
C	-5.453559	-1.236976	-2.714125	C	4.992600	0.168241	-1.293077
C	-4.114540	-3.226027	-1.895682	H	3.911019	1.233938	1.647806
H	-2.507471	-2.723985	-0.517320	C	3.202884	2.794718	0.344987
H	-4.116283	-2.389966	0.089770	C	1.931774	1.826061	2.282299
H	3.271476	-4.578513	1.850369	H	-3.899478	1.960922	-0.588136
H	4.637025	-3.481244	2.035650	C	-2.340625	2.259421	-2.047792
C	3.098965	-3.203735	3.529100	C	-2.270258	2.969951	0.381836
H	4.499902	-1.593687	3.864858	H	-2.496532	0.767715	2.130910
H	3.052328	-1.483912	4.861599	C	-4.547320	0.236593	1.776641
H	3.480221	-2.177475	-4.349753	C	-2.639109	-1.349406	2.296900
H	3.654225	-0.427652	-4.258028	H	-2.699659	-0.880092	-2.248406
C	5.341492	-1.507263	-3.443217	C	-4.734975	-0.372261	-1.781312
H	5.758740	0.566488	-2.986980	C	-3.465158	-2.375703	-0.925353
H	6.910117	-0.557762	-2.270515	H	2.285887	-3.038866	0.103370
H	4.853480	3.926680	0.603182	H	3.781476	-2.618499	-0.723962
H	4.091841	4.770467	-0.741326	C	4.068111	-3.864400	1.013436
C	2.909405	4.733412	1.085141	C	3.542278	-2.752614	3.213793
H	1.810479	4.191559	2.881948	H	2.905294	-0.699063	3.060914
H	3.454109	3.562411	2.821434	H	1.738612	-1.850009	2.415278
H	-2.574483	3.896590	-3.490958	H	3.213825	-1.688451	-2.464838
H	-3.982797	3.745004	-2.443978	H	1.921993	-0.553069	-2.794722
C	-2.312834	4.751939	-1.507268	C	3.730112	-0.203417	-3.945314
H	-2.221625	5.168682	0.626267	C	5.716285	0.589104	-2.585009
H	-3.765852	4.524540	0.077432	H	5.326812	0.797206	-0.458466
H	-4.295032	1.134160	3.838981	H	5.285843	-0.859885	-1.042570
H	-5.841813	0.340767	3.555100	H	2.275474	3.069115	-0.178229
C	-4.231723	-1.011451	4.117524	H	3.964940	2.637007	-0.423384
H	-2.384356	-2.141102	4.328866	C	3.656789	3.966915	1.234332
H	-2.167037	-0.392978	4.317389	C	2.402411	2.978104	3.185635
H	-6.463532	-0.869124	-2.937857	H	0.979736	2.098422	1.809246
H	-4.873624	-1.142245	-3.644177	H	1.720747	0.942424	2.890545
C	-5.504391	-2.714365	-2.300335	H	-1.247555	2.171959	-2.097014
H	-3.456926	-3.238121	-2.777581	H	-2.740977	1.539074	-2.770682
H	-4.179012	-4.261806	-1.537427	C	-2.758820	3.683060	-2.453283
H	2.016811	-3.376986	3.625503	C	-2.680264	4.395290	-0.028343
H	3.589174	-3.869055	4.251624	H	-2.640155	2.770516	1.394158
H	5.898765	-1.477271	-4.388392	H	-1.175427	2.900906	0.425510
H	5.538472	-2.493079	-2.995533	H	-4.842774	1.182764	1.307049
H	3.332034	5.659879	1.495556	H	-5.121246	-0.554835	1.276578
H	1.989083	5.015790	0.552730	C	-4.931949	0.263874	3.268034
H	-2.676771	5.750174	-1.783443	C	-3.017929	-1.314506	3.787625
H	-1.217829	4.775919	-1.609557	H	-3.148766	-2.195875	1.822109
H	-4.424022	-0.940441	5.195907	H	-1.565148	-1.527441	2.182167
H	-4.784103	-1.893087	3.758827	H	-5.420242	-0.394895	-0.923862
H	-6.191022	-2.828027	-1.448041	H	-4.687395	0.668796	-2.115312
H	-5.914996	-3.324761	-3.114904	C	-5.318703	-1.231237	-2.919944
C	-0.152333	-2.662144	-1.654231	C	-4.027840	-3.237384	-2.068586
O	0.039246	-3.448713	-0.804553	H	-2.502419	-2.773880	-0.593634
O	-0.360980	-1.984309	-2.591716	H	-4.148561	-2.445280	-0.068024
H	0.185483	1.279886	-0.855123	H	3.999060	-4.794727	0.435348
				H	5.138411	-3.616311	1.081553
				C	3.505904	-4.067481	2.425359
				H	4.589906	-2.459084	3.379871
				H	3.095671	-2.887133	4.207606

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Ru	0.083898	-0.187471	-0.152567
P	2.457870	-0.016689	0.125351

H	3.413147	-0.847120	-4.775535
H	3.424249	0.820158	-4.210005
C	5.256831	-0.249114	-3.786825
H	5.510856	1.651753	-2.783666
H	6.802168	0.501521	-2.448768
H	4.642889	3.728897	1.660670
H	3.795300	4.862083	0.614070
C	2.671214	4.251256	2.373857
H	1.647522	3.169244	3.959440
H	3.321013	2.679875	3.713405
H	-2.393130	3.900204	-3.465114
H	-3.856793	3.742877	-2.498206
C	-2.235249	4.728343	-1.458948
H	-2.257922	5.117896	0.682081
H	-3.774115	4.492411	0.042127
H	-4.441094	1.123270	3.748761
H	-6.013099	0.425418	3.369660
C	-4.513222	-1.026411	3.987455
H	-2.747808	-2.267593	4.260231
H	-2.426588	-0.536257	4.293279
H	-6.313991	-0.855656	-3.191745
H	-4.686113	-1.114987	-3.812283
C	-5.391880	-2.717268	-2.542730
H	-3.315737	-3.231108	-2.906049
H	-4.112005	-4.280420	-1.737348
H	2.467134	-4.420885	2.354438
H	4.069505	-4.846337	2.955239
H	5.747975	0.101370	-4.703737
H	5.574565	-1.292393	-3.641369
H	3.055246	5.050134	3.021252
H	1.723335	4.616470	1.951704
H	-2.578237	5.731926	-1.741660
H	-1.136140	4.747747	-1.501163
H	-4.751665	-0.959161	5.056778
H	-5.099207	-1.868154	3.588957
H	-6.128422	-2.849054	-1.735738
H	-5.753536	-3.307604	-3.394460
C	-0.071600	-1.951886	-1.145440
O	-0.074254	-2.720964	-0.189469
O	-0.122465	-1.822857	-2.353618
H	0.190827	1.332114	-0.628189

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Ru	-0.096769	-0.616358	-0.098834
P	-2.504144	-0.419095	0.183735
P	2.211751	-1.281615	0.009892
H	-0.234389	-1.443568	1.273806
C	-3.625549	0.705091	-0.876517
C	-3.363449	-2.102278	-0.003408
C	-2.943549	0.052314	1.974872
C	2.503515	-3.146115	-0.118727
C	2.986679	-0.866945	1.686818
C	3.296712	-0.593593	-1.382793
H	-4.602623	0.201280	-0.888065
C	-3.113299	0.782907	-2.333022
C	-3.869714	2.132190	-0.340893
H	-2.783880	-2.736222	0.682246
C	-3.212767	-2.716606	-1.412254
C	-4.846945	-2.166187	0.424234
H	-4.012548	0.313027	1.979583
C	-2.733795	-1.092831	2.993071
C	-2.141024	1.283120	2.454093
H	3.589235	-3.296607	-0.020521
C	2.065338	-3.696103	-1.495614
C	1.819804	-3.948949	1.010055
H	2.519422	-1.618744	2.338851
C	4.515197	-1.022366	1.827118

C	2.526478	0.504113	2.225926
H	2.664055	-0.789257	-2.260782
C	4.669731	-1.247680	-1.657389
C	3.445864	0.939281	-1.291604
H	-2.140691	1.287624	-2.342803
H	-2.940152	-0.216776	-2.743075
C	-4.096324	1.546152	-3.236912
C	-4.857284	2.898827	-1.241015
H	-4.273156	2.103746	0.677578
H	-2.922753	2.684357	-0.299390
H	-3.804331	-2.132059	-2.130778
H	-2.174972	-2.672494	-1.751598
C	-3.717786	-4.170076	-1.435536
C	-5.361540	-3.618399	0.412521
H	-5.001238	-1.730359	1.416789
H	-5.458626	-1.576199	-0.271967
H	-1.673358	-1.376123	2.996146
H	-3.294054	-1.988399	2.710026
C	-3.158372	-0.668829	4.411152
C	-2.568789	1.727890	3.862924
H	-1.076454	1.011504	2.473265
H	-2.234004	2.120111	1.757629
H	0.995795	-3.505748	-1.639220
H	2.574824	-3.166720	-2.308122
C	2.342821	-5.203972	-1.619929
C	2.097056	-5.457141	0.881236
H	2.160772	-3.608791	1.994830
H	0.738379	-3.768854	0.974120
H	4.841607	-2.008780	1.476646
H	5.018912	-0.279898	1.194908
C	4.967438	-0.811583	3.283785
C	2.994616	0.725010	3.674910
H	2.906686	1.314117	1.591214
H	1.432523	0.560169	2.182960
H	5.349334	-1.064546	-0.816663
H	4.580472	-2.334580	-1.756212
C	5.299570	-0.674935	-2.941527
C	4.078714	1.512128	-2.570364
H	2.473852	1.405991	-1.121588
H	4.081194	1.199914	-0.433509
H	-3.692172	1.600512	-4.255911
H	-5.041977	0.986976	-3.305929
C	-4.379203	2.954795	-2.698082
H	-5.840323	2.405624	-1.202430
H	-5.002619	3.913163	-0.845846
H	-3.615090	-4.579934	-2.448398
H	-3.078239	-4.783959	-0.783535
C	-5.174791	-4.273620	-0.962984
H	-4.815774	-4.199626	1.170720
H	-6.419510	-3.639312	0.705676
H	-4.242028	-0.477343	4.421611
H	-2.982997	-1.497415	5.109772
C	-2.418027	0.590407	4.881677
H	-1.975647	2.598683	4.172391
H	-3.617720	2.059615	3.836519
H	1.993605	-5.560104	-2.597483
H	3.429001	-5.381116	-1.592009
C	1.673150	-5.997780	-0.490620
H	1.575876	-5.995440	1.683780
H	3.171805	-5.643413	1.027546
H	4.546220	-1.608972	3.913987
H	6.059283	-0.905246	3.350460
C	4.513387	0.553482	3.819685
H	2.689147	1.723276	4.014800
H	2.486441	0.002379	4.331112
H	6.281813	-1.136368	-3.108911
H	4.673489	-0.951210	-3.802664

C	5.430428	0.853665	-2.880614	H	4.395499	-0.274376	-1.487919
H	3.389461	1.348744	-3.411377	C	3.288065	1.511187	-1.927004
H	4.198159	2.599029	-2.468252	C	2.887050	-0.789509	-2.936105
H	-3.456331	3.551557	-2.752070	H	2.220213	-2.838796	-0.735371
H	-5.121481	3.466296	-3.324915	C	4.324754	-2.783410	-0.317674
H	-5.496403	-5.322792	-0.931172	C	2.472895	-2.992552	1.381464
H	-5.826242	-3.768946	-1.692110	H	2.957030	1.483442	0.909772
H	-2.784424	0.904601	5.867658	C	4.702772	0.324160	1.419083
H	-1.349962	0.356488	5.003166	C	2.462561	0.296807	2.601515
H	1.917369	-7.064848	-0.573555	C	-0.815817	4.504227	0.240711
H	0.580804	-5.915486	-0.590290	C	0.677744	4.427348	0.756086
H	4.813339	0.670700	4.869045	H	-1.190519	-3.519586	-0.755406
H	5.023290	1.349700	3.256849	H	-2.257735	-3.793947	0.613331
H	6.153060	1.122841	-2.095297	C	-2.797144	-4.904957	-1.164567
H	5.837787	1.238219	-3.824747	C	-3.574913	-3.491272	-3.102910
C	-0.126961	-0.779648	-2.190100	H	-3.677370	-1.379705	-2.695999
O	0.167847	0.428691	-2.118108	H	-2.034583	-1.994487	-2.760865
O	-0.329909	-1.659686	-2.991926	H	-1.493790	-2.757882	2.326062
H	-0.381139	-2.129529	-0.356934	H	-0.762650	-1.170671	2.497222
C	-0.055842	5.019932	-0.553270	C	-2.026504	-1.749371	4.164376
C	1.409540	4.930997	0.031269	C	-4.497306	-1.864716	3.619851
B	0.365045	2.915063	0.205603	H	-4.991971	-1.398205	1.558377
H	0.190045	1.770949	0.483973	H	-4.080688	-2.886854	1.765580
O	1.602542	3.489340	0.177607	H	-3.498468	2.028006	0.891120
O	-0.657495	3.774549	-0.074528	H	-4.650037	0.825447	1.485500
C	2.507758	5.472496	-0.881343	C	-5.507407	2.221723	0.096476
H	2.373015	6.545693	-1.058688	C	-4.637456	2.059992	-2.268388
H	3.483027	5.328655	-0.405291	H	-2.632719	1.907718	-1.482068
H	2.523775	4.958456	-1.844882	H	-3.067867	0.597384	-2.561734
C	1.548913	5.527702	1.437985	H	2.247693	1.829358	-2.048930
H	2.526029	5.249845	1.844914	H	3.675496	2.056033	-1.058911
H	1.480970	6.620471	1.422063	C	4.100616	1.902088	-3.174083
H	0.779679	5.141602	2.114318	C	3.706226	-0.384742	-4.174061
C	-0.891590	6.187866	-0.034524	H	2.977104	-1.871020	-2.777448
H	-0.437127	7.145041	-0.314740	H	1.827442	-0.589564	-3.125955
H	-1.892577	6.147920	-0.475547	H	4.630730	-2.386188	-1.290218
H	-1.000469	6.158451	1.052020	H	5.015532	-2.363816	0.424290
C	-0.109404	4.964881	-2.085046	C	4.476212	-4.316855	-0.334760
H	-1.150049	4.838340	-2.399384	C	2.610556	-4.524275	1.364754
H	0.275616	5.886475	-2.534113	H	3.126702	-2.591023	2.166893
H	0.462759	4.117917	-2.475748	H	1.446956	-2.712737	1.644963

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Ru	-0.054613	-0.372896	-0.199350	H	5.225465	0.454133	0.464290
P	-2.440633	-0.807696	0.009850	C	5.233143	1.346398	2.441067
P	2.381267	-0.549406	-0.147056	C	2.994343	1.314954	3.625161
B	-0.161207	2.313564	0.388259	H	1.382697	0.431403	2.475325
H	-0.071010	-1.881192	0.273078	H	2.614879	-0.715507	2.995854
H	-0.267865	1.241106	0.995086	C	-1.726508	5.439569	1.038092
H	0.087207	-1.498082	-1.297510	C	-0.925837	4.833437	-1.256363
C	-3.030220	-2.381223	-0.866970	C	0.806299	4.693363	2.263602
C	-2.839363	-1.104193	1.842714	C	1.669861	5.304310	-0.009655
C	-3.831781	0.401945	-0.509309	H	-2.202513	-5.778949	-0.868067
C	3.344803	-0.013153	-1.679062	H	-3.824217	-5.093169	-0.816972
C	2.871870	-2.378870	0.021651	C	-2.797937	-4.747247	-2.690201
C	3.175845	0.458293	1.239485	H	-4.637510	-3.627241	-2.849763
O	-1.279899	3.145629	0.448027	H	-3.529391	-3.351703	-4.190459
O	1.025840	3.038394	0.536034	H	-1.208437	-2.224861	4.720898
H	-4.070460	-2.515480	-0.535093	H	-2.093248	-0.714056	4.530577
C	-2.241950	-3.647759	-0.472112	C	-3.352633	-2.471258	4.443796
C	-3.046598	-2.224958	-2.404802	H	-4.684177	-0.835201	3.959684
H	-2.948006	-0.079772	2.224059	H	-5.427439	-2.422785	3.788463
C	-1.690088	-1.731848	2.662355	H	-6.367265	1.562749	-0.098631
C	-4.163845	-1.849971	2.117416	H	-5.818466	2.909256	0.894103
H	-4.676009	-0.253893	-0.775615	C	-5.169676	3.001043	-1.180430
C	-4.323487	1.368960	0.593599	H	-4.330433	2.632412	-3.153058
C	-3.447613	1.230911	-1.757013	H	-5.444132	1.386492	-2.596522
				H	4.013854	2.983472	-3.341466

H	5.167493	1.698542	-2.993661
C	3.643012	1.129104	-4.418309
H	3.334478	-0.929466	-5.051284
H	4.755722	-0.688170	-4.037685
H	3.867829	-4.726395	-1.154691
H	5.517874	-4.581681	-0.557971
C	4.035396	-4.954739	0.990147
H	2.334176	-4.932472	2.345634
H	1.897717	-4.942482	0.638724
H	6.316170	1.217649	2.566958
H	5.081511	2.361717	2.046480
C	4.517264	1.213546	3.792782
H	2.730584	2.326322	3.287320
H	2.494186	1.165195	4.591012
H	-2.741009	5.400191	0.627209
H	-1.378065	6.477042	0.973050
H	-1.779258	5.153697	2.091267
H	-0.304204	4.168204	-1.859346
H	-0.641415	5.872103	-1.458930
H	-1.965119	4.697421	-1.573022
H	0.122794	4.058440	2.835863
H	0.601111	5.740168	2.513182
H	1.828456	4.462276	2.580733
H	2.676417	5.160436	0.397976
H	1.415477	6.366364	0.089025
H	1.696104	5.048305	-1.071074
H	-1.760221	-4.666320	-3.045867
H	-3.226324	-5.637527	-3.168528
H	-3.590684	-2.431155	5.514397
H	-3.246786	-3.535820	4.186398
H	-6.052263	3.547662	-1.537852
H	-4.401949	3.753489	-0.950429
H	4.258399	1.402303	-5.285415
H	2.608681	1.411353	-4.660724
H	4.101987	-6.048432	0.926795
H	4.726826	-4.645182	1.788137
H	4.769814	0.240568	4.240783
H	4.876313	1.980556	4.491072
C	-0.277571	0.593631	-1.967031
O	-0.474611	0.275723	-3.115632
O	-0.086471	1.728850	-1.386723

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Ru	-0.073524	-0.475351	-0.361427
H	0.231058	-1.859912	-1.475598
H	-0.328058	-2.177167	-0.968989
H	-0.071611	1.070708	0.361671
C	0.873814	4.274159	0.350715
C	-0.610393	4.112617	0.848186
B	-0.009054	2.296793	-0.459867
O	-1.105570	3.091460	-0.035633
O	1.202577	2.928133	-0.050542
C	-0.134737	0.522486	-2.069730
O	-0.203718	0.071883	-3.198611
O	-0.092212	1.856341	-1.844354
C	-0.703177	3.593556	2.293218
H	-0.416979	4.359020	3.023359
H	-1.738211	3.299323	2.498438
H	-0.064441	2.716970	2.437941
C	-1.485185	5.357291	0.686940
H	-2.498390	5.148315	1.047860
H	-1.087911	6.197642	1.268885
H	-1.557171	5.659305	-0.360371
C	0.988306	5.172324	-0.893374
H	0.816066	6.227950	-0.653991
H	1.997030	5.073583	-1.307312
H	0.277141	4.865384	-1.665757

C	1.867643	4.742554	1.413271
H	2.875774	4.779227	0.985630
H	1.616942	5.750057	1.766180
H	1.890335	4.071197	2.274756
P	-2.502458	-0.631809	-0.048024
P	2.352222	-0.630004	-0.206120
C	-3.287055	-2.287619	-0.551804
C	-2.777250	-0.524510	1.820940
C	-3.807251	0.563978	-0.766636
C	3.400317	-0.330598	-1.746879
C	2.731852	-2.445957	0.197652
C	3.145057	0.484712	1.099017
H	-4.326334	-2.228986	-0.195335
C	-2.638936	-3.523122	0.108669
C	-3.326953	-2.459767	-2.088163
H	-2.744987	0.560397	1.992003
C	-1.602824	-1.114785	2.633271
C	-4.123430	-1.049726	2.363485
H	-4.705974	-0.059788	-0.895845
C	-4.190105	1.751579	0.145082
C	-3.388117	1.107529	-2.152711
H	4.436179	-0.574218	-1.467810
C	3.365496	1.149882	-2.192807
C	3.003231	-1.250876	-2.924344
H	2.424033	-2.939137	-0.736450
C	4.200298	-2.846991	0.453357
C	1.827761	-3.034384	1.305376
H	2.742335	1.465512	0.812154
C	4.687212	0.586179	1.111602
C	2.623526	0.186541	2.521777
H	-1.577104	-3.577912	-0.168592
H	-2.668748	-3.439252	1.199414
C	-3.326773	-4.832873	-0.316529
C	-3.997070	-3.780227	-2.507462
H	-3.867367	-1.628507	-2.549928
H	-2.305364	-2.423046	-2.489997
H	-1.553066	-2.203564	2.504235
H	-0.653086	-0.705303	2.260561
C	-1.752591	-0.797177	4.131466
C	-4.274936	-0.735325	3.863308
H	-4.965877	-0.621393	1.808002
H	-4.180914	-2.137461	2.223995
H	-3.303206	2.374349	0.304641
H	-4.535926	1.406280	1.124962
C	-5.307972	2.600229	-0.491491
C	-4.516862	1.931618	-2.793886
H	-2.510505	1.747296	-2.025127
H	-3.083360	0.301350	-2.826166
H	2.340847	1.432380	-2.451961
H	3.662405	1.813629	-1.374292
C	4.275190	1.382072	-3.411195
C	3.905170	-1.007510	-4.148353
H	3.077410	-2.306976	-2.636104
H	1.959181	-1.059097	-3.197919
H	4.859372	-2.448373	-0.326339
H	4.538659	-2.415567	1.404247
C	4.348227	-4.378341	0.523317
C	1.968284	-4.564741	1.379777
H	2.096608	-2.605822	2.278460
H	0.779082	-2.765078	1.125969
H	5.130158	-0.380272	1.382015
H	5.071453	0.840479	0.118901
C	5.162234	1.649163	2.119890
C	3.103110	1.242380	3.532730
H	1.527854	0.143338	2.521028
H	2.983660	-0.796581	2.853387
H	-2.820323	-5.683302	0.158109

H	-4.361340	-4.836601	0.057678
C	-3.340093	-4.995187	-1.841422
H	-5.061564	-3.749791	-2.230597
H	-3.961901	-3.874901	-3.600088
H	-0.923463	-1.246412	4.693353
H	-1.677430	0.290424	4.276073
C	-3.099378	-1.292428	4.680056
H	-4.327914	0.354838	3.999250
H	-5.224043	-1.142723	4.235001
H	-6.226597	1.997173	-0.559681
H	-5.540939	3.446452	0.168519
C	-4.927234	3.101392	-1.890497
H	-4.185966	2.301524	-3.772468
H	-5.390080	1.286974	-2.980482
H	4.213905	2.434603	-3.715857
H	5.323811	1.197357	-3.130374
C	3.891736	0.464864	-4.580536
H	3.578676	-1.651682	-4.974832
H	4.936727	-1.306336	-3.905991
H	4.101003	-4.808602	-0.458472
H	5.394460	-4.642003	0.724922
C	3.429404	-4.988147	1.592138
H	1.336673	-4.957926	2.186983
H	1.593332	-5.007434	0.444737
H	6.259408	1.687934	2.124192
H	4.815064	2.638627	1.789074
C	4.632715	1.371239	3.533069
H	2.657764	2.213329	3.277005
H	2.740571	0.984866	4.536633
H	-2.306856	-5.097083	-2.205683
H	-3.863754	-5.917492	-2.123476
H	-3.205240	-1.014808	5.736483
H	-3.122469	-2.391897	4.642033
H	-5.761136	3.660360	-2.335129
H	-4.082998	3.799675	-1.805668
H	4.572967	0.618629	-5.427635
H	2.883693	0.728659	-4.929345
H	3.513691	-6.082314	1.587849
H	3.760863	-4.653209	2.586421
H	5.075404	0.436089	3.908495
H	4.948705	2.164532	4.222652

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Ru	0.062490	0.487602	-0.381460
H	-0.275531	1.890435	-1.501008
H	0.349964	2.177447	-1.070133
H	0.055494	-1.023578	0.363626
C	-0.835398	-4.293749	0.401337
C	0.652267	-4.086301	0.873754
B	0.015000	-2.362003	-0.523449
O	1.123405	-3.100758	-0.066649
O	-1.182510	-2.979919	-0.090956
C	0.119960	-0.522997	-2.077155
O	0.173936	-0.081889	-3.210426
O	0.090092	-1.869795	-1.868455
C	0.755510	-3.494937	2.288911
H	0.479451	-4.225679	3.057303
H	1.790908	-3.186960	2.470324
H	0.114821	-2.614712	2.395759
C	1.543451	-5.324327	0.760807
H	2.558070	-5.082207	1.095504
H	1.167211	-6.139610	1.390275
H	1.605223	-5.678077	-0.270821
C	-0.955359	-5.269559	-0.781613
H	-0.774963	-6.306665	-0.477016
H	-1.968217	-5.202432	-1.191435
H	-0.252879	-5.010147	-1.579212

C	-1.815277	-4.698877	1.501299
H	-2.826992	-4.769456	1.086954
H	-1.553555	-5.679782	1.915523
H	-1.833377	-3.973432	2.317447
P	2.489755	0.630092	-0.048040
P	-2.358353	0.623868	-0.221798
C	3.271665	2.311810	-0.469163
C	2.777159	0.438831	1.813373
C	3.797808	-0.515101	-0.836088
C	-3.409249	0.327650	-1.761662
C	-2.743730	2.436565	0.192209
C	-3.152821	-0.493472	1.082294
H	4.307033	2.243174	-0.103020
C	2.606168	3.510384	0.239950
C	3.332302	2.562347	-1.993945
H	2.756362	-0.652814	1.937142
C	1.599511	0.982537	2.653152
C	4.119620	0.954359	2.374259
H	4.683404	0.128534	-0.955500
C	4.225137	-1.736020	0.008619
C	3.359095	-1.001965	-2.236154
H	-4.445892	0.565578	-1.480333
C	-3.367324	-1.150961	-2.213470
C	-3.017832	1.252626	-2.937303
H	-2.458530	2.932770	-0.747315
C	-4.208630	2.828962	0.478947
C	-1.817565	3.027433	1.280640
H	-2.737450	-1.472393	0.807548
C	-4.694148	-0.610495	1.079006
C	-2.650975	-0.174919	2.507929
H	1.549585	3.573299	-0.055011
H	2.615999	3.371874	1.325424
C	3.297068	4.842121	-0.104817
C	4.013991	3.900362	-2.331915
H	3.872966	1.753977	-2.495097
H	2.315531	2.557852	-2.410048
H	1.536529	2.074841	2.565523
H	0.655783	0.575763	2.264712
C	1.757247	0.609750	4.137555
C	4.278487	0.579510	3.859343
H	4.965573	0.558870	1.800003
H	4.165639	2.047673	2.281092
H	3.358016	-2.389687	0.152361
H	4.578592	-1.431723	0.999381
C	5.353403	-2.518976	-0.691096
C	4.493052	-1.760352	-2.943860
H	2.502450	-1.671498	-2.117943
H	3.013415	-0.173147	-2.860385
H	-2.341917	-1.424957	-2.478464
H	-3.656759	-1.820323	-1.396732
C	-4.279443	-1.384395	-3.429798
C	-3.921692	1.009524	-4.159987
H	-3.095207	2.307688	-2.646178
H	-1.973621	1.065051	-3.213207
H	-4.880518	2.429764	-0.289615
H	-4.526509	2.391974	1.434311
C	-4.363351	4.359161	0.558149
C	-1.966888	4.556517	1.365060
H	-2.058137	2.592617	2.258225
H	-0.771205	2.767467	1.073366
H	-5.149071	0.355382	1.330467
H	-5.064365	-0.882184	0.085719
C	-5.172066	-1.663537	2.096258
C	-3.135455	-1.218722	3.528982
H	-1.555878	-0.123285	2.519301
H	-3.022278	0.809685	2.821848
H	2.777199	5.666520	0.400311

H	4.323233	4.829945	0.291803	C	2.833554	4.582325	1.416715
C	3.343196	5.080823	-1.619051	H	3.825500	4.610648	0.953421
H	5.072166	3.852960	-2.034022	H	2.701846	5.508552	1.987933
H	4.002411	4.050840	-3.418822	H	2.808709	3.739717	2.110902
H	0.926252	1.030437	4.718582	P	-2.589641	-0.335097	-0.041736
H	1.691174	-0.483149	4.241441	P	2.160901	-1.030947	-0.209629
C	3.101573	1.094107	4.701486	C	-3.721277	-1.659367	-0.809136
H	4.339895	-0.514919	3.950409	C	-2.893650	-0.500931	1.821673
H	5.225878	0.978362	4.244566	C	-3.586764	1.230614	-0.488670
H	6.253358	-1.886970	-0.743395	C	3.280121	-0.915144	-1.730772
H	5.622817	-3.391460	-0.080946	C	2.308007	-2.877231	0.222496
C	4.961994	-2.958883	-2.108140	C	3.084262	-0.031953	1.106953
H	4.148040	-2.094158	-3.930507	H	-4.722005	-1.477831	-0.389407
H	5.341533	-1.081085	-3.121406	C	-3.302495	-3.096916	-0.432317
H	-4.213366	-2.435587	-3.738165	C	-3.823067	-1.511260	-2.344053
H	-5.328229	-1.206211	-3.145378	H	-2.616633	0.497687	2.184780
C	-3.903773	-0.461381	-4.597145	C	-1.918061	-1.475968	2.514977
H	-3.599573	1.657406	-4.985303	C	-4.345035	-0.780998	2.263532
H	-4.953850	1.303676	-3.914423	H	-4.616310	0.867466	-0.637287
H	-4.138482	4.794674	-0.426698	C	-3.628574	2.318106	0.607717
H	-5.406594	4.616498	0.782290	C	-3.102415	1.878721	-1.806538
C	-3.425888	4.969453	1.610363	H	4.238060	-1.375225	-1.442652
H	-1.320783	4.950511	2.160319	C	3.561156	0.541537	-2.165781
H	-1.615082	5.005830	0.424242	C	2.716623	-1.707133	-2.933361
H	-6.268787	-1.712862	2.086804	H	2.092425	-3.344390	-0.749619
H	-4.811485	-2.654398	1.784278	C	3.670742	-3.427586	0.690209
C	-4.663728	-1.360485	3.511996	C	1.189087	-3.349804	1.177581
H	-2.679644	-2.190364	3.295643	H	2.829228	0.997532	0.819007
H	-2.787749	-0.942263	4.533115	C	4.626762	-0.132913	1.152360
H	2.317863	5.201129	-1.999791	C	2.498758	-0.267202	2.517099
H	3.872126	6.015950	-1.843205	H	-2.267363	-3.270527	-0.756296
H	3.213556	0.775839	5.745809	H	-3.313684	-3.227776	0.654685
H	3.115747	2.194379	4.706840	C	-4.209366	-4.161531	-1.074827
H	5.805943	-3.464525	-2.595717	C	-4.716318	-2.592162	-2.978464
H	4.145278	-3.691666	-2.045434	H	-4.230309	-0.529111	-2.600753
H	-4.587237	-0.615077	-5.442487	H	-2.818304	-1.553511	-2.786575
H	-2.895829	-0.719882	-4.950121	H	-2.105158	-2.507658	2.189742
H	-3.516884	6.063108	1.613070	H	-0.889301	-1.226323	2.225207
H	-3.734390	4.627933	2.609791	C	-2.058112	-1.403986	4.045818
H	-5.119031	-0.423728	3.867677	C	-4.484075	-0.708891	3.795166
H	-4.982036	-2.146165	4.209222	H	-5.041729	-0.075489	1.794493
				H	-4.646219	-1.783126	1.929774
				H	-2.608997	2.680976	0.783143
				H	-4.004211	1.917897	1.554703
				C	-4.530063	3.496927	0.192093
				C	-4.030052	3.026201	-2.238276
				H	-2.099478	2.281542	-1.643835
				H	-3.008387	1.145820	-2.610772
				H	2.621449	1.021714	-2.454110
				H	3.960799	1.136043	-1.337958
				C	4.539473	0.583597	-3.352580
				C	3.684725	-1.667174	-4.129672
				H	2.528728	-2.754422	-2.666026
				H	1.753135	-1.273614	-3.227590
				H	4.473950	-3.113631	0.013493
				H	3.912575	-3.019687	1.679906
				C	3.642734	-4.964349	0.787035
				C	1.159338	-4.884356	1.290567
				H	1.336651	-2.916845	2.175175
				H	0.213202	-2.991414	0.820974
				H	4.934238	-1.146259	1.434599
				H	5.063290	0.064068	0.168492
				C	5.212587	0.860254	2.173457
				C	3.093835	0.705082	3.550240
				H	1.408180	-0.164118	2.488867
				H	2.718813	-1.293605	2.842147
				H	-3.850265	-5.162070	-0.800315

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Ru	-0.210704	-0.597307	-0.399502
H	0.010805	-2.038570	-1.635220
H	-0.780770	-1.946249	-1.635673
H	-0.050654	0.615717	0.662271
C	1.765487	4.455613	0.332847
C	0.280456	4.348253	0.859060
B	0.680518	2.763297	-0.744920
O	-0.329962	3.475761	-0.128951
O	1.938986	3.189682	-0.355605
C	-0.069469	0.625976	-1.940056
O	-0.373488	0.338087	-3.081621
O	0.512981	1.898389	-1.782029
C	0.168307	3.649756	2.220854
H	0.574679	4.270745	3.026665
H	-0.887082	3.457239	2.437791
H	0.688225	2.687771	2.216450
C	-0.490474	5.668189	0.882197
H	-1.510485	5.494090	1.240104
H	-0.014434	6.386777	1.559640
H	-0.554224	6.115529	-0.112381
C	1.955878	5.558424	-0.719268
H	1.907505	6.557991	-0.274213
H	2.937987	5.435314	-1.186230
H	1.198353	5.490891	-1.506473

H	-5.225487	-4.070584	-0.662644
C	-4.267518	-4.008211	-2.599152
H	-5.754994	-2.444104	-2.646153
H	-4.717607	-2.468128	-4.068870
H	-1.378008	-2.125377	4.517403
H	-1.743236	-0.406940	4.387886
C	-3.503916	-1.661373	4.495924
H	-4.289332	0.321823	4.127088
H	-5.516452	-0.940980	4.087590
H	-5.570512	3.144283	0.122551
H	-4.515540	4.261476	0.980766
C	-4.111136	4.106445	-1.152288
H	-3.663425	3.457366	-3.178487
H	-5.037841	2.633834	-2.445274
H	4.711170	1.626740	-3.647607
H	5.515889	0.181942	-3.039666
C	4.013973	-0.227077	-4.545430
H	3.247409	-2.217390	-4.972807
H	4.614956	-2.191435	-3.861887
H	3.491106	-5.387339	-0.217044
H	4.615535	-5.333032	1.137387
C	2.521990	-5.449367	1.718342
H	0.379375	-5.191198	1.999520
H	0.880724	-5.310003	0.314978
H	6.305950	0.763477	2.197342
H	4.995878	1.886573	1.843456
C	4.627610	0.642277	3.575672
H	2.776742	1.728867	3.305534
H	2.685762	0.483264	4.545217
H	-3.271031	-4.201381	-3.023493
H	-4.944121	-4.754997	-3.034227
H	-3.588137	-1.560041	5.585569
H	-3.777615	-2.700044	4.256657
H	-4.810896	4.900574	-1.444532
H	-3.122564	4.573421	-1.043478
H	4.746446	-0.224977	-5.363298
H	3.103920	0.252075	-4.932977
H	2.489804	-6.546199	1.737964
H	2.741541	-5.124625	2.746426
H	4.942941	-0.343688	3.949211
H	5.028908	1.384322	4.278064

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Ru	-0.749982	0.343205	0.317196
H	-0.749761	0.746810	2.169449
H	-1.183430	0.071750	2.142082
H	-0.575934	0.273873	-1.287338
C	4.198021	-3.579746	-0.422979
C	4.861849	-2.460746	0.477405
B	2.807914	-1.787909	-0.219707
O	4.025977	-1.303985	0.196654
O	2.820121	-3.127582	-0.515862
C	0.783650	-0.860063	0.596292
O	1.012002	-1.522405	1.604717
O	1.718817	-0.959969	-0.442858
C	4.732288	-2.737466	1.981748
H	5.357928	-3.580294	2.294766
H	5.053203	-1.847601	2.532623
H	3.692844	-2.941998	2.255143
C	6.306570	-2.114948	0.123228
H	6.658799	-1.306320	0.772039
H	6.963445	-2.979443	0.274429
H	6.401394	-1.781055	-0.912735
C	4.747973	-3.614073	-1.855718
H	5.769217	-4.008473	-1.889995
H	4.108551	-4.260718	-2.465010
H	4.745732	-2.616532	-2.306864

C	4.205085	-4.984034	0.178363
H	3.699224	-5.676798	-0.502200
H	5.230570	-5.342407	0.325887
H	3.682168	-5.011539	1.136814
P	-2.363972	-1.373222	-0.093614
P	0.635092	2.311860	0.161775
C	-2.987661	-2.530132	1.275831
C	-3.894555	-0.407715	-0.644651
C	-2.069836	-2.618524	-1.502588
C	1.366830	2.969442	1.781089
C	-0.405097	3.782481	-0.427466
C	2.181684	2.133154	-0.917847
H	-3.835233	-3.082240	0.840789
C	-3.500039	-1.773489	2.518378
C	-1.910274	-3.559364	1.690338
H	-3.647524	-0.140456	-1.680430
C	-4.024234	0.932358	0.115412
C	-5.238524	-1.162987	-0.664920
H	-2.683133	-3.498854	-1.254191
C	-2.505468	-2.123114	-2.899053
C	-0.585929	-3.045072	-1.560466
H	1.990683	3.835282	1.522228
C	2.274812	1.903204	2.436530
C	0.305245	3.461724	2.787698
H	-1.145343	3.858979	0.384909
C	0.297574	5.152699	-0.531769
C	-1.209253	3.507277	-1.718113
H	2.609221	1.210965	-0.507211
C	3.275413	3.221294	-0.831552
C	1.860008	1.824349	-2.395814
H	-2.683781	-1.166558	2.931656
H	-4.302192	-1.078146	2.248770
C	-4.009138	-2.730214	3.610425
C	-2.416740	-4.507625	2.791465
H	-1.605975	-4.157962	0.825906
H	-1.013959	-3.027165	2.034421
H	-4.225961	0.754940	1.178778
H	-3.069806	1.482694	0.069812
C	-5.148219	1.802625	-0.473512
C	-6.359991	-0.286855	-1.252076
H	-5.149979	-2.091131	-1.243266
H	-5.516641	-1.458677	0.355416
H	-1.950983	-1.206114	-3.144039
H	-3.570507	-1.868289	-2.914042
C	-2.246461	-3.184542	-3.985278
C	-0.337605	-4.123626	-2.625791
H	0.017702	-2.162651	-1.794381
H	-0.231566	-3.397962	-0.588005
H	1.682692	1.005191	2.653410
H	3.062067	1.584637	1.744005
C	2.914640	2.419222	3.736290
C	0.948765	3.967589	4.091967
H	-0.299930	4.265911	2.352830
H	-0.386805	2.642420	3.026503
H	0.870790	5.375145	0.375566
H	1.017512	5.129432	-1.359906
C	-0.720610	6.278909	-0.788327
C	-2.233816	4.625854	-1.976123
H	-0.526200	3.445664	-2.574337
H	-1.708717	2.534345	-1.657458
H	2.915206	4.163061	-1.266063
H	3.543624	3.437075	0.208017
C	4.541713	2.771923	-1.585939
C	3.123729	1.375566	-3.148567
H	1.090464	1.049664	-2.453358
H	1.460420	2.723564	-2.886291
H	-4.340240	-2.149332	4.481298

H	-4.894260	-3.268502	3.239206
C	-2.932042	-3.743555	4.017484
H	-3.228850	-5.132273	2.388844
H	-1.610089	-5.193632	3.080021
H	-5.245798	2.730247	0.105233
H	-4.876723	2.098052	-1.497642
C	-6.486486	1.047415	-0.501519
H	-6.144828	-0.087316	-2.312307
H	-7.312872	-0.831077	-1.223922
H	-2.894874	-4.053472	-3.795915
H	-2.542696	-2.783861	-4.963842
C	-0.783268	-3.644498	-4.013194
H	0.728723	-4.381023	-2.628875
H	-0.884357	-5.042651	-2.363364
H	3.524446	1.625166	4.185632
H	3.600752	3.247852	3.503468
C	1.854022	2.906476	4.732030
H	0.162563	4.275691	4.793678
H	1.543411	4.867716	3.875373
H	-1.384835	6.368884	0.084241
H	-0.197536	7.239616	-0.881716
C	-1.563176	6.006231	-2.043065
H	-2.779137	4.423628	-2.907341
H	-2.982264	4.624169	-1.169292
H	5.304636	3.559810	-1.528774
H	4.960689	1.889128	-1.081431
C	4.242738	2.422012	-3.050439
H	3.472828	0.425654	-2.719092
H	2.878963	1.175603	-4.200222
H	-2.094707	-3.211034	4.491496
H	-3.326819	-4.441511	4.767244
H	-7.263724	1.670643	-0.961757
H	-6.812884	0.851790	0.530824
H	-0.648697	-4.436860	-4.761329
H	-0.145839	-2.804190	-4.325020
H	2.330276	3.308477	5.635714
H	1.240723	2.051813	5.053789
H	-2.317744	6.792625	-2.173879
H	-0.912479	6.047077	-2.929245
H	3.934238	3.333728	-3.584630
H	5.152306	2.061351	-3.548538

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Ru	0.563805	0.386878	0.005781
H	0.065568	-0.290428	1.346358
H	1.128819	1.088353	1.411328
H	0.237910	0.009912	-1.596985
C	-5.034531	-2.732052	-0.902445
C	-4.337433	-3.514350	0.280949
B	-2.968318	-1.875830	-0.492669
O	-2.956967	-3.069563	0.179285
O	-4.196885	-1.550626	-1.026803
C	-0.587279	-1.266078	-0.448838
O	-0.218468	-2.413404	-0.541230
O	-1.942250	-0.967682	-0.610175
C	-4.839136	-3.090767	1.668559
H	-5.856905	-3.448155	1.858153
H	-4.176675	-3.516024	2.428828
H	-4.827437	-2.001680	1.781699
C	-4.361257	-5.037040	0.157418
H	-3.827900	-5.480975	1.004079
H	-5.390309	-5.414714	0.168166
H	-3.872930	-5.374065	-0.759518
C	-4.957666	-3.470796	-2.245982
H	-5.614014	-4.347334	-2.266194
H	-5.268947	-2.788290	-3.043051
H	-3.935304	-3.797188	-2.461486

C	-6.469223	-2.283641	-0.630734
H	-6.848411	-1.724477	-1.492400
H	-7.125054	-3.147666	-0.473103
H	-6.530809	-1.634353	0.245687
P	-1.175183	2.032219	0.116518
P	2.605802	-0.916975	0.066083
C	-0.264083	3.672678	-0.198112
C	-2.543810	2.094422	-1.191376
C	-2.162482	2.218444	1.723850
C	2.955176	-1.801966	1.700501
C	4.068137	0.284273	-0.084492
C	2.826441	-2.317480	-1.190771
H	-0.938637	4.308297	-0.788582
C	0.977370	3.351853	-1.065338
C	0.163777	4.483348	1.040994
H	-3.097458	1.164914	-1.021113
C	-1.994057	2.008478	-2.630532
C	-3.532487	3.275512	-1.073612
H	-2.611747	3.222691	1.704347
C	-3.308598	1.180316	1.802583
C	-1.301227	2.099421	3.000840
H	3.946587	-2.266281	1.595305
C	1.941300	-2.930192	1.994378
C	3.016371	-0.829699	2.899249
H	3.756508	1.085604	0.602537
C	5.469467	-0.181678	0.370978
C	4.166019	0.915741	-1.491629
H	2.082749	-3.036024	-0.827271
C	4.196679	-3.027023	-1.229072
C	2.379948	-1.955311	-2.624001
H	1.638704	2.681612	-0.482230
H	0.688301	2.814166	-1.973734
C	1.771144	4.613193	-1.447180
C	0.925716	5.760432	0.642529
H	-0.709738	4.752202	1.645959
H	0.815016	3.865589	1.672864
H	-1.421400	2.917295	-2.869533
H	-1.306471	1.160650	-2.713677
C	-3.138619	1.865543	-3.648770
C	-4.675617	3.148190	-2.099090
H	-3.961027	3.338391	-0.066952
H	-3.006363	4.225311	-1.247980
H	-2.869390	0.173775	1.798497
H	-3.961716	1.235706	0.926997
C	-4.157689	1.364506	3.072797
C	-2.143765	2.303350	4.272470
H	-0.841581	1.104664	3.020630
H	-0.473980	2.812354	2.989892
H	0.933223	-2.502864	2.056689
H	1.912549	-3.654030	1.174093
C	2.280985	-3.662176	3.304664
C	3.369977	-1.564900	4.203361
H	3.744886	-0.029635	2.722776
H	2.043016	-0.337972	3.006954
H	5.434789	-0.617731	1.374463
H	5.839215	-0.966963	-0.298583
C	6.466530	0.992637	0.362392
C	5.157905	2.091662	-1.509277
H	4.507514	0.157325	-2.208419
H	3.180634	1.248251	-1.839728
H	4.955394	-2.349037	-1.642990
H	4.534447	-3.300383	-0.222451
C	4.134486	-4.289798	-2.108540
C	2.318441	-3.212343	-3.508758
H	1.400656	-1.470810	-2.595636
H	3.080935	-1.238060	-3.072439
H	2.664618	4.332366	-2.019223

H	1.152120	5.229093	-2.116568	C	-6.014628	-2.973134	1.561394
C	2.158762	5.438395	-0.213418	H	-6.566916	-2.132119	1.993622
H	0.254474	6.424613	0.077876	H	-6.739662	-3.745847	1.280232
H	1.221217	6.309696	1.545786	H	-5.356222	-3.376087	2.334209
H	-2.727730	1.818410	-4.665838	P	2.568417	-1.208172	0.108629
H	-3.653662	0.910685	-3.470879	P	-0.845078	2.063578	-0.183276
C	-4.144750	3.019257	-3.533530	C	2.971900	-2.791064	-0.858136
H	-5.275883	2.259781	-1.854548	C	3.947558	0.002664	-0.378364
H	-5.346784	4.013335	-2.015196	C	3.054913	-1.726489	1.878247
H	-4.671773	2.336382	3.024823	C	-1.754789	2.551666	-1.777061
H	-4.944615	0.598964	3.102569	C	0.278646	3.576391	0.097920
C	-3.305505	1.304270	4.346370	C	-2.246530	2.084249	1.085166
H	-1.500654	2.206393	5.156916	H	4.044085	-2.977945	-0.692969
H	-2.542904	3.329035	4.288794	C	2.742418	-2.617977	-2.372818
H	1.525790	-4.434931	3.498446	C	2.196478	-4.025209	-0.344606
H	3.241151	-4.187664	3.187916	H	4.022864	0.647655	0.506184
C	2.377093	-2.697949	4.495175	C	3.522125	0.938744	-1.532679
H	3.389562	-0.849537	5.036096	C	5.346800	-0.588070	-0.641431
H	4.385409	-1.982786	4.126789	H	3.755658	-2.566831	1.754074
H	6.152746	1.736434	1.109958	C	3.780678	-0.633086	2.693119
H	7.458478	0.638833	0.672463	C	1.827802	-2.223097	2.677455
C	6.547643	1.662502	-1.016933	H	-2.251904	3.511148	-1.577337
H	5.224894	2.507621	-2.523194	C	-2.847459	1.536691	-2.179140
H	4.775808	2.896933	-0.864088	C	-0.782147	2.765565	-2.958230
H	5.120406	-4.772773	-2.136552	H	1.092217	3.384213	-0.621094
H	3.443703	-5.012017	-1.649421	C	-0.276766	4.983259	-0.225539
C	3.656941	-3.964791	-3.531252	C	0.925751	3.588816	1.501131
H	1.531705	-3.877068	-3.124235	H	-2.928421	1.346086	0.647949
H	2.022515	-2.933692	-4.528830	C	-3.030625	3.401982	1.259512
H	2.879652	4.869172	0.392401	C	-1.858497	1.517356	2.468505
H	2.666272	6.362846	-0.517274	H	1.683391	-2.383108	-2.544212
H	-4.977269	2.874458	-4.234346	H	3.318398	-1.769521	-2.760206
H	-3.652491	3.960090	-3.823546	C	3.107162	-3.886776	-3.163052
H	-3.925097	1.497731	5.231681	C	2.556845	-5.292705	-1.140199
H	-2.899726	0.288492	4.461866	H	2.417323	-4.199591	0.713567
H	2.668695	-3.239822	5.404452	H	1.119531	-3.830537	-0.407263
H	1.384717	-2.265550	4.690830	H	3.380845	0.369661	-2.460124
H	7.224893	2.525600	-0.983333	H	2.546843	1.403444	-1.307058
H	6.980758	0.952625	-1.737348	C	4.565386	2.045196	-1.769742
H	4.414555	-3.342409	-4.031549	C	6.386987	0.522184	-0.876356
H	3.570122	-4.885553	-4.122859	H	5.661234	-1.221827	0.197380
				H	5.315679	-1.237053	-1.527104
				H	3.127283	0.247073	2.775784
				H	4.697580	-0.307235	2.191215
				C	4.159316	-1.122403	4.104037
				C	2.223271	-2.736236	4.071116
				H	1.125872	-1.386648	2.778180
				H	1.282279	-2.991747	2.128910
				H	-2.388839	0.552061	-2.335264
				H	-3.575286	1.410216	-1.370843
				C	-3.583704	1.973048	-3.458083
				C	-1.518710	3.202619	-4.237125
				H	-0.015916	3.508912	-2.709179
				H	-0.248909	1.826785	-3.158960
				H	-0.726730	5.016435	-1.222913
				H	-1.072151	5.241020	0.483856
				C	0.833353	6.047632	-0.138728
				C	2.036361	4.648632	1.595603
				H	0.156930	3.815145	2.252370
				H	1.320566	2.597338	1.744134
				H	-2.397562	4.145921	1.761356
				H	-3.317150	3.831882	0.292393
				C	-4.292690	3.175953	2.113366
				C	-3.116277	1.283518	3.324500
				H	-1.305547	0.582891	2.348700
				H	-1.190428	2.216636	2.989958
				H	2.904998	-3.726651	-4.230278

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Ru	0.613312	0.133035	-0.260537
H	0.071570	0.016560	-2.042202
H	0.630545	-0.576521	-1.987238
H	0.826179	0.478110	1.306831
C	-5.224949	-2.497096	0.343336
C	-4.343446	-3.605355	-0.361086
B	-3.099781	-1.744022	0.014528
O	-3.187689	-2.844642	-0.801294
O	-4.222192	-1.544397	0.788559
C	-0.730170	-1.228255	0.222195
O	-0.556495	-2.356436	0.648920
O	-2.073670	-0.826611	0.016850
C	-3.825183	-4.676795	0.608306
H	-4.628246	-5.339752	0.948320
H	-3.070923	-5.280237	0.094402
H	-3.347311	-4.223441	1.481898
C	-4.984436	-4.264397	-1.580968
H	-4.286703	-4.987987	-2.014813
H	-5.898049	-4.801151	-1.300164
H	-5.232670	-3.532161	-2.352874
C	-6.148510	-1.746675	-0.626291
H	-6.981970	-2.372983	-0.961996
H	-6.560695	-0.870215	-0.116120
H	-5.599522	-1.398306	-1.507170

H	4.187893	-4.073854	-3.074127	C	-5.177076	-3.264798	1.364302
C	2.336102	-5.108439	-2.647048	H	-5.902661	-2.448655	1.282064
H	3.612354	-5.548416	-0.959868	H	-5.733840	-4.202936	1.472487
H	1.963808	-6.137958	-0.767794	H	-4.586766	-3.101432	2.268665
H	4.259275	2.673142	-2.616497	P	2.604555	-0.796756	0.079266
H	4.599581	2.701984	-0.887588	P	-1.108154	2.195556	-0.222814
C	5.963478	1.458406	-2.017967	C	2.651898	-2.607701	-0.497876
H	6.505911	1.107298	0.047624	C	4.058398	0.019694	-0.838064
H	7.366974	0.077233	-1.092389	C	3.273653	-0.937740	1.858524
H	4.911717	-1.920524	4.013941	C	-2.080452	2.505281	-1.820744
H	4.641221	-0.303642	4.654869	C	-0.393437	3.921383	0.129074
C	2.950593	-1.656798	4.881519	C	-2.476426	1.764069	1.010049
H	1.325487	-3.074772	4.604233	H	3.715542	-2.886225	-0.519728
H	2.876378	-3.616927	3.970077	C	2.079360	-2.761370	-1.923957
H	-4.333249	1.217301	-3.726813	C	1.943600	-3.591031	0.462781
H	-4.136341	2.903687	-3.259425	H	4.300556	0.869519	-0.186111
C	-2.615517	2.202298	-4.625887	C	3.664935	0.643146	-2.196171
H	-0.797455	3.319369	-5.056599	C	5.336218	-0.831568	-0.983266
H	-1.970912	4.192684	-4.075710	H	3.920737	-1.828959	1.860725
H	1.583840	5.849649	-0.918891	C	4.133540	0.264065	2.310328
H	0.413132	7.038363	-0.356221	C	2.132228	-1.152542	2.880085
C	1.518400	6.048102	1.234997	H	-2.804682	3.304323	-1.611245
H	2.463648	4.649425	2.606885	C	-2.874486	1.255094	-2.259532
H	2.854636	4.375924	0.911485	C	-1.166219	2.994204	-2.965730
H	-4.828825	4.125769	2.242618	H	0.333260	4.019718	-0.693932
H	-4.974070	2.501558	1.574305	C	-1.354477	5.127088	0.030383
C	-3.948161	2.565506	3.479526	C	0.422186	4.012597	1.437825
H	-3.725292	0.501928	2.848873	H	-2.773786	0.771262	0.642286
H	-2.825842	0.900007	4.311573	C	-3.747831	2.641069	1.025493
H	1.262888	-4.967104	-2.841414	C	-1.968309	1.550870	2.453632
H	2.639489	-6.011129	-3.193209	H	1.030530	-2.440227	-1.918649
H	6.696728	2.265644	-2.141029	H	2.609115	-2.106684	-2.626317
H	5.956721	0.895415	-2.963222	C	2.153303	-4.213251	-2.428435
H	3.269022	-2.048790	5.856459	C	2.020508	-5.039582	-0.053102
H	2.254906	-0.829734	5.086405	H	2.400609	-3.547989	1.456240
H	-3.158981	2.555844	-5.511619	H	0.892251	-3.305081	0.582680
H	-2.150219	1.244964	-4.904334	H	3.371748	-0.140087	-2.907557
H	2.338035	6.778036	1.252786	H	2.785538	1.289975	-2.072989
H	0.794671	6.371517	1.997998	C	4.826502	1.458167	-2.792397
H	-3.376233	3.300416	4.066440	C	6.495575	-0.010723	-1.575860
H	-4.866343	2.361627	4.045953	H	5.634405	-1.254018	-0.015465
				H	5.136079	-1.683405	-1.647327
				H	3.528306	1.180262	2.250415
				H	4.995351	0.405401	1.650085
				C	4.658311	0.088475	3.748186
				C	2.671117	-1.359008	4.304585
				H	1.481330	-0.271920	2.856007
				H	1.490563	-1.988097	2.597169
				H	-2.186439	0.411805	-2.391243
				H	-3.573683	0.949032	-1.473814
				C	-3.649855	1.498894	-3.565693
				C	-1.947111	3.224936	-4.271557
				H	-0.653844	3.922053	-2.684990
				H	-0.380922	2.246494	-3.145032
				H	-1.934190	5.101417	-0.898329
				H	-2.079039	5.085759	0.853629
				C	-0.584952	6.458908	0.109592
				C	1.199624	5.337912	1.513801
				H	-0.256593	3.951696	2.298255
				H	1.103647	3.160458	1.519303
				H	-3.512981	3.630592	1.439501
				H	-4.136264	2.806751	0.014468
				C	-4.844073	1.986001	1.887383
				C	-3.058255	0.889417	3.313492
				H	-1.069963	0.930340	2.448296
				H	-1.702187	2.519543	2.899020
				H	1.710168	-4.273683	-3.431072
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Ru	0.648705	0.541047	-0.293678				
H	0.153288	0.319200	-2.115721				
H	0.710615	-0.248871	-2.016647				
H	0.855610	0.991573	1.237205				
C	-4.295776	-3.294611	0.116733				
C	-3.166612	-4.404332	0.121628				
B	-2.272414	-2.382268	-0.402613				
O	-2.071128	-3.732825	-0.560199				
O	-3.523649	-2.064791	0.068340				
C	-0.570152	-0.888921	0.278250				
O	-0.759834	-1.382572	1.382211				
O	-1.339262	-1.430516	-0.783727				
C	-2.658273	-4.746362	1.529044				
H	-3.409629	-5.290451	2.111306				
H	-1.770044	-5.379805	1.438004				
H	-2.369415	-3.841716	2.072149				
C	-3.509579	-5.680066	-0.644884				
H	-2.656623	-6.365925	-0.615362				
H	-4.368049	-6.188798	-0.191078				
H	-3.739929	-5.474059	-1.692773				
C	-5.166960	-3.318581	-1.146518				
H	-5.834823	-4.186466	-1.162854				
H	-5.780252	-2.412210	-1.171368				
H	-4.552610	-3.335473	-2.052504				

H	3.207325	-4.513422	-2.532631
C	1.442116	-5.173851	-1.467057
H	3.070456	-5.370955	-0.055450
H	1.487271	-5.699673	0.643609
H	4.534281	1.861282	-3.770684
H	5.026896	2.324371	-2.143939
C	6.105962	0.618612	-2.921228
H	6.776684	0.784405	-0.869255
H	7.380749	-0.648908	-1.695268
H	5.361759	-0.757672	3.768444
H	5.235013	0.977680	4.035773
C	3.530737	-0.171957	4.754375
H	1.829763	-1.504475	4.994249
H	3.272116	-2.280676	4.347175
H	-4.171404	0.578706	-3.859202
H	-4.428678	2.257558	-3.394494
C	-2.725916	1.973139	-4.695247
H	-1.253711	3.533469	-5.064889
H	-2.650898	4.058965	-4.130936
H	0.067489	6.549940	-0.771885
H	-1.291606	7.297746	0.061010
C	0.267185	6.550936	1.382989
H	1.757599	5.386615	2.457925
H	1.947694	5.366196	0.706934
H	-5.735496	2.627407	1.903544
H	-5.145499	1.038391	1.417675
C	-4.356387	1.709659	3.316965
H	-3.253518	-0.116502	2.917026
H	-2.689891	0.757192	4.339283
H	0.369517	-4.936467	-1.440782
H	1.535193	-6.208727	-1.822223
H	6.928326	1.234709	-3.306736
H	5.941439	-0.180790	-3.659074
H	3.947496	-0.348106	5.754772
H	2.897179	0.723953	4.829703
H	-3.304026	2.173495	-5.606628
H	-2.015565	1.170486	-4.943328
H	0.846167	7.483526	1.387571
H	-0.396816	6.590559	2.259305
H	-4.177811	2.668247	3.827719
H	-5.137538	1.192667	3.889870

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Ru	0.541073	0.816856	-0.064823
P	-1.540467	2.015158	-0.040642
P	2.660504	-0.346584	0.073697
B	-1.702187	-2.600587	-0.212034
H	1.434192	2.370498	-0.404686
H	1.333006	2.073942	-1.166627
H	0.859124	1.429588	1.341401
C	-1.523552	3.852483	-0.524310
C	-2.786680	1.229702	-1.228403
C	-2.482830	2.112314	1.614898
C	3.364018	-0.550451	1.815981
C	4.055337	0.606003	-0.803363
C	2.600254	-2.128080	-0.560953
O	-3.036790	-2.315853	-0.012340
O	-1.453799	-3.947103	-0.355089
H	-2.577439	4.168132	-0.488561
C	-1.003575	4.109783	-1.954272
C	-0.744462	4.722882	0.487227
H	-3.114119	0.340874	-0.673120
C	-2.125675	0.692559	-2.518762
C	-4.039103	2.063312	-1.571206
H	-3.014339	3.077162	1.588696
C	-3.541736	1.006623	1.832727
C	-1.508819	2.126074	2.817999

H	4.336254	-1.050361	1.702715
C	2.479801	-1.445433	2.711918
C	3.611842	0.810397	2.503334
H	3.929445	1.606853	-0.361850
C	5.517441	0.181127	-0.543549
C	3.830328	0.765732	-2.323042
H	1.813076	-2.546223	0.081370
C	3.857775	-3.005428	-0.386508
C	2.065661	-2.250323	-2.005838
C	-3.703005	-3.576038	0.269758
C	-2.737698	-4.623803	-0.417768
H	0.029690	3.748729	-2.037900
H	-1.589408	3.543873	-2.684686
C	-1.043383	5.603719	-2.322765
C	-0.775312	6.214953	0.110241
H	-1.157600	4.604257	1.493632
H	0.298501	4.379541	0.536028
H	-1.753337	1.519919	-3.136891
H	-1.261482	0.069899	-2.261153
C	-3.130597	-0.135789	-3.338626
C	-5.043368	1.238800	-2.397702
H	-4.525849	2.434657	-0.661121
H	-3.749011	2.949764	-2.151660
H	-3.054951	0.025225	1.822055
H	-4.280417	1.006819	1.024934
C	-4.282720	1.198103	3.169751
C	-2.253983	2.338413	4.146041
H	-0.982545	1.166249	2.842259
H	-0.742015	2.897725	2.694622
H	1.479963	-1.007179	2.799021
H	2.343739	-2.433362	2.256515
C	3.095456	-1.618295	4.111550
C	4.221219	0.635131	3.905239
H	4.274528	1.440914	1.897626
H	2.656684	1.344911	2.582831
H	5.716655	0.080215	0.528146
H	5.702379	-0.803406	-0.991364
C	6.503756	1.200465	-1.145260
C	4.799952	1.797891	-2.923557
H	3.996003	-0.197976	-2.821030
H	2.793179	1.051317	-2.533255
H	4.655813	-2.648124	-1.051043
H	4.248242	-2.944159	0.635618
C	3.549721	-4.475078	-0.729304
C	1.753895	-3.717136	-2.352276
H	1.161965	-1.644951	-2.124692
H	2.811699	-1.870165	-2.715048
C	-5.115935	-3.520707	-0.307724
C	-3.761040	-3.713027	1.797609
C	-3.046744	-4.855322	-1.903272
C	-2.613079	-5.962252	0.308105
H	-0.642988	5.743103	-3.335412
H	-2.089693	5.942822	-2.351732
C	-0.263425	6.457198	-1.314907
H	-1.808336	6.585207	0.190608
H	-0.182226	6.788318	0.834445
H	-2.655350	-0.493368	-4.261522
H	-3.407121	-1.026768	-2.756688
C	-4.395527	0.670439	-3.668992
H	-5.420432	0.409864	-1.781147
H	-5.912134	1.858621	-2.656123
H	-4.867265	2.130396	3.129619
H	-5.007449	0.383709	3.302995
C	-3.319936	1.257196	4.362821
H	-1.534120	2.335567	4.975081
H	-2.732172	3.330469	4.150873
H	2.430872	-2.236179	4.728884

H	4.046407	-2.167069	4.029544
C	3.350959	-0.266362	4.791059
H	4.355130	1.619151	4.373469
H	5.225520	0.193784	3.814222
H	6.393677	2.159474	-0.617170
H	7.534532	0.865767	-0.970144
C	6.261555	1.417632	-2.645630
H	4.628094	1.886256	-4.004181
H	4.590738	2.787506	-2.490426
H	4.459394	-5.080242	-0.619150
H	2.821953	-4.867189	-0.004111
C	2.980544	-4.618919	-2.148040
H	0.925379	-4.063574	-1.720260
H	1.406260	-3.783223	-3.392062
H	-5.689876	-2.740087	0.202308
H	-5.636461	-4.473871	-0.158631
H	-5.109405	-3.291350	-1.375935
H	-2.757727	-3.719703	2.233744
H	-4.287925	-4.623422	2.103298
H	-4.295117	-2.850706	2.208649
H	-3.134318	-3.907752	-2.444523
H	-3.973720	-5.422034	-2.041656
H	-2.225609	-5.423876	-2.351153
H	-1.901779	-6.603196	-0.223160
H	-3.577905	-6.481635	0.340718
H	-2.250986	-5.832062	1.330351
H	0.804180	6.195908	-1.367380
H	-0.338520	7.521145	-1.573898
H	-5.114940	0.045715	-4.214282
H	-4.130728	1.500267	-4.341772
H	-3.875072	1.441930	5.292106
H	-2.824164	0.282845	4.475063
H	3.825475	-0.412454	5.770238
H	2.388101	0.231086	4.977652
H	6.939198	2.189069	-3.033414
H	6.500239	0.490357	-3.187671
H	3.758857	-4.344705	-2.876691
H	2.722128	-5.666950	-2.348251
C	-0.416474	-0.746631	0.750951
O	-0.786706	-1.107528	1.851345
O	-0.720980	-1.649337	-0.351244

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Ru	-0.019323	0.239259	0.070355
P	2.417591	0.566531	0.033128
P	-2.411033	0.637860	0.076248
B	0.090941	-2.639780	-1.205127
H	-0.021531	1.116565	1.680261
H	-0.003954	0.333407	1.922209
H	0.008300	1.748563	-0.363215
C	2.871537	2.418984	0.004991
C	3.407966	-0.060800	1.547406
C	3.568258	-0.029306	-1.389028
C	-2.852101	2.423816	-0.377844
C	-3.195685	0.484981	1.799506
C	-3.445832	-0.346700	-1.173049
O	0.304408	-3.970600	-1.491940
O	-0.001447	-2.402640	0.167582
H	3.966822	2.444483	0.096829
C	2.277683	3.201829	1.195762
C	2.513786	3.125544	-1.321205
H	3.551501	-1.120393	1.302270
C	2.647083	-0.051783	2.891439
C	4.810562	0.561757	1.728622
H	4.370862	0.724476	-1.406225
C	4.244961	-1.406269	-1.198490
C	2.880721	-0.027152	-2.773486

H	-3.948625	2.484253	-0.334297
C	-2.413771	2.781137	-1.815903
C	-2.298022	3.461772	0.622037
H	-2.653653	1.269115	2.350282
C	-4.702113	0.791463	1.934730
C	-2.861959	-0.840538	2.516406
H	-2.815357	-0.273597	-2.069577
C	-4.847586	0.175212	-1.561469
C	-3.536317	-1.844329	-0.813893
C	0.103277	-4.729895	-0.279053
C	0.335672	-3.649672	0.855701
H	1.183407	3.145741	1.144139
H	2.570913	2.745898	2.147435
C	2.710073	4.679047	1.193917
C	2.935399	4.606503	-1.315288
H	3.004893	2.631412	-2.163929
H	1.433459	3.047294	-1.496374
H	2.429305	0.976863	3.206194
H	1.678968	-0.548829	2.774155
C	3.452966	-0.754904	3.999311
C	5.612751	-0.156216	2.828872
H	5.374972	0.540498	0.788747
H	4.710462	1.618922	2.007877
H	3.476639	-2.192661	-1.202510
H	4.769885	-1.476889	-0.241157
C	5.260664	-1.687961	-2.323977
C	3.900339	-0.256482	-3.901357
H	2.141081	-0.832335	-2.801680
H	2.323857	0.893660	-2.953088
H	-1.328274	2.667409	-1.901922
H	-2.838052	2.078360	-2.540233
C	-2.826913	4.214367	-2.190989
C	-2.706544	4.895262	0.238791
H	-2.650060	3.253815	1.639496
H	-1.203525	3.387718	0.643032
H	-4.959593	1.739985	1.450362
H	-5.281390	0.010553	1.424977
C	-5.130195	0.839231	3.413585
C	-3.285578	-0.796722	3.995373
H	-3.380519	-1.672717	2.023862
H	-1.790906	-1.050091	2.434837
H	-5.531653	0.097788	-0.706933
H	-4.815409	1.231855	-1.843561
C	-5.420701	-0.636937	-2.739092
C	-4.095516	-2.662967	-1.990222
H	-2.553010	-2.221764	-0.517964
H	-4.200904	-1.972798	0.052217
C	1.095327	-5.894425	-0.271625
C	-1.330128	-5.280482	-0.319049
C	1.797606	-3.555056	1.300715
C	-0.564428	-3.804368	2.079650
H	2.245678	5.197991	2.042847
H	3.798140	4.742049	1.347575
C	2.345909	5.371533	-0.124740
H	4.033530	4.670427	-1.274840
H	2.631817	5.074146	-2.260746
H	2.900898	-0.702498	4.946877
H	3.547968	-1.823110	3.752396
C	4.855230	-0.154200	4.163608
H	5.805846	-1.194626	2.520591
H	6.594058	0.322149	2.944682
H	6.082840	-0.960702	-2.244822
H	5.708348	-2.679086	-2.171604
C	4.631919	-1.592669	-3.719982
H	3.384920	-0.233106	-4.869526
H	4.632229	0.565958	-3.914176
H	-2.476648	4.441699	-3.205905

H	-3.925341	4.286473	-2.216108
C	-2.279965	5.243670	-1.193231
H	-2.269967	5.605132	0.953813
H	-3.798871	4.997484	0.325994
H	-4.627208	1.684350	3.906795
H	-6.208178	1.035204	3.482217
C	-4.776152	-0.461103	4.148643
H	-3.060296	-1.757898	4.476078
H	-2.686830	-0.037007	4.520308
H	-6.422998	-0.265813	-2.990440
H	-4.792347	-0.469833	-3.625746
C	-5.470370	-2.139926	-2.430245
H	-3.390222	-2.606886	-2.831058
H	-4.165707	-3.722282	-1.709301
H	0.869665	-6.564661	-1.107062
H	1.019500	-6.472513	0.656556
H	2.125361	-5.550319	-0.388150
H	-2.071274	-4.476397	-0.332343
H	-1.539191	-5.932225	0.536039
H	-1.454533	-5.864068	-1.236265
H	2.470087	-3.432425	0.447289
H	2.102827	-4.448213	1.856063
H	1.915308	-2.689478	1.956702
H	-0.337898	-3.021760	2.810809
H	-0.391417	-4.773369	2.562135
H	-1.622022	-3.729249	1.819915
H	1.250927	5.411430	-0.223563
H	2.698830	6.411002	-0.122976
H	5.420205	-0.706144	4.925702
H	4.767428	0.880495	4.527337
H	5.401774	-1.724099	-4.491603
H	3.912382	-2.413809	-3.849917
H	-2.617808	6.254327	-1.457125
H	-1.181230	5.253885	-1.250971
H	-5.044225	-0.384387	5.210245
H	-5.376133	-1.284837	3.733579
H	-6.199786	-2.320010	-1.625814
H	-5.828235	-2.696386	-3.305939
C	-0.161779	-0.236375	-1.880279
O	-0.382629	0.392970	-2.884403
O	-0.033105	-1.698622	-2.159626

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Ru	-0.428966	-0.689451	-0.068184
P	1.718014	-1.782698	-0.091469
P	-2.696622	0.194466	0.044656
B	1.446753	2.609192	-0.156504
H	-1.109675	-2.088012	-0.979360
H	-0.866278	-1.584209	-1.594809
H	-0.863267	-1.756070	1.013072
C	1.757459	-3.595774	-0.666583
C	2.961057	-0.903417	-1.212432
C	2.634936	-1.943512	1.572095
C	-3.628772	-0.353608	1.593429
C	-3.809563	-0.448736	-1.349072
C	-2.796090	2.085439	0.117430
O	2.764371	2.346701	0.231362
O	1.266139	3.964075	-0.427496
H	2.817759	-3.883572	-0.601088
C	1.309959	-3.810517	-2.129050
C	0.964570	-4.532351	0.272619
H	3.233808	-0.023332	-0.615963
C	2.318776	-0.340228	-2.501757
C	4.247273	-1.692045	-1.539099
H	3.224429	-2.870145	1.485736
C	3.621695	-0.793535	1.881318
C	1.658569	-2.104926	2.762858

H	-4.602652	0.154555	1.573147
C	-2.887794	0.087791	2.875722
C	-3.898832	-1.873545	1.636309
H	-3.769347	-1.533855	-1.168080
C	-5.296489	-0.033672	-1.307697
C	-3.252983	-0.231317	-2.775280
H	-1.974141	2.317835	0.807514
C	-4.079881	2.726508	0.689542
C	-2.426419	2.754368	-1.226070
C	3.410870	3.614740	0.488509
C	2.555318	4.612146	-0.391049
H	0.269845	-3.483074	-2.249597
H	1.909018	-3.200144	-2.811101
C	1.414406	-5.286772	-2.553434
C	1.054027	-6.005454	-0.164858
H	1.336315	-4.449780	1.297983
H	-0.087404	-4.216239	0.295564
H	1.961441	-1.153450	-3.146880
H	1.448286	0.269063	-2.238679
C	3.329588	0.514326	-3.286612
C	5.249090	-0.827814	-2.325978
H	4.721811	-2.067005	-0.623902
H	3.999281	-2.575349	-2.143431
H	3.080615	0.158740	1.929952
H	4.362894	-0.687715	1.083786
C	4.366643	-1.038187	3.207243
C	2.410929	-2.376804	4.076139
H	1.077412	-1.183953	2.868054
H	0.932634	-2.901712	2.576485
H	-1.896158	-0.378442	2.891324
H	-2.717345	1.170408	2.876689
C	-3.662884	-0.311051	4.143073
C	-4.665982	-2.275735	2.909040
H	-4.473483	-2.193312	0.758972
H	-2.940871	-2.408690	1.601787
H	-5.722070	-0.183328	-0.309149
H	-5.380843	1.038586	-1.528005
C	-6.120677	-0.823689	-2.341680
C	-4.062294	-1.036327	-3.806905
H	-3.305329	0.830988	-3.037980
H	-2.194853	-0.508388	-2.826942
H	-4.927267	2.542342	0.015751
H	-4.347023	2.288364	1.656919
C	-3.896478	4.246580	0.862622
C	-2.240460	4.271365	-1.054674
H	-1.505711	2.316462	-1.620605
H	-3.230449	2.579971	-1.954053
C	4.884665	3.506097	0.097102
C	3.289116	3.884371	1.995991
C	3.050290	4.723718	-1.841030
C	2.380096	6.010253	0.204193
H	1.067596	-5.394487	-3.589366
H	2.470726	-5.594219	-2.544630
C	0.613105	-6.201866	-1.619905
H	2.092315	-6.352045	-0.052943
H	0.446029	-6.623611	0.508300
H	2.865974	0.881537	-4.211502
H	3.580514	1.399879	-2.685634
C	4.616384	-0.260117	-3.604403
H	5.588318	0.002288	-1.689151
H	6.140450	-1.420880	-2.569801
H	5.009456	-1.925361	3.099632
H	5.036887	-0.192222	3.408732
C	3.408175	-1.252650	4.385307
H	1.689645	-2.484172	4.896746
H	2.948366	-3.335065	4.004422
H	-3.096840	-0.002703	5.031319

H	-4.618414	0.234058	4.176154
C	-3.939580	-1.819978	4.181633
H	-4.812522	-3.363746	2.920199
H	-5.670260	-1.826469	2.884617
H	-6.120784	-1.887944	-2.062299
H	-7.167345	-0.494071	-2.312066
C	-5.553235	-0.671101	-3.760531
H	-3.659155	-0.861895	-4.812792
H	-3.943586	-2.111390	-3.603466
H	-4.823496	4.686969	1.253389
H	-3.120015	4.426475	1.620486
C	-3.488466	4.929234	-0.450788
H	-1.365979	4.451533	-0.417137
H	-2.008918	4.721965	-2.028791
H	5.382505	2.770712	0.738282
H	5.397771	4.466528	0.225523
H	5.005452	3.185448	-0.940626
H	2.240351	3.942648	2.302600
H	3.793791	4.812284	2.286637
H	3.750104	3.055997	2.543360
H	3.185168	3.735535	-2.292254
H	3.997750	5.269636	-1.909225
H	2.299410	5.260737	-2.429297
H	1.754315	6.615720	-0.460093
H	3.346010	6.517422	0.314135
H	1.892517	5.971806	1.181109
H	-0.457839	-5.966326	-1.711188
H	0.729649	-7.251698	-1.918004
H	5.332447	0.386634	-4.127867
H	4.383384	-1.087880	-4.291523
H	3.972717	-1.477307	5.299758
H	2.853059	-0.323015	4.575018
H	-4.528363	-2.080337	5.070739
H	-2.985045	-2.359793	4.266298
H	-6.121804	-1.290285	-4.466154
H	-5.677908	0.371590	-4.088385
H	-4.321677	4.857956	-1.166960
H	-3.314773	6.000023	-0.281772
C	0.191146	0.675415	1.170253
O	0.437106	1.200495	2.195839
O	0.466505	1.697686	-0.252709

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Ru	-0.057307	0.426651	-0.001226
P	2.401442	0.734248	0.001531
P	-2.477670	0.619780	0.076566
B	0.284539	-2.635103	-1.100456
H	-0.098717	1.017676	1.718403
H	-0.020787	0.213641	1.836158
H	-0.087907	1.991078	-0.135531
C	2.877518	2.575049	-0.045176
C	3.351799	0.082793	1.525878
C	3.513572	0.061670	-1.411235
C	-3.079646	2.382457	-0.239374
C	-3.170747	0.252994	1.797739
C	-3.412962	-0.386268	-1.225058
O	0.763895	-3.916682	-1.415676
O	-0.043730	-2.580511	0.284020
H	3.975700	2.595102	0.006626
C	2.327379	3.362488	1.164913
C	2.471377	3.274280	-1.361773
H	3.444128	-0.985340	1.294087
C	2.610583	0.136910	2.880105
C	4.779351	0.657352	1.673734
H	4.358273	0.768214	-1.440054
C	4.097710	-1.353189	-1.187514
C	2.817482	0.071605	-2.791806

H	-4.177948	2.342778	-0.223082
C	-2.643708	2.881851	-1.635183
C	-2.638169	3.386053	0.848047
H	-2.662863	1.024145	2.397325
C	-4.688201	0.437392	2.016656
C	-2.722329	-1.106123	2.377691
H	-2.806336	-0.202473	-2.121704
C	-4.863642	0.017549	-1.568077
C	-3.347289	-1.904468	-0.954367
C	0.460924	-4.801451	-0.328208
C	0.381399	-3.815930	0.904891
H	1.231964	3.291627	1.165602
H	2.671500	2.919508	2.105290
C	2.739990	4.845176	1.134425
C	2.881160	4.758097	-1.378660
H	2.934869	2.776210	-2.217718
H	1.385168	3.191505	-1.496746
H	2.415233	1.174444	3.180405
H	1.637075	-0.352605	2.789767
C	3.416020	-0.565732	3.989249
C	5.573933	-0.062520	2.777627
H	5.326632	0.593822	0.726117
H	4.719369	1.723320	1.929726
H	3.277126	-2.083025	-1.161142
H	4.632177	-1.428385	-0.235601
C	5.079089	-1.735376	-2.313653
C	3.809517	-0.258316	-3.919323
H	2.031714	-0.689658	-2.774932
H	2.332222	1.028279	-2.995211
H	-1.548775	2.880591	-1.687393
H	-2.986354	2.198212	-2.419690
C	-3.168252	4.298756	-1.922562
C	-3.153582	4.806827	0.552312
H	-3.000191	3.075529	1.835424
H	-1.541645	3.397601	0.901038
H	-5.034633	1.396343	1.615018
H	-5.233582	-0.346420	1.474769
C	-5.037502	0.347415	3.514295
C	-3.051453	-1.191601	3.877190
H	-3.238595	-1.920362	1.856204
H	-1.654358	-1.267666	2.203956
H	-5.521394	-0.181757	-0.711978
H	-4.943145	1.088032	-1.784455
C	-5.367699	-0.775111	-2.790459
C	-3.822503	-2.694328	-2.184826
H	-2.333747	-2.197596	-0.670837
H	-4.004146	-2.148041	-0.107656
C	1.559613	-5.862817	-0.236992
C	-0.883366	-5.480000	-0.642937
C	1.751880	-3.572772	1.552788
C	-0.628524	-4.216363	1.981885
H	2.300093	5.363857	1.996323
H	3.831858	4.922671	1.248183
C	2.321015	5.524050	-0.174736
H	3.979179	4.831369	-1.372011
H	2.544755	5.216263	-2.317530
H	2.878425	-0.478309	4.942398
H	3.474561	-1.640290	3.761676
C	4.837424	-0.005113	4.122351
H	5.727767	-1.113180	2.490390
H	6.571924	0.386038	2.866249
H	5.951728	-1.065792	-2.265588
H	5.456817	-2.750512	-2.134215
C	4.441213	-1.639460	-3.704887
H	3.286492	-0.224919	-4.883255
H	4.599885	0.507664	-3.962969
H	-2.816226	4.626303	-2.909039

H	-4.267533	4.281253	-1.973489
C	-2.728311	5.292310	-0.839387
H	-2.791870	5.495784	1.326741
H	-4.252014	4.814004	0.617790
H	-4.572993	1.194280	4.041185
H	-6.121637	0.453754	3.649576
C	-4.549146	-0.968818	4.138069
H	-2.738903	-2.167068	4.271982
H	-2.469578	-0.432359	4.421742
H	-6.408682	-0.498798	-3.003867
H	-4.779032	-0.480245	-3.671254
C	-5.249120	-2.292777	-2.587100
H	-3.130209	-2.507364	-3.017128
H	-3.777078	-3.771263	-1.976592
H	1.549398	-6.473754	-1.145758
H	1.401757	-6.528152	0.620244
H	2.550448	-5.409821	-0.151769
H	-1.691591	-4.744881	-0.711429
H	-1.155759	-6.227464	0.110690
H	-0.803700	-5.979874	-1.613299
H	2.500537	-3.302232	0.802129
H	2.108709	-4.456790	2.093053
H	1.667826	-2.747044	2.266458
H	-0.612543	-3.487968	2.800004
H	-0.380910	-5.197790	2.403581
H	-1.645827	-4.255980	1.585501
H	1.222681	5.548987	-0.236981
H	2.660026	6.567877	-0.191318
H	5.395025	-0.558463	4.888719
H	4.788307	1.039701	4.464032
H	5.189755	-1.850198	-4.479948
H	3.660578	-2.407035	-3.798564
H	-3.144181	6.288277	-1.038755
H	-1.633354	5.397202	-0.867932
H	-4.756286	-0.977194	5.215811
H	-5.116954	-1.805343	3.704372
H	-5.948877	-2.606984	-1.797653
H	-5.552899	-2.820181	-3.500396
C	-0.187472	0.233826	-1.913816
O	-0.406316	0.550436	-3.015453
O	0.160697	-1.647007	-1.961886

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Ru	-0.181411	0.643268	-0.316839
P	2.185950	1.288283	-0.102889
P	-2.595039	0.201781	-0.191926
B	0.581679	-2.333496	0.714589
H	-0.586740	1.838383	1.105345
H	-0.174117	1.318314	1.514008
H	-0.437468	2.070320	-1.060428
C	2.478954	3.164912	0.010840
C	2.959863	0.609773	1.495811
C	3.503810	0.817844	-1.400765
C	-3.318054	-1.057140	-1.400875
C	-3.682165	1.720638	-0.489345
C	-2.988797	-0.566398	1.500322
O	1.507764	-2.655156	-0.310115
O	0.335430	-3.483344	1.496652
H	3.534413	3.262811	0.303608
C	1.621206	3.850236	1.096290
C	2.302994	3.907464	-1.332220
H	3.125510	-0.440646	1.223962
C	2.034798	0.566330	2.733744
C	4.319901	1.239861	1.871822
H	4.276557	1.595895	-1.295508
C	4.181973	-0.552335	-1.173550
C	2.975251	0.863483	-2.852437

H	-4.332581	-1.260506	-1.032299
C	-2.535511	-2.389849	-1.372125
C	-3.466547	-0.542920	-2.851126
H	-3.507639	1.914242	-1.557990
C	-5.198279	1.504726	-0.287807
C	-3.215637	2.994509	0.249269
H	-2.096389	-1.195759	1.628249
C	-4.245152	-1.461149	1.611262
C	-2.991321	0.451853	2.662970
C	1.699663	-4.082369	-0.319938
C	1.304793	-4.483858	1.154725
H	0.562043	3.746343	0.828655
H	1.755098	3.361371	2.066640
C	1.948794	5.347209	1.231962
C	2.603300	5.412419	-1.200700
H	2.970389	3.491799	-2.092084
H	1.275642	3.762300	-1.693010
H	1.790342	1.583270	3.070411
H	1.107170	0.049888	2.471243
C	2.711349	-0.187085	3.894347
C	4.993121	0.473513	3.024348
H	4.995872	1.277218	1.009305
H	4.163648	2.279937	2.190286
H	3.423497	-1.341777	-1.233204
H	4.622657	-0.617046	-0.174486
C	5.305073	-0.797196	-2.200752
C	4.115605	0.682268	-3.867695
H	2.263955	0.046641	-2.991572
H	2.427465	1.786919	-3.059099
H	-1.512351	-2.220663	-1.722005
H	-2.445208	-2.770215	-0.349007
C	-3.203696	-3.445099	-2.269672
C	-4.117062	-1.610174	-3.751475
H	-4.081375	0.363565	-2.879552
H	-2.486461	-0.274942	-3.259252
H	-5.546329	0.625064	-0.841121
H	-5.399369	1.307236	0.773421
C	-6.005682	2.738767	-0.730125
C	-4.025787	4.223352	-0.200301
H	-3.332012	2.869524	1.333016
H	-2.152144	3.162674	0.052086
H	-5.154817	-0.856845	1.488757
H	-4.262581	-2.220385	0.824575
C	-4.290832	-2.176618	2.975464
C	-3.016735	-0.263831	4.024894
H	-2.116415	1.105861	2.618086
H	-3.876061	1.099789	2.590395
C	3.146232	-4.393188	-0.710796
C	0.747483	-4.671808	-1.373160
C	2.476571	-4.349786	2.142788
C	0.665356	-5.866099	1.302489
H	1.310923	5.793111	2.006168
H	2.987137	5.465868	1.576013
C	1.767329	6.080140	-0.102540
H	3.671161	5.546692	-0.970952
H	2.429981	5.903099	-2.167166
H	2.048776	-0.179518	4.769458
H	2.831185	-1.241936	3.608064
C	4.081224	0.402423	4.256639
H	5.234000	-0.546136	2.689023
H	5.947752	0.952241	3.279312
H	6.115258	-0.073881	-2.021307
H	5.736810	-1.792626	-2.033697
C	4.825411	-0.660466	-3.651365
H	3.712502	0.741574	-4.886733
H	4.839970	1.505129	-3.767869
H	-2.614222	-4.370562	-2.248838

H	-4.195774	-3.697951	-1.865372
C	-3.353312	-2.940603	-3.711354
H	-4.175505	-1.232582	-4.780407
H	-5.153367	-1.778037	-3.420915
H	-5.894153	2.870477	-1.816566
H	-7.074039	2.567476	-0.545019
C	-5.534922	4.012315	-0.014680
H	-3.692786	5.108738	0.356655
H	-3.814861	4.424023	-1.261263
H	-5.199027	-2.790683	3.036213
H	-3.438134	-2.867105	3.040816
C	-4.234108	-1.188684	4.147881
H	-2.095193	-0.851909	4.136091
H	-3.018873	0.479861	4.832760
H	3.328270	-4.071074	-1.742203
H	3.347878	-5.469757	-0.655850
H	3.858709	-3.873758	-0.065095
H	-0.296987	-4.492914	-1.100112
H	0.892382	-5.750589	-1.500904
H	0.935568	-4.182019	-2.334265
H	2.962990	-3.373649	2.042236
H	3.233372	-5.129798	2.000730
H	2.086908	-4.428361	3.162926
H	0.404923	-6.039338	2.352345
H	1.354796	-6.659579	0.989590
H	-0.251211	-5.947231	0.713259
H	0.705020	6.056137	-0.387246
H	2.042225	7.137928	-0.001891
H	4.556412	-0.190098	5.049059
H	3.945635	1.416367	4.662638
H	5.670754	-0.768422	-4.343350
H	4.123713	-1.475402	-3.880844
H	-3.864843	-3.690325	-4.328748
H	-2.354832	-2.798471	-4.148795
H	-6.091358	4.883487	-0.383399
H	-5.760178	3.928699	1.059065
H	-5.151553	-0.580650	4.156493
H	-4.209324	-1.730526	5.102004
C	-0.061208	-0.061742	-2.010069
O	-0.030264	-0.487145	-3.093482
O	0.029013	-1.162818	0.944281

TS12_2

Ru	0.018890	0.086842	-0.094265
P	-2.392520	0.016717	-0.048674
P	2.436210	-0.041077	0.131950
H	0.151822	-0.898053	-1.429552
H	-0.037518	0.633155	1.591515
H	-0.085649	-1.240802	0.774946
H	0.002936	1.363618	1.177138
C	-3.267618	1.638285	-0.474571
C	-3.107320	-1.225325	-1.280812
C	-3.194019	-0.522420	1.601761
C	3.560566	-0.337596	-1.377126
C	3.031467	1.625980	0.821717
C	3.037863	-1.279317	1.422869
H	-4.336998	1.493042	-0.271486
C	-2.761768	2.787680	0.425563
C	-3.126562	2.043557	-1.958629
H	-2.720004	-0.858899	-2.239017
C	-4.643895	-1.311829	-1.393802
C	-2.512343	-2.637610	-1.085063
H	-3.272027	-1.612235	1.473996
C	-4.619656	0.015547	1.869299
C	-2.317838	-0.292094	2.852192
H	3.618619	0.662858	-1.831512
C	5.003906	-0.797471	-1.059199

C	2.957475	-1.277384	-2.445775
H	2.395403	1.733387	1.712878
C	4.493691	1.776476	1.291053
C	2.665200	2.792167	-0.123876
H	4.132692	-1.194157	1.457811
C	2.684315	-2.733680	1.040795
C	2.496501	-0.962456	2.834264
H	-1.687841	2.930674	0.241606
H	-2.863667	2.528859	1.486905
C	-3.509316	4.101802	0.141129
C	-3.888069	3.349655	-2.247661
H	-3.497488	1.251847	-2.618993
H	-2.066780	2.187661	-2.198710
H	-5.087735	-0.319962	-1.541367
H	-5.063026	-1.713176	-0.461288
C	-5.057723	-2.237836	-2.552697
C	-2.930313	-3.575432	-2.231031
H	-2.859326	-3.061267	-0.130217
H	-1.421749	-2.577088	-1.026593
H	-5.274555	-0.144429	1.008326
H	-4.576278	1.100543	2.032623
C	-5.244493	-0.641559	3.113330
C	-2.939281	-0.933567	4.105499
H	-2.192466	0.787146	3.024520
H	-1.318961	-0.704811	2.686656
H	5.471140	-0.159998	-0.304256
H	4.977308	-1.811319	-0.637654
C	5.877938	-0.818439	-2.326478
C	3.825754	-1.314630	-3.715669
H	2.869246	-2.293998	-2.038527
H	1.947022	-0.967498	-2.711918
H	4.783876	0.959947	1.962811
H	5.167257	1.731035	0.425829
C	4.704325	3.128405	1.998768
C	2.882830	4.152285	0.562352
H	3.291976	2.744718	-1.026115
H	1.628969	2.699935	-0.463088
H	1.594023	-2.820394	0.953456
H	3.096684	-2.987502	0.057796
C	3.201771	-3.738273	2.085342
C	3.016159	-1.966039	3.878813
H	2.774478	0.052836	3.141247
H	1.399558	-0.998482	2.808630
H	-4.567207	3.985272	0.420794
H	-3.106023	4.902342	0.775075
C	-3.415137	4.494210	-1.340127
H	-3.760656	3.623565	-3.302730
H	-4.965442	3.185294	-2.094582
H	-4.716159	-1.800811	-3.502202
H	-6.152806	-2.294985	-2.609103
C	-4.456134	-3.640914	-2.392409
H	-2.478340	-3.212470	-3.164836
H	-2.523411	-4.579701	-2.054259
H	-6.249011	-0.231390	3.280698
H	-5.373930	-1.718145	2.927373
C	-4.370366	-0.441074	4.357929
H	-2.950070	-2.026459	3.978206
H	-2.304697	-0.728820	4.977667
H	5.976854	0.206162	-2.714582
H	6.891201	-1.153897	-2.069017
C	5.274393	-1.718799	-3.412201
H	3.816397	-0.318951	-4.183429
H	3.379768	-2.003734	-4.443884
H	4.094420	3.155405	2.914121
H	5.750492	3.221580	2.318276
C	4.316093	4.305102	1.091774
H	2.174657	4.247655	1.399374

H	2.647320	4.963083	-0.138870
H	4.302184	-3.722203	2.093696
H	2.907636	-4.755135	1.794863
C	2.680978	-3.412491	3.491965
H	2.593275	-1.725231	4.862874
H	4.107252	-1.859342	3.973592
H	-2.370328	4.737218	-1.582906
H	-4.001477	5.402127	-1.532037
H	-4.895306	-4.121337	-1.504817
H	-4.723209	-4.269709	-3.251605
H	-4.346500	0.628871	4.613403
H	-4.807902	-0.958897	5.221126
H	5.294869	-2.763062	-3.066143
H	5.883656	-1.679564	-4.324280
H	5.012448	4.347887	0.240897
H	4.425503	5.254404	1.631770
H	1.589793	-3.549127	3.514171
H	3.100184	-4.111504	4.227114
C	-0.174703	0.254336	-2.488276
O	0.273134	1.340755	-2.140269
O	-0.664496	-0.356349	-3.397452

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Ru	-0.006088	-0.051731	-0.043966
P	2.431646	0.004143	0.007388
P	-2.414856	0.138476	-0.027326
H	-0.038601	-1.838499	-0.906074
H	0.005978	1.511471	-0.285558
H	0.006942	0.635189	-1.489531
H	-0.010633	0.938538	1.200818
C	3.200785	-0.204922	1.718015
C	3.137887	-1.430537	-1.000248
C	3.297622	1.535534	-0.728198
C	-3.334322	-1.026714	-1.207290
C	-3.137757	-0.217297	1.695998
C	-3.057076	1.873455	-0.402945
H	4.280881	-0.044627	1.597281
C	2.671961	0.861243	2.702881
C	2.999712	-1.618633	2.309665
H	2.669086	-2.304032	-0.526653
C	4.664191	-1.659232	-0.979583
C	2.640925	-1.403350	-2.463327
H	3.392012	1.272540	-1.792376
C	4.722410	1.812998	-0.191257
C	2.461436	2.832274	-0.663834
H	-3.267656	-1.989934	-0.680548
C	-4.831337	-0.724690	-1.441717
C	-2.615036	-1.221801	-2.563599
H	-2.391747	0.264126	2.345156
C	-4.518364	0.376705	2.060642
C	-3.117007	-1.725469	2.037522
H	-4.148891	1.822589	-0.286207
C	-2.769436	2.350822	-1.843536
C	-2.519901	2.916865	0.604777
H	1.586974	0.735301	2.810255
H	2.828747	1.871668	2.305601
C	3.340896	0.736322	4.082420
C	3.668577	-1.740582	3.690671
H	3.418889	-2.379578	1.641688
H	1.929275	-1.835074	2.391483
H	5.048395	-1.680678	0.046640
H	5.169669	-0.829610	-1.492446
C	5.026358	-2.976093	-1.692682
C	2.989868	-2.716848	-3.183694
H	3.107175	-0.562720	-2.998629
H	1.559780	-1.234442	-2.498064
H	5.345414	0.915270	-0.240412

H	4.664091	2.096316	0.868103
C	5.404614	2.954824	-0.965681
C	3.143840	3.985549	-1.420371
H	2.308900	3.123685	0.384953
H	1.468275	2.657745	-1.084537
H	-5.363040	-0.623208	-0.490871
H	-4.934790	0.236640	-1.963097
C	-5.503094	-1.823794	-2.286168
C	-3.286994	-2.326517	-3.396957
H	-2.627779	-0.285075	-3.135741
H	-1.561717	-1.469462	-2.403390
H	-4.570480	1.448194	1.842442
H	-5.302700	-0.103290	1.461471
C	-4.832985	0.149743	3.551658
C	-3.441945	-1.964230	3.522666
H	-3.866764	-2.248728	1.426121
H	-2.140142	-2.155553	1.804685
H	-1.684679	2.374349	-2.009898
H	-3.182281	1.648775	-2.574637
C	-3.360942	3.748568	-2.102424
C	-3.123910	4.308845	0.352089
H	-2.720907	2.610666	1.637476
H	-1.428776	2.974530	0.509825
H	4.414996	0.956938	3.988335
H	2.925915	1.490981	4.763268
C	3.161052	-0.671191	4.667599
H	3.487591	-2.744221	4.095790
H	4.759202	-1.639764	3.579818
H	4.597189	-3.817224	-1.129677
H	6.115354	-3.114914	-1.682937
C	4.497175	-3.005873	-3.134455
H	2.437083	-3.536642	-2.704220
H	2.646354	-2.670926	-4.225295
H	6.406360	3.131376	-0.552941
H	5.547479	2.648878	-2.012735
C	4.571447	4.242037	-0.919982
H	3.176196	3.739843	-2.492531
H	2.536660	4.895423	-1.328473
H	-5.504154	-2.764217	-1.715673
H	-6.555426	-1.562967	-2.458957
C	-4.778341	-2.041582	-3.621125
H	-3.173023	-3.288558	-2.876661
H	-2.768203	-2.428889	-4.358651
H	-4.102260	0.702914	4.160393
H	-5.818504	0.572081	3.787969
C	-4.784250	-1.338216	3.924408
H	-2.638077	-1.533411	4.137249
H	-3.445619	-3.042216	3.727753
H	-4.458554	3.690974	-2.050213
H	-3.114815	4.067780	-3.123432
C	-2.861160	4.781967	-1.084127
H	-2.710524	5.026002	1.072906
H	-4.208960	4.275286	0.531919
H	2.094033	-0.844139	4.870065
H	3.681844	-0.753513	5.630377
H	5.030233	-2.248684	-3.729432
H	4.714920	-3.976550	-3.597770
H	4.532959	4.610810	0.115875
H	5.050416	5.030005	-1.515104
H	-4.886652	-1.140608	-4.243583
H	-5.246155	-2.863628	-4.177653
H	-5.599688	-1.865579	3.406817
H	-4.962649	-1.467051	4.999778
H	-1.780324	4.933476	-1.222265
H	-3.338709	5.754174	-1.261325
C	0.072028	-2.588589	0.014583
O	-0.003352	-1.984765	1.129321

O 0.232237 -3.751359 -0.309935

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Ru 0.012803 0.217985 -0.036300
P 2.436371 0.068126 0.027384
P -2.398762 0.263482 0.032306
H -0.253150 -2.573000 -1.564086
H 0.030797 1.897124 0.159045
H 0.049972 1.764940 -0.739133
H -0.004766 0.557101 1.490496
C 3.179010 -0.651182 1.606150
C 2.913254 -1.155357 -1.325393
C 3.508170 1.599445 -0.355246
C -3.190303 -0.816882 -1.303216
C -3.070396 -0.364621 1.694848
C -3.208964 1.964646 -0.122160
H 4.270395 -0.590002 1.495337
C 2.777444 0.197500 2.834038
C 2.812934 -2.134914 1.834124
H 2.410947 -2.072877 -0.992112
C 4.406348 -1.480042 -1.529186
C 2.267727 -0.751989 -2.670287
H 3.567102 1.590341 -1.454643
C 4.955959 1.556447 0.186809
C 2.850940 2.940102 0.042181
H -3.047258 -1.830255 -0.900008
C -4.697912 -0.630303 -1.580171
C -2.400204 -0.755366 -2.632268
H -2.454076 0.207762 2.403941
C -4.550917 -0.078595 2.031406
C -2.758408 -1.858310 1.942027
H -4.293571 1.798788 -0.060227
C -2.924470 2.653587 -1.474661
C -2.805976 2.895664 1.044950
H 1.683958 0.186413 2.926982
H 3.065965 1.247224 2.694164
C 3.406109 -0.342838 4.129265
C 3.439330 -2.666617 3.135238
H 3.162924 -2.749022 0.996172
H 1.724298 -2.247293 1.857991
H 4.869079 -1.791000 -0.584973
H 4.939722 -0.579920 -1.865131
C 4.595143 -2.582487 -2.587663
C 2.462732 -1.841066 -3.739257
H 2.709534 0.189148 -3.030001
H 1.194893 -0.553530 -2.532571
H 5.454286 0.624047 -0.093756
H 4.933975 1.582976 1.284217
C 5.783707 2.753482 -0.314146
C 3.679619 4.145869 -0.436065
H 2.734755 2.986872 1.134290
H 1.845562 3.006693 -0.380326
H -5.278241 -0.702272 -0.655628
H -4.877791 0.375244 -1.985018
C -5.212337 -1.674565 -2.588800
C -2.907274 -1.807293 -3.632614
H -2.496111 0.241250 -3.082514
H -1.330465 -0.907229 -2.443158
H -4.808545 0.974541 1.876928
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C -4.867925 -0.463535 3.488171
C -3.083595 -2.255844 3.393116
H -3.366975 -2.475880 1.265141
H -1.712208 -2.075727 1.714703
H -1.840476 2.773841 -1.605173
H -3.268254 2.026887 -2.303495
C -3.604623 4.030869 -1.570394

C -3.492821 4.268883 0.942741
H -3.047852 2.436888 2.009884
H -1.716964 3.035933 1.036953
H 4.500606 -0.239379 4.075914
H 3.076509 0.266734 4.980870
C 3.045920 -1.817862 4.351829
H 3.134879 -3.710193 3.283508
H 4.536319 -2.670564 3.039653
H 4.146436 -3.516541 -2.220415
H 5.665400 -2.782336 -2.727711
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H 1.909898 -2.741203 -3.435513
H 2.027561 -1.510408 -4.691226
H 6.799911 2.695355 0.096816
H 5.885430 2.693154 -1.408028
C 5.128583 4.088134 0.064121
H 3.678433 4.165017 -1.536402
H 3.198024 5.076360 -0.108647
H -5.137433 -2.674637 -2.137562
H -6.277637 -1.501018 -2.789047
C -4.411507 -1.648974 -3.898257
H -2.709573 -2.810713 -3.229195
H -2.344085 -1.729764 -4.571549
H -4.282902 0.177914 4.164256
H -5.925425 -0.259480 3.701935
C -4.536824 -1.935444 3.769147
H -2.405307 -1.718348 4.072654
H -2.878962 -3.324749 3.531425
H -4.696382 3.894950 -1.567508
H -3.351898 4.500160 -2.529921
C -3.207146 4.945222 -0.404495
H -3.160855 4.908480 1.770623
H -4.579192 4.142556 1.062581
H 1.962288 -1.904297 4.517755
H 3.534993 -2.197680 5.258287
H 4.476331 -1.328010 -4.345972
H 4.052666 -3.010454 -4.650395
H 5.140165 4.198666 1.158656
H 5.707038 4.928072 -0.341180
H -4.589612 -0.693124 -4.413804
H -4.763989 -2.438333 -4.574151
H -5.212272 -2.574602 3.180888
H -4.723086 -2.173031 4.824587
H -2.133575 5.176155 -0.473600
H -3.738162 5.903255 -0.471864
C -0.162779 -2.855734 -0.486270
O 0.013807 -1.856263 0.326692
O -0.224637 -4.034508 -0.168041

TS12_2

Ru 0.018890 0.086842 -0.094265
P -2.392520 0.016717 -0.048674
P 2.436210 -0.041077 0.131950
H 0.151822 -0.898053 -1.429552
H -0.037518 0.633155 1.591515
H -0.085649 -1.240802 0.774946
H 0.002936 1.363618 1.177138
C -3.267618 1.638285 -0.474571
C -3.107320 -1.225325 -1.280812
C -3.194019 -0.522420 1.601761
C 3.560566 -0.337596 -1.377126
C 3.031467 1.625980 0.821717
C 3.037863 -1.279317 1.422869
H -4.336998 1.493042 -0.271486
C -2.761768 2.787680 0.425563
C -3.126562 2.043557 -1.958629
H -2.720004 -0.858899 -2.239017

C	-4.643895	-1.311829	-1.393802
C	-2.512343	-2.637610	-1.085063
H	-3.272027	-1.612235	1.473996
C	-4.619656	0.015547	1.869299
C	-2.317838	-0.292094	2.852192
H	3.618619	0.662858	-1.831512
C	5.003906	-0.797471	-1.059199
C	2.957475	-1.277384	-2.445775
H	2.395403	1.733387	1.712878
C	4.493691	1.776476	1.291053
C	2.665200	2.792167	-0.123876
H	4.132692	-1.194157	1.457811
C	2.684315	-2.733680	1.040795
C	2.496501	-0.962456	2.834264
H	-1.687841	2.930674	0.241606
H	-2.863667	2.528859	1.486905
C	-3.509316	4.101802	0.141129
C	-3.888069	3.349655	-2.247661
H	-3.497488	1.251847	-2.618993
H	-2.066780	2.187661	-2.198710
H	-5.087735	-0.319962	-1.541367
H	-5.063026	-1.713176	-0.461288
C	-5.057723	-2.237836	-2.552697
C	-2.930313	-3.575432	-2.231031
H	-2.859326	-3.061267	-0.130217
H	-1.421749	-2.577088	-1.026593
H	-5.274555	-0.144429	1.008326
H	-4.576278	1.100543	2.032623
C	-5.244493	-0.641559	3.113330
C	-2.939281	-0.933567	4.105499
H	-2.192466	0.787146	3.024520
H	-1.318961	-0.704811	2.686656
H	5.471140	-0.159998	-0.304256
H	4.977308	-1.811319	-0.637654
C	5.877938	-0.818439	-2.326478
C	3.825754	-1.314630	-3.715669
H	2.869246	-2.293998	-2.038527
H	1.947022	-0.967498	-2.711918
H	4.783876	0.959947	1.962811
H	5.167257	1.731035	0.425829
C	4.704325	3.128405	1.998768
C	2.882830	4.152285	0.562352
H	3.291976	2.744718	-1.026115
H	1.628969	2.699935	-0.463088
H	1.594023	-2.820394	0.953456
H	3.096684	-2.987502	0.057796
C	3.201771	-3.738273	2.085342
C	3.016159	-1.966039	3.878813
H	2.774478	0.052836	3.141247
H	1.399558	-0.998482	2.808630
H	-4.567207	3.985272	0.420794
H	-3.106023	4.902342	0.775075
C	-3.415137	4.494210	-1.340127
H	-3.760656	3.623565	-3.302730
H	-4.965442	3.185294	-2.094582
H	-4.716159	-1.800811	-3.502202
H	-6.152806	-2.294985	-2.609103
C	-4.456134	-3.640914	-2.392409
H	-2.478340	-3.212470	-3.164836
H	-2.523411	-4.579701	-2.054259
H	-6.249011	-0.231390	3.280698
H	-5.373930	-1.718145	2.927373
C	-4.370366	-0.441074	4.357929
H	-2.950070	-2.026459	3.978206
H	-2.304697	-0.728820	4.977667
H	5.976854	0.206162	-2.714582
H	6.891201	-1.153897	-2.069017

C	5.274393	-1.718799	-3.412201
H	3.816397	-0.318951	-4.183429
H	3.379768	-2.003734	-4.443884
H	4.094420	3.155405	2.914121
H	5.750492	3.221580	2.318276
C	4.316093	4.305102	1.091774
H	2.174657	4.247655	1.399374
H	2.647320	4.963083	-0.138870
H	4.302184	-3.722203	2.093696
H	2.907636	-4.755135	1.794863
C	2.680978	-3.412491	3.491965
H	2.593275	-1.725231	4.862874
H	4.107252	-1.859342	3.973592
H	-2.370328	4.737218	-1.582906
H	-4.001477	5.402127	-1.532037
H	-4.895306	-4.121337	-1.504817
H	-4.723209	-4.269709	-3.251605
H	-4.346500	0.628871	4.613403
H	-4.807902	-0.958897	5.221126
H	5.294869	-2.763062	-3.066143
H	5.883656	-1.679564	-4.324280
H	5.012448	4.347887	0.240897
H	4.425503	5.254404	1.631770
H	1.589793	-3.549127	3.514171
H	3.100184	-4.111504	4.227114
C	-0.174703	0.254336	-2.488276
O	0.273134	1.340755	-2.140269
O	-0.664496	-0.356349	-3.397452

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C	0.056346	-1.296440	2.871781
H	0.040810	-2.311542	3.325506
O	-0.022347	-1.314041	1.583648
O	0.136895	-0.311635	3.605942
Ru	0.025365	0.446221	0.182345
P	2.448222	0.646562	-0.062034
P	-2.392543	0.746459	0.047052
H	0.035426	1.378169	-1.130212
C	3.060706	2.394003	-0.543446
C	3.085450	-0.426487	-1.487650
C	3.537155	0.163148	1.399364
C	-2.791721	2.592285	-0.220178
C	-3.231501	-0.271273	-1.307006
C	-3.418633	0.342989	1.582252
H	2.989999	2.376117	-1.640909
C	2.154869	3.550690	-0.068281
C	4.530786	2.713540	-0.179502
H	2.765351	-1.431498	-1.183852
C	2.370810	-0.111946	-2.821735
C	4.611424	-0.468508	-1.720656
H	4.570563	0.431023	1.140024
C	3.498069	-1.356360	1.673015
C	3.137056	0.960870	2.662150
H	-2.108015	3.068077	0.498972
C	-2.396025	3.113777	-1.619349
C	-4.216648	3.086010	0.124243
H	-3.082349	-1.290238	-0.926009
C	-4.748086	-0.061465	-1.505181
C	-2.512126	-0.225008	-2.674064
H	-4.445752	0.681118	1.384665
C	-3.477411	-1.171988	1.873735
C	-2.888771	1.122794	2.808362
H	2.166465	3.605213	1.030015
H	1.121984	3.356549	-0.367172
C	2.607483	4.902437	-0.648785
C	4.982465	4.057199	-0.780246
H	4.633595	2.768196	0.911984

C	-2.678799	0.957339	2.905093	H	4.320585	5.216157	1.054010
H	2.211461	3.547095	1.102305	H	4.688821	6.030712	-0.463978
H	1.291133	3.372179	-0.390385	H	4.546433	-1.636979	-5.018428
C	2.856716	4.857024	-0.498227	H	4.653362	0.045639	-4.508610
C	5.196012	3.914997	-0.433078	H	2.892929	-1.690853	4.305261
H	4.643886	2.609903	1.192121	H	4.545887	-1.615493	4.918869
H	5.311414	1.769603	-0.199809	H	-3.753416	6.431653	-0.957691
H	1.283858	-0.031732	-2.674650	H	-4.505146	5.058866	-1.765741
H	2.620494	1.040039	-3.067653	H	-5.117697	-1.451524	-4.518171
C	2.769341	-0.895242	-4.006360	H	-4.842363	0.269506	-4.264173
C	4.996475	-1.364607	-2.906788	H	-2.693238	-1.350591	4.493808
H	4.964691	0.573763	-1.971824	H	-4.263982	-1.082240	5.252460
H	5.139691	-0.755697	-0.830771	H	0.132664	1.702063	1.430319
H	2.550905	-1.958824	1.652967	H	0.078725	2.143893	0.671231
H	3.982480	-2.005886	0.656342	C	-1.137537	-4.133355	-0.593027
C	4.402631	-1.974410	2.779251	C	0.412677	-4.162105	-0.898030
C	3.859104	0.203454	3.942404	B	-0.155616	-2.119068	0.055469
H	3.013005	1.725702	2.650054	H	0.001688	-1.016460	-0.725641
H	1.964356	0.335245	2.909676	O	0.906601	-3.051101	-0.125646
H	-1.359046	2.912019	-1.731706	O	-1.379822	-2.736305	-0.342175
H	-3.061379	2.903926	-2.185760	C	1.138582	-5.427666	-0.436057
C	-2.384840	4.805336	-1.431679	H	0.750172	-6.315507	-0.948808
H	-4.407619	2.853165	1.353911	H	2.206026	-5.344711	-0.667213
H	-4.893654	2.821080	-0.335856	H	1.040589	-5.577483	0.641812
C	-4.179455	4.746865	0.349472	C	0.731284	-3.900926	-2.377977
H	-5.278206	0.084819	-0.482867	H	1.811884	-3.765978	-2.487989
H	-4.911069	1.200379	-1.793936	H	0.426651	-4.737400	-3.016395
C	-5.391691	-0.793825	-2.462993	H	0.236159	-2.992916	-2.735592
C	-3.172020	-0.971395	-3.668031	C	-2.028247	-4.585535	-1.753574
H	-2.590423	1.010694	-3.044047	H	-1.837629	-5.633827	-2.012888
H	-1.470785	-0.242581	-2.526385	H	-3.081034	-4.498395	-1.463588
H	-2.618821	-1.675319	1.833910	H	-1.873309	-3.973451	-2.644668
H	-4.134761	-1.559836	0.966191	C	-1.529507	-4.928059	0.665391
C	-4.357547	-1.465696	3.113717	H	-2.566271	-4.689068	0.923581
C	-3.468689	0.639726	4.186024	H	-1.456941	-6.009371	0.503488
H	-1.667499	0.542772	2.997759	H	-0.904166	-4.672155	1.525389
H	-2.568573	2.045378	2.803456				
H	2.821178	4.866571	-1.598101				
H	2.206435	5.674298	-0.159934				
C	4.300583	5.095956	-0.039438				
H	6.215362	4.062532	-0.053108				
H	5.275226	3.866511	-1.529503				
H	2.393932	-1.912750	-3.834091				
H	2.278496	-0.532871	-4.919217				
C	4.290172	-0.947475	-4.203677				
H	6.085869	-1.355340	-3.043017				
H	4.721013	-2.399729	-2.656306				
H	4.391457	-3.068583	2.869543				
H	5.451818	-1.686754	2.610570				
C	3.903053	-1.324656	4.077784				
H	4.882943	0.590868	3.825226				
H	3.454451	0.655911	4.856706				
H	-1.616080	5.184919	-0.741885				
H	-2.122804	5.182300	-2.428864				
C	-3.760174	5.335051	-1.004529				
H	-5.188917	5.084950	0.617544				
H	-3.506198	5.126467	1.132640				
H	-5.330690	-1.820348	-2.072375				
H	-6.459480	-0.564972	-2.577301				
C	-4.679847	-0.724927	-3.821422				
H	-2.669468	-0.869011	-4.639009				
H	-3.007675	-2.006026	-3.335866				
H	-5.375905	-1.055408	3.032769				
H	-4.468753	-2.552828	3.221086				
C	-3.672310	-0.872147	4.351882				
H	-2.938700	1.051540	5.054368				
H	-4.448961	1.139546	4.149207				
				46			
				C	-0.304001	1.273155	2.516769
				H	-0.442362	1.434391	3.595208
				O	-0.241999	2.351095	1.835488
				O	-0.235281	0.093063	2.119158
				Ru	-0.152827	-0.482484	0.039763
				P	-2.570742	-0.608229	-0.067365
				P	2.251665	-0.881645	0.061600
				C	-3.276670	-1.980080	-1.186467
				C	-3.493859	0.940143	-0.660146
				C	-3.463995	-1.004840	1.573863
				C	2.597561	-2.702821	-0.404893
				C	3.265906	0.262389	-1.054195
				C	3.145884	-0.748226	1.721402
				H	-4.353966	-1.764958	-1.230022
				C	-2.733478	-1.934551	-2.632113
				C	-3.124836	-3.411707	-0.627200
				H	-3.323104	1.636447	0.173056
				C	-2.880299	1.628143	-1.900296
				C	-5.019074	0.788274	-0.854751
				H	-4.401583	-1.498849	1.272999
				C	-3.852874	0.229769	2.420764
				C	-2.665257	-1.988630	2.464460
				H	1.821347	-3.212175	0.183378
				C	2.314392	-3.031331	-1.887046
				C	3.957153	-3.320342	-0.001156
				H	3.095406	1.234968	-0.570952
				C	4.786486	-0.001919	-1.105417
				C	2.694368	0.398207	-2.484911
				H	4.160166	-1.135127	1.552717

C	3.301736	0.703089	2.224971
C	2.475464	-1.635455	2.795726
H	-1.657693	-2.150674	-2.619453
H	-2.845289	-0.935819	-3.062594
C	-3.428071	-2.964764	-3.539507
C	-3.795018	-4.456226	-1.539689
H	-2.058109	-3.647356	-0.513473
H	-3.574743	-3.487605	0.366483
H	-1.804804	1.761563	-1.764782
H	-3.032283	1.007139	-2.792942
C	-3.537997	2.999313	-2.134107
C	-5.684668	2.158620	-1.077329
H	-5.213334	0.159389	-1.734797
H	-5.488425	0.282144	-0.002727
H	-2.945309	0.761232	2.733543
H	-4.448001	0.942442	1.843707
C	-4.654709	-0.177982	3.670760
C	-3.477887	-2.413012	3.699726
H	-2.357457	-2.873027	1.901668
H	-1.740066	-1.498312	2.781929
H	1.357124	-2.605854	-2.204702
H	3.089527	-2.575020	-2.516585
C	2.312735	-4.549539	-2.136917
H	4.178881	-3.139736	1.054673
H	4.768809	-2.856539	-0.575744
C	3.970210	-4.840872	-0.250514
H	5.208323	-0.063892	-0.095524
H	4.978148	-0.971083	-1.585732
C	5.521235	1.091044	-1.901983
C	3.444489	1.473021	-3.291722
H	2.769892	-0.556332	-3.020471
H	1.630929	0.653262	-2.434012
H	2.320616	1.175203	2.329593
H	3.843600	1.309006	1.492161
C	4.047779	0.752698	3.570316
C	3.238243	-1.575902	4.130353
H	1.444833	-1.298211	2.946725
H	2.415331	-2.675940	2.454649
H	-4.495932	-2.714413	-3.626882
H	-3.009329	-2.903311	-4.552345
C	-3.281922	-4.386215	-2.982885
H	-3.634978	-5.459415	-1.123640
H	-4.882625	-4.288435	-1.536581
H	-3.278159	3.653125	-1.291709
H	-3.109452	3.462596	-3.032808
C	-5.063734	2.895541	-2.272799
H	-6.764776	2.028032	-1.226307
H	-5.564831	2.768672	-0.169853
H	-4.897896	0.717528	4.257501
H	-5.614919	-0.610976	3.352068
C	-3.903021	-1.198261	4.534866
H	-4.374412	-2.966703	3.380603
H	-2.884768	-3.106453	4.310125
H	1.486083	-5.006504	-1.573165
H	2.117431	-4.750038	-3.198492
C	3.639605	-5.189658	-1.707370
H	4.950034	-5.250489	0.027681
H	3.233306	-5.317764	0.412784
H	5.414013	2.052759	-1.379543
H	6.595944	0.868251	-1.933549
C	4.958024	1.219936	-3.323341
H	3.042864	1.512670	-4.312837
H	3.253251	2.456507	-2.841514
H	5.085040	0.415590	3.421940
H	4.106043	1.792092	3.918443
C	3.382185	-0.132573	4.632503
H	2.721759	-2.191969	4.878035

H	4.239681	-2.014652	4.002642
H	-2.221150	-4.676979	-3.007449
H	-3.818760	-5.105088	-3.615183
H	-5.508052	3.894263	-2.374755
H	-5.309770	2.349410	-3.196235
H	-3.006663	-0.722879	4.960247
H	-4.524804	-1.510260	5.384053
H	3.602110	-6.278436	-1.840924
H	4.445545	-4.821494	-2.359718
H	5.468797	2.025867	-3.865984
H	5.161106	0.291331	-3.878239
H	2.385658	0.269470	4.868755
H	3.958766	-0.107579	5.566346
C	1.461593	4.394777	0.044524
C	0.109214	4.575693	-0.747110
B	0.155261	2.512384	0.324846
H	0.008617	1.369721	-0.219635
O	-0.703689	3.510456	-0.224818
O	1.510129	2.966455	0.226904
C	-0.608762	5.904215	-0.497029
H	0.006565	6.753903	-0.817454
H	-1.543262	5.931444	-1.068130
H	-0.857269	6.030567	0.559329
C	0.275849	4.355287	-2.260055
H	-0.715072	4.300457	-2.722240
H	0.829684	5.172023	-2.737237
H	0.797863	3.415084	-2.462996
C	2.718628	4.837145	-0.707009
H	2.693100	5.913008	-0.917968
H	3.604104	4.636714	-0.093311
H	2.835306	4.302384	-1.652120
C	1.441861	5.070815	1.428630
H	2.310934	4.725506	1.999163
H	1.497688	6.162543	1.348214
H	0.543103	4.806123	1.990896
H	-0.273085	-2.025434	0.475837
H	-0.130831	-1.393749	-1.335750
H	-0.131871	-0.456562	-1.619325

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C	-0.187449	-1.955075	2.779638
H	-0.473272	-3.016687	2.858439
O	0.072333	-1.569380	1.514078
O	-0.103905	-1.212914	3.723219
Ru	0.054317	0.473942	0.241825
P	2.450596	0.574869	-0.011334
P	-2.325157	0.814713	0.075253
H	0.075988	1.455414	-1.009420
C	3.174976	2.329726	-0.318324
C	3.080307	-0.364276	-1.535230
C	3.537101	-0.081230	1.397434
C	-2.676821	2.690218	-0.116403
C	-3.186876	-0.105320	-1.338828
C	-3.434231	0.405001	1.562581
H	3.169921	2.396582	-1.415955
C	2.285630	3.485068	0.187954
C	4.631195	2.569489	0.146138
H	2.726177	-1.386369	-1.341029
C	2.382002	0.121389	-2.825934
C	4.607850	-0.411427	-1.752809
H	4.566943	0.235071	1.186832
C	3.549356	-1.619928	1.513427
C	3.115132	0.549230	2.744402
H	-1.976783	3.109647	0.620961
C	-2.256697	3.257348	-1.490124

C	-4.079660	3.231272	0.247117
H	-3.070372	-1.148829	-1.010622
C	-4.693555	0.166152	-1.536137
C	-2.445781	0.002431	-2.690657
H	-4.419737	0.845980	1.362675
C	-3.656347	-1.105506	1.781085
C	-2.875232	1.059623	2.847156
H	2.244237	3.467334	1.287116
H	1.262230	3.344296	-0.168723
C	2.811587	4.855026	-0.275307
C	5.160825	3.932515	-0.336116
H	4.675292	2.547464	1.243245
H	5.299751	1.779208	-0.207529
H	1.298085	0.110142	-2.681353
H	2.662051	1.165507	-3.029133
C	2.771599	-0.727442	-4.049339
C	4.980945	-1.293005	-2.958564
H	4.984601	0.602746	-1.941576
H	5.123990	-0.777722	-0.858014
H	2.531973	-1.985086	1.678176
H	3.888448	-2.079300	0.578351
C	4.453194	-2.085024	2.669698
C	4.020776	0.084213	3.897742
H	3.134912	1.644601	2.681503
H	2.077871	0.269677	2.965914
H	-1.268768	2.879841	-1.769809
H	-2.963782	2.911758	-2.256134
C	-2.256597	4.795479	-1.488813
H	-4.399149	2.883611	1.233856
H	-4.823844	2.864630	-0.471679
C	-4.095760	4.772400	0.246301
H	-5.240300	0.067307	-0.591195
H	-4.838963	1.200212	-1.876017
C	-5.303434	-0.784097	-2.583358
C	-3.057584	-0.942332	-3.739632
H	-2.504587	1.028323	-3.073462
H	-1.384736	-0.217188	-2.542611
H	-2.692596	-1.608917	1.903459
H	-4.121257	-1.558248	0.898325
C	-4.539713	-1.378563	3.012028
C	-3.771557	0.784569	4.066684
H	-1.869892	0.669071	3.046871
H	-2.765199	2.142711	2.709951
H	2.735901	4.914174	-1.371683
H	2.169178	5.651323	0.123343
C	4.269987	5.086186	0.141388
H	6.191453	4.072802	0.015939
H	5.203189	3.935671	-1.435734
H	2.374189	-1.744617	-3.926518
H	2.294757	-0.316166	-4.948991
C	4.292379	-0.805248	-4.240415
H	6.071251	-1.302267	-3.088809
H	4.681783	-2.332253	-2.755102
H	4.422705	-3.180362	2.744372
H	5.497089	-1.817706	2.444977
C	4.045689	-1.446635	4.005346
H	5.044400	0.454263	3.733713
H	3.674755	0.526690	4.840816
H	-1.494980	5.156258	-0.781342
H	-1.963159	5.167272	-2.479393
C	-3.629070	5.356998	-1.093059
H	-5.105286	5.129921	0.488654
H	-3.436288	5.135543	1.048771
H	-5.251364	-1.816480	-2.206015
H	-6.368701	-0.554759	-2.718908
C	-4.561820	-0.696933	-3.924655
H	-2.532083	-0.823700	-4.696522

H	-2.901679	-1.985434	-3.426480
H	-5.552232	-0.990584	2.823346
H	-4.645309	-2.462343	3.155889
C	-3.976765	-0.721427	4.279731
H	-3.326166	1.238979	4.961039
H	-4.749633	1.268563	3.922113
H	4.328072	5.156656	1.237919
H	4.636433	6.042878	-0.253167
H	4.540123	-1.463227	-5.083723
H	4.678512	0.192427	-4.498308
H	3.043437	-1.800647	4.287438
H	4.728642	-1.764030	4.804290
H	-3.597648	6.453109	-1.040757
H	-4.361379	5.101815	-1.873813
H	-4.983381	-1.413675	-4.641620
H	-4.714184	0.303522	-4.356919
H	-3.010794	-1.181250	4.531986
H	-4.645835	-0.900959	5.131447
H	0.124835	1.581529	1.688060
H	0.083186	2.089635	1.032390
C	-1.098023	-4.308711	-0.464538
C	0.378102	-4.163604	-1.010540
B	-0.108202	-2.436671	0.393839
H	-0.015808	-0.774854	-0.850537
O	0.943481	-3.170121	-0.107888
O	-1.339462	-3.003971	0.136802
C	1.230643	-5.428293	-0.912325
H	0.809503	-6.230910	-1.528717
H	2.240414	-5.216782	-1.278222
H	1.314021	-5.784900	0.116823
C	0.442861	-3.596330	-2.432414
H	1.486160	-3.381369	-2.679457
H	0.059138	-4.312153	-3.166965
H	-0.121266	-2.663724	-2.515182
C	-2.162329	-4.564998	-1.528673
H	-1.985059	-5.521283	-2.034052
H	-3.149799	-4.609841	-1.057793
H	-2.180484	-3.772315	-2.278694
C	-1.231989	-5.342627	0.663015
H	-2.218446	-5.238312	1.125755
H	-1.136618	-6.366237	0.285856
H	-0.473923	-5.193218	1.439046

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C	-0.625468	1.510312	2.572741
H	-0.868139	1.705778	3.624985
O	-0.859710	2.562391	1.813578
O	-0.249666	0.406571	2.216828
Ru	-0.134317	-0.509057	0.120202
P	-2.525593	-0.669699	-0.072105
P	2.240959	-0.869719	0.104799
C	-3.135911	-2.119155	-1.146389
C	-3.486618	0.809311	-0.782935
C	-3.514115	-1.026858	1.537265
C	2.617668	-2.714263	-0.210564
C	3.264742	0.169069	-1.109784
C	3.157757	-0.575437	1.737709
H	-4.228852	-2.003431	-1.184503
C	-2.601915	-2.055296	-2.593534
C	-2.847621	-3.508481	-0.536801
H	-3.447762	1.527378	0.048585
C	-2.795021	1.518055	-1.966974
C	-4.971869	0.555239	-1.123587
H	-4.382519	-1.622732	1.214604
C	-4.071527	0.219282	2.263888
C	-2.702026	-1.874075	2.545650

H	-1.693133	-3.240893	-2.04084
C	-2.276969	-4.784596	-0.66318
C	0.081293	-4.135207	-1.26662
H	2.321546	2.746072	0.37766
C	4.054825	2.878520	-0.87816
C	1.663089	2.592642	-1.65026
H	3.372699	-0.647990	1.96567
C	5.151197	0.502071	1.65071
C	2.984773	1.332558	2.65865
H	4.853900	0.142785	-1.09094
C	3.514109	-0.331155	-2.70162
C	4.169394	-1.881093	-0.82542
H	-0.206606	-2.702426	2.66342
H	-0.592091	-4.224311	1.86785
C	-1.539391	-3.971032	3.80298
C	-3.266590	-2.126190	3.89373
H	-3.577202	-1.076042	2.03120
H	-1.994823	-0.795844	2.73756
H	-4.552770	-2.332814	0.21147
H	-4.222128	-2.751304	-1.46842
C	-5.446154	-0.991322	-1.24014
C	-3.790119	0.351035	-2.60404
H	-2.514402	-1.376616	-2.84089
H	-1.705109	-0.007171	-2.08819
H	-3.310201	-4.454534	-0.52213
H	-1.947190	-5.197467	0.29960
C	-2.242973	-5.910173	-1.71349
C	0.126256	-5.267654	-2.30785
H	0.478747	-4.508503	-0.31098
H	0.731762	-3.315544	-1.58164
H	4.784446	2.679923	-0.08831
H	4.452480	2.419791	-1.79384
C	3.943160	4.399692	-1.08995
C	1.551513	4.111828	-1.86140
H	1.969781	2.123407	-2.59329
H	0.683420	2.173133	-1.40805
H	5.625942	-0.180895	0.93846
H	5.448388	1.516723	1.35747
C	5.700269	0.223291	3.06301
C	3.537060	1.070836	4.07100
H	3.218502	2.371097	2.37957
H	1.896314	1.223821	2.66078
H	2.547126	-0.830541	-2.84280
H	3.376930	0.709053	-3.01254
C	4.579988	-0.981135	-3.60333
C	5.250272	-2.520497	-1.71365
H	4.458394	-1.971669	0.22828
H	3.235276	-2.443760	-0.94334
H	-2.290837	-4.750764	3.60602
H	-0.717594	-4.459569	4.34329
C	-2.166828	-2.867062	4.66601
H	-3.671098	-1.306282	4.50149
H	-4.103087	-2.817049	3.70558
H	-5.587065	-0.185087	-0.50599
H	-6.387301	-1.556152	-1.27406
C	-5.141335	-0.378501	-2.61446
H	-3.861150	1.220452	-1.93474
H	-3.556432	0.735743	-3.60601
H	-2.898196	-6.731511	-1.39450
H	-2.654153	-5.533323	-2.66197
C	-0.816142	-6.423147	-1.94634
H	-0.160240	-4.861228	-3.28960
H	1.156510	-5.633038	-2.41201
H	3.649270	4.872520	-0.14088
H	4.927502	4.810132	-1.35101
C	2.912472	4.750522	-2.17078
H	1.126139	4.568579	-0.95582

H	0.844389	4.317307	-2.67612
H	5.490780	-0.823341	3.33038
H	6.792917	0.332247	3.06361
C	5.069334	1.150695	4.11112
H	3.214571	0.072376	4.40107
H	3.098947	1.787449	4.77783
H	5.509773	-0.395421	-3.54240
H	4.252511	-0.935854	-4.65022
C	4.874162	-2.431681	-3.19876
H	5.398734	-3.567463	-1.41852
H	6.210936	-2.010040	-1.54753
H	-1.385373	-2.150163	4.95652
H	-2.568881	-3.291082	5.59568
H	-5.116530	-1.178092	-3.37033
H	-5.944820	0.307846	-2.91268
H	-0.454447	-6.912396	-1.02960
H	-0.806853	-7.187905	-2.73382
H	3.271594	4.384809	-3.14451
H	2.813962	5.839967	-2.26411
H	5.383681	2.186166	3.91036
H	5.441199	0.900994	5.11342
H	3.980947	-3.047231	-3.38111
H	5.675074	-2.847884	-3.82352
C	-2.630663	4.724979	-0.43567
C	-4.011974	4.275629	0.18982
B	-2.435163	2.689345	0.56619
O	-3.792338	2.860024	0.44535
O	-1.696900	3.781398	0.17056
O	-1.919397	1.526192	1.06503
C	-0.538891	1.297839	1.15868
H	0.035857	2.200006	0.91383
O	-0.149964	0.503867	2.05334
C	-5.220068	4.420100	-0.73313
H	-6.116217	4.053086	-0.22260
H	-5.386606	5.471220	-0.99547
H	-5.097544	3.845207	-1.65374
C	-4.304491	4.929308	1.54760
H	-4.547920	5.991699	1.44147
H	-5.159278	4.423462	2.00689
H	-3.452465	4.835459	2.22875
C	-2.185063	6.139931	-0.07322
H	-1.208464	6.344939	-0.52365
H	-2.895734	6.881655	-0.45555
H	-2.092745	6.269676	1.00736
C	-2.556060	4.518320	-1.95348
H	-3.190111	5.234088	-2.48727
H	-1.522671	4.663253	-2.28180
H	-2.862090	3.506340	-2.23594

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Ru	-0.947723	0.440759	-0.071578
P	0.128620	2.602626	0.008904
P	-2.172302	-1.659579	-0.053326
H	0.756246	-2.074006	1.125203
H	-2.275756	0.998761	-0.970336
H	-1.607651	0.882103	-1.580337
H	-2.019388	0.994405	0.933282
C	0.538513	3.308402	1.713075
C	1.795363	2.431442	-0.858431
C	-0.731457	4.050125	-0.888196
C	-1.251290	-3.224873	-0.613780
C	-2.834410	-2.051510	1.679518
C	-3.758148	-1.665012	-1.094471
H	0.851093	4.348667	1.547150
C	-0.724327	3.327152	2.604106
C	1.692704	2.586513	2.444964

H	2.278361	1.654282	-0.251429
C	2.720089	3.664439	-0.908780
C	1.627678	1.835444	-2.275349
H	-0.438408	3.893459	-1.937916
C	-0.276041	5.472230	-0.483204
C	-2.275823	3.995510	-0.842718
H	-0.725819	-3.540199	0.300270
C	-2.091582	-4.427636	-1.098772
C	-0.167001	-2.887512	-1.664276
H	-3.392047	-1.133029	1.913983
C	-3.802161	-3.243626	1.837171
C	-1.701663	-2.150572	2.723835
H	-4.184401	-2.672902	-0.994401
C	-3.494216	-1.426601	-2.598433
C	-4.810510	-0.660467	-0.574499
H	-1.073806	2.295634	2.736058
H	-1.539694	3.870617	2.110765
C	-0.444552	3.961022	3.977169
C	1.970571	3.233438	3.813275
H	2.607646	2.613506	1.841371
H	1.422486	1.532824	2.561809
H	2.855843	4.096355	0.089921
H	2.261985	4.444475	-1.532093
C	4.088536	3.305001	-1.514937
C	2.987757	1.501529	-2.914173
H	1.091385	2.548832	-2.919831
H	1.012134	0.928626	-2.228723
H	0.813861	5.559672	-0.486104
H	-0.603421	5.675825	0.545380
C	-0.882647	6.541446	-1.409525
C	-2.904657	5.062119	-1.757123
H	-2.619212	4.155229	0.188763
H	-2.636049	3.006531	-1.133557
H	-2.857057	-4.699231	-0.365571
H	-2.623843	-4.159519	-2.021036
C	-1.197437	-5.648938	-1.385796
C	0.726432	-4.104043	-1.958220
H	-0.648801	-2.563399	-2.597684
H	0.452274	-2.052038	-1.324121
H	-4.624965	-3.191185	1.114753
H	-3.264982	-4.180501	1.638188
C	-4.377207	-3.304456	3.264997
C	-2.267503	-2.222759	4.152664
H	-1.107667	-3.057612	2.534537
H	-1.026455	-1.295935	2.625025
H	-3.024360	-0.445236	-2.737174
H	-2.784914	-2.163808	-2.988980
C	-4.793385	-1.482526	-3.421490
C	-6.105159	-0.708133	-1.405402
H	-5.051763	-0.859517	0.475483
H	-4.391688	0.353935	-0.607166
H	-0.197245	5.025530	3.844714
H	-1.353771	3.926949	4.591898
C	0.715132	3.258406	4.695768
H	2.779623	2.689356	4.318399
H	2.331010	4.264141	3.669363
H	4.591254	2.573680	-0.865282
H	4.729783	4.196107	-1.542453
C	3.931599	2.712937	-2.922881
H	3.450606	0.677426	-2.356404
H	2.831245	1.137872	-3.938614
H	-0.543803	7.537703	-1.096365
H	-0.505713	6.390397	-2.432092
C	-2.415696	6.476211	-1.415499
H	-2.647565	4.832787	-2.802516
H	-3.999107	5.010003	-1.687578
H	-0.735483	-5.985309	-0.445651

H	-1.814912	-6.482623	-1.745432
C	-0.095135	-5.321772	-2.403719
H	1.290781	-4.359252	-1.048457
H	1.469232	-3.841453	-2.722273
H	-4.989873	-2.408413	3.444493
H	-5.050784	-4.166743	3.356976
C	-3.263864	-3.377918	4.320035
H	-2.770132	-1.272408	4.386813
H	-1.443582	-2.323007	4.871028
H	-5.210339	-2.499769	-3.375287
H	-4.569026	-1.285286	-4.477782
C	-5.835472	-0.484761	-2.899318
H	-6.812191	0.041752	-1.027554
H	-6.587138	-1.687845	-1.268475
H	0.420272	2.225720	4.932120
H	0.927942	3.753324	5.652568
H	3.529862	3.487508	-3.594096
H	4.911375	2.427932	-3.328302
H	-2.791312	6.758322	-0.420640
H	-2.828211	7.206220	-2.123871
H	-0.556970	-5.109130	-3.379592
H	0.556703	-6.192699	-2.550686
H	-2.730634	-4.334686	4.213946
H	-3.695576	-3.371642	5.329370
H	-5.464260	0.539598	-3.052403
H	-6.767598	-0.568817	-3.472685
C	5.149218	-2.872844	0.593710
C	5.504231	-1.940466	-0.631729
B	3.370179	-1.544120	0.065776
O	4.199376	-1.459045	-1.040473
O	3.938776	-2.260491	1.105576
O	2.150595	-0.964866	0.091963
C	1.268145	-1.107214	1.279132
H	1.931240	-1.190373	2.154147
O	0.449527	-0.051530	1.395337
C	6.155409	-2.647346	-1.819393
H	6.331129	-1.926426	-2.624628
H	7.121581	-3.080953	-1.536045
H	5.517540	-3.441831	-2.213381
C	6.332754	-0.711061	-0.230576
H	7.362430	-0.979340	0.029626
H	6.361258	-0.013083	-1.073325
H	5.883639	-0.193100	0.623133
C	6.188650	-2.901603	1.713500
H	5.835856	-3.547120	2.524582
H	7.143638	-3.301596	1.353329
H	6.361095	-1.905934	2.128659
C	4.784630	-4.305061	0.176291
H	5.661552	-4.865640	-0.164928
H	4.356203	-4.826772	1.037993
H	4.038739	-4.305659	-0.625300

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Ru	-0.639953	-0.557058	-0.539245
P	-2.813547	0.442864	-0.147037
P	1.373699	-1.755174	-1.377800
H	1.558779	1.368700	2.249892
H	-1.080275	-1.340269	-1.840517
H	-0.900604	0.155853	-1.920167
H	-1.497411	-1.856804	-0.384542
C	-3.657355	0.109809	1.506416
C	-2.730474	2.331236	-0.262009
C	-4.147455	-0.005904	-1.442817
C	3.060222	-1.708393	-0.508792
C	0.939974	-3.595711	-1.494601
C	1.762518	-1.278993	-3.167071

H	-4.692630	0.454288	1.384187	H	-4.745832	-0.848516	-4.076662
C	-3.695038	-1.404498	1.811789	H	-4.780918	-2.574763	-3.732857
C	-3.061521	0.883573	2.702326	H	5.451617	-2.985630	0.224374
H	-2.057106	2.593949	0.565595	H	6.419896	-2.432646	-1.139908
C	-4.058075	3.093065	-0.056005	C	5.826243	-0.854214	0.238488
C	-2.046144	2.807284	-1.563348	H	4.431118	-1.150054	1.873264
H	-4.004992	0.766323	-2.214085	H	4.774379	0.539606	1.535749
C	-5.612752	0.090931	-0.952412	H	0.368208	-5.859832	-3.040137
C	-3.940298	-1.370596	-2.137958	H	1.979481	-6.570513	-2.994525
H	2.944302	-2.461015	0.284172	C	0.957193	-6.549572	-1.072829
C	4.289363	-2.086470	-1.367306	H	-0.931820	-5.554062	-0.720367
C	3.322836	-0.367748	0.207512	H	-0.109743	-6.049183	0.755713
H	-0.016891	-3.567726	-2.035977	H	3.420454	0.103570	-5.001841
C	1.893269	-4.520155	-2.281954	H	2.674454	1.684681	-4.785414
C	0.650147	-4.210799	-0.108000	C	1.388348	0.207736	-5.733995
H	2.659093	-1.848160	-3.448026	H	0.228919	-1.546110	-6.295653
C	2.097855	0.224255	-3.290357	H	1.915322	-1.883022	-5.916111
C	0.650039	-1.655823	-4.170192	H	-2.901524	-1.254537	4.492241
H	-2.668023	-1.770319	1.926895	H	-4.522463	-1.091642	5.188640
H	-4.138687	-1.958489	0.974142	H	-3.836072	4.935046	-2.172370
C	-4.488697	-1.690261	3.098271	H	-2.962844	6.175452	-1.277474
C	-3.867567	0.598007	3.983368	H	-6.639363	-2.261475	-2.122600
H	-3.068154	1.963057	2.506703	H	-7.085969	-1.542204	-3.667706
H	-2.025495	0.578325	2.870514	H	6.063016	-0.068819	-0.495932
H	-4.552182	2.778123	0.869858	H	6.708051	-0.952245	0.885102
H	-4.745995	2.858901	-0.879437	H	1.894682	-6.728496	-0.525310
C	-3.833105	4.615492	-0.034473	H	0.481626	-7.529883	-1.205926
C	-1.845690	4.332263	-1.571138	H	0.484079	0.803891	-5.540750
H	-2.659382	2.522236	-2.431396	H	1.705842	0.443022	-6.758068
H	-1.075867	2.316616	-1.680754	C	3.377398	4.409099	0.515821
H	-5.807593	1.047784	-0.460729	C	2.673758	4.672415	-0.878765
H	-5.796160	-0.689405	-0.202094	B	1.630404	2.976111	0.221743
C	-6.610854	-0.100956	-2.108248	O	1.830116	3.498344	-1.036124
C	-4.944442	-1.586231	-3.284283	O	2.413826	3.555664	1.193979
H	-4.046839	-2.179951	-1.401606	O	0.722459	1.987537	0.446557
H	-2.923765	-1.443995	-2.529332	C	0.587567	1.390076	1.745493
H	4.141777	-3.033582	-1.893718	H	-0.122623	1.997669	2.323788
H	4.443640	-1.320748	-2.140537	O	0.102938	0.113165	1.531586
C	5.562736	-2.170296	-0.505524	C	3.618963	4.748029	-2.076873
C	4.600123	-0.433712	1.059151	H	3.037357	4.898311	-2.992256
H	3.416379	0.438009	-0.534684	H	4.314170	5.589417	-1.975954
H	2.476933	-0.135829	0.849805	H	4.197788	3.828896	-2.192815
H	2.127797	-4.108283	-3.270342	C	1.745988	5.894883	-0.866610
H	2.844871	-4.611721	-1.742986	H	2.311192	6.831138	-0.809961
C	1.286209	-5.926961	-2.437186	H	1.156362	5.902856	-1.788297
C	0.056845	-5.623935	-0.242090	H	1.050089	5.859651	-0.022153
H	1.582446	-4.267935	0.471928	C	3.603071	5.652155	1.375060
H	-0.026414	-3.568755	0.462896	H	4.057880	5.360540	2.327251
H	1.228738	0.814806	-2.971592	H	4.281132	6.354665	0.876986
H	2.915577	0.495895	-2.614533	H	2.665415	6.167343	1.594520
C	2.479483	0.605932	-4.730908	C	4.681558	3.609842	0.398512
C	1.045124	-1.283073	-5.610333	H	5.482895	4.207818	-0.048366
H	0.426097	-2.727601	-4.121244	H	4.999772	3.300773	1.398950
H	-0.274986	-1.128591	-3.905861	H	4.543936	2.707865	-0.205371
H	-5.544950	-1.418694	2.944660	C	0.533120	-0.846086	4.875808
H	-4.470540	-2.767839	3.307572	C	1.777436	-1.581509	4.240072
C	-3.920985	-0.905619	4.288844	B	0.289665	-1.040739	2.525133
H	-3.413087	1.138104	4.823998	H	-0.210083	-1.963184	1.872814
H	-4.890738	0.991161	3.873166	O	1.700448	-1.193645	2.869330
H	-3.205065	4.876967	0.829932	O	-0.401208	-0.820387	3.796135
H	-4.792513	5.129436	0.108776	C	3.133527	-1.152987	4.809440
C	-3.153306	5.095386	-1.324328	H	3.193341	-1.350659	5.886840
H	-1.118402	4.594448	-0.790921	H	3.936820	-1.716995	4.321575
H	-1.397532	4.637274	-2.525583	H	3.320775	-0.089374	4.640084
H	-7.635961	-0.029005	-1.722189	C	1.658464	-3.116882	4.319242
H	-6.491748	0.718885	-2.832558	H	2.439551	-3.560596	3.691936
C	-6.398425	-1.443690	-2.817860	H	1.785115	-3.492948	5.341207

H	0.689347	-3.454959	3.940248
C	-0.103073	-1.577101	6.065286
H	0.608748	-1.696390	6.891963
H	-0.956614	-1.000089	6.439263
H	-0.469746	-2.564855	5.775365
C	0.845165	0.602416	5.299315
H	-0.098380	1.116928	5.512661
H	1.467620	0.645899	6.201157
H	1.358083	1.152893	4.505372

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Ru	-0.161491	-0.595773	-0.204313
P	2.222424	-1.060662	-0.022718
P	-2.606076	-0.514631	0.073329
H	-1.380369	0.965491	-2.662339
H	-0.225127	-1.622029	1.004615
H	-0.082894	-0.015077	1.261625
H	-0.447179	-2.161830	-0.333749
C	3.420615	-0.601647	-1.411072
C	2.901992	-0.093471	1.471774
C	2.587021	-2.883157	0.376429
C	-3.722315	0.861488	-0.627882
C	-3.307229	-2.099054	-0.705509
C	-3.160180	-0.662629	1.875105
H	4.427232	-0.829602	-1.030041
C	3.209487	-1.422027	-2.703453
C	3.358196	0.907957	-1.734323
H	2.406087	0.877997	1.337940
C	4.423653	0.172021	1.565022
C	2.403644	-0.671485	2.815959
H	2.159449	-2.980154	1.385610
C	4.078430	-3.278466	0.461597
C	1.831794	-3.901600	-0.509861
H	-3.829423	0.560097	-1.681847
C	-5.145171	0.978253	-0.033045
C	-3.062523	2.258400	-0.629609
H	-2.651380	-2.863535	-0.265398
C	-4.763249	-2.512758	-0.403101
C	-3.064273	-2.135990	-2.230377
H	-4.257831	-0.691241	1.845458
C	-2.741478	0.558134	2.723859
C	-2.686114	-1.964161	2.557432
H	2.183538	-1.269865	-3.057998
H	3.323284	-2.491918	-2.503322
C	4.214913	-1.021371	-3.798812
C	4.376045	1.299344	-2.818479
H	3.530797	1.508119	-0.834958
H	2.347318	1.156594	-2.069963
H	4.812204	0.599615	0.635813
H	4.967298	-0.767197	1.726972
C	4.743196	1.127581	2.730625
C	2.715270	0.280282	3.983834
H	2.894924	-1.636207	3.010475
H	1.326587	-0.862326	2.775222
H	4.628400	-2.595938	1.114990
H	4.538095	-3.197026	-0.533051
C	4.254990	-4.718421	0.978930
C	1.997470	-5.334860	0.023694
H	2.211022	-3.862796	-1.538145
H	0.771519	-3.642145	-0.563621
H	-5.651691	0.010270	-0.000313
H	-5.074902	1.330188	1.005043
C	-6.001096	1.978253	-0.832478
C	-3.905375	3.265601	-1.431063
H	-2.965576	2.617816	0.404839
H	-2.048426	2.206923	-1.027575

H	-4.975245	-2.490420	0.672463
H	-5.456038	-1.806371	-0.878165
C	-5.054361	-3.920906	-0.956760
C	-3.364233	-3.531323	-2.806883
H	-3.722191	-1.404106	-2.723296
H	-2.033728	-1.847664	-2.458164
H	-1.646215	0.627298	2.736946
H	-3.103131	1.488104	2.271635
C	-3.269419	0.452465	4.165344
C	-3.224272	-2.071480	3.995135
H	-2.999681	-2.843968	1.983772
H	-1.589578	-1.980391	2.581777
H	5.231520	-1.292831	-3.475268
H	4.013498	-1.600931	-4.709278
C	4.171214	0.482003	-4.100608
H	4.291094	2.373099	-3.031859
H	5.397568	1.135435	-2.442281
H	4.286313	2.106489	2.526179
H	5.827283	1.293072	2.785705
C	4.214818	0.595111	4.069579
H	2.151311	1.213488	3.844209
H	2.364744	-0.162146	4.925770
H	5.322422	-4.974753	0.998638
H	3.902793	-4.770066	2.020076
C	3.475858	-5.732586	0.131776
H	1.527097	-5.408971	1.016010
H	1.460501	-6.035575	-0.628879
H	-6.146288	1.592834	-1.852748
H	-7.000004	2.051192	-0.382370
C	-5.341823	3.362771	-0.899497
H	-3.929675	2.953872	-2.486460
H	-3.422122	4.250031	-1.410299
H	-4.419867	-4.652433	-0.434443
H	-6.094156	-4.198186	-0.738903
C	-4.787044	-3.998027	-2.466799
H	-2.637207	-4.248663	-2.398380
H	-3.215645	-3.523296	-3.894421
H	-4.368970	0.497856	4.154372
H	-2.927757	1.318149	4.747354
C	-2.825544	-0.853163	4.839466
H	-2.855115	-2.995542	4.458761
H	-4.321423	-2.152076	3.968562
H	3.194223	0.736158	-4.537614
H	4.929002	0.744611	-4.850309
H	4.762625	-0.321571	4.335607
H	4.410170	1.318862	4.871560
H	3.913180	-5.773911	-0.877029
H	3.574277	-6.739955	0.556642
H	-5.324525	3.801747	0.109279
H	-5.939154	4.039627	-1.524074
H	-5.512369	-3.358317	-2.991852
H	-4.952693	-5.020212	-2.831060
H	-1.732602	-0.842318	4.963754
H	-3.254945	-0.928718	5.846841
C	0.651973	4.969123	-0.616746
C	1.479639	4.393257	0.601951
B	0.520466	2.668438	-0.595302
O	1.037698	3.020974	0.662029
O	0.427534	3.797886	-1.423280
O	0.160624	1.452039	-0.977776
C	-0.363544	0.593933	-2.840818
H	0.265849	1.226229	-3.486388
O	-0.037357	-0.572861	-2.579374
C	1.196322	5.056561	1.951281
H	1.796974	4.574767	2.730459
H	1.458979	6.121060	1.932665
H	0.145025	4.960862	2.232812

C	2.993579	4.385952	0.340244
H	3.413826	5.397645	0.344345
H	3.488614	3.807776	1.127212
H	3.226961	3.918684	-0.621418
C	1.381856	6.015732	-1.461112
H	0.737308	6.333564	-2.287778
H	1.629880	6.902514	-0.865770
H	2.302818	5.615362	-1.891495
C	-0.723718	5.514436	-0.200442
H	-0.640900	6.447393	0.368085
H	-1.312343	5.712694	-1.102085
H	-1.269303	4.785126	0.406792

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Ru	-0.053810	-0.922752	-0.110403
P	-2.458771	-0.778722	-0.104632
P	2.356304	-0.967304	-0.140153
H	-0.114259	-2.485227	-0.493473
H	-0.081552	-1.350515	-1.629289
H	-0.096816	-2.212908	0.833410
C	-3.162237	-0.367372	1.597840
C	-3.001527	0.660183	-1.194706
C	-3.499730	-2.240096	-0.736698
C	3.273156	-2.473611	-0.855174
C	2.994362	0.476773	-1.167606
C	3.101840	-0.705633	1.574107
H	-4.257890	-0.396820	1.523010
C	-2.727592	-1.424299	2.639418
C	-2.755317	1.045040	2.072622
H	-2.440788	1.496299	-0.759347
C	-4.500605	1.022973	-1.197901
C	-2.491016	0.506503	-2.644414
H	-3.604388	-2.015594	-1.809084
C	-4.925395	-2.356197	-0.149416
C	-2.782450	-3.604189	-0.639070
H	3.388853	-2.206764	-1.916564
C	4.688865	-2.728085	-0.286811
C	2.449823	-3.779198	-0.813248
H	2.498877	1.330899	-0.689593
C	4.514422	0.736827	-1.173197
C	2.458810	0.426360	-2.615643
H	4.190936	-0.822562	1.487334
C	2.581223	-1.778708	2.557127
C	2.820345	0.705727	2.135910
H	-1.630152	-1.448570	2.683909
H	-3.043601	-2.428413	2.330329
C	-3.287024	-1.112341	4.037964
C	-3.307538	1.351886	3.475454
H	-3.121255	1.804813	1.372298
H	-1.663634	1.133832	2.072672
H	-4.881313	1.144922	-0.176585
H	-5.075815	0.205816	-1.655141
C	-4.754896	2.311753	-2.001423
C	-2.744003	1.788337	-3.456558
H	-2.999296	-0.337111	-3.135843
H	-1.421565	0.274580	-2.638192
H	-5.463304	-1.406105	-0.225751
H	-4.862731	-2.596041	0.920488
C	-5.734083	-3.463002	-0.850082
C	-3.592251	-4.720152	-1.321847
H	-2.621317	-3.863725	0.417169
H	-1.790499	-3.536928	-1.093500
H	5.299294	-1.820642	-0.328125
H	4.612874	-3.006495	0.772812
C	5.402334	-3.864208	-1.041320
C	3.164539	-4.923752	-1.551998

H	2.274753	-4.073366	0.231574
H	1.463887	-3.611115	-1.254933
H	4.910920	0.788285	-0.152006
H	5.031300	-0.094721	-1.672323
C	4.846662	2.041778	-1.920254
C	2.787750	1.727039	-3.368019
H	2.904429	-0.424857	-3.152843
H	1.376192	0.266085	-2.604886
H	1.487175	-1.699615	2.616709
H	2.795458	-2.787364	2.183046
C	3.182617	-1.606208	3.961315
C	3.413582	0.876927	3.545523
H	3.243179	1.471761	1.476565
H	1.740350	0.890151	2.158943
H	-4.384795	-1.187488	4.016375
H	-2.936993	-1.868728	4.752624
C	-2.883618	0.293353	4.502266
H	-2.966752	2.346454	3.789928
H	-4.406870	1.394746	3.435378
H	-4.258294	3.153317	-1.497157
H	-5.828917	2.540187	-2.007867
C	-4.225273	2.194404	-3.437796
H	-2.130696	2.594966	-3.031520
H	-2.403041	1.645433	-4.490344
H	-6.734188	-3.528578	-0.401950
H	-5.882204	-3.190654	-1.905754
C	-5.020536	-4.819042	-0.769656
H	-3.636616	-4.519117	-2.402919
H	-3.069968	-5.678680	-1.205643
H	5.566945	-3.558530	-2.085299
H	6.395854	-4.029825	-0.604512
C	4.582190	-5.160848	-1.014153
H	3.221908	-4.678012	-2.623175
H	2.567702	-5.841830	-1.475367
H	4.413507	2.889887	-1.369615
H	5.933456	2.198343	-1.930588
C	4.293307	2.030456	-3.352761
H	2.234449	2.549555	-2.894891
H	2.426514	1.657613	-4.402516
H	4.268821	-1.777128	3.916174
H	2.774211	-2.370587	4.635331
C	2.912499	-0.200831	4.516487
H	3.166600	1.876733	3.924839
H	4.511701	0.826189	3.487569
H	-1.791958	0.332075	4.631543
H	-3.324347	0.512830	5.483407
H	-4.815361	1.438082	-3.977420
H	-4.368828	3.141460	-3.974093
H	-4.982342	-5.144938	0.280580
H	-5.589836	-5.583756	-1.313585
H	4.521233	-5.527688	0.021432
H	5.086426	-5.944496	-1.594116
H	4.824568	1.263024	-3.936212
H	4.495100	2.990685	-3.845062
H	1.830537	-0.074753	4.670166
H	3.385369	-0.080299	5.499809
C	0.529535	4.561590	0.977016
C	0.045560	4.624711	-0.525966
B	0.125732	2.431935	0.188640
O	0.183792	3.255064	-0.954592
O	0.186908	3.216455	1.354745
O	0.025349	1.119880	0.184743
C	0.882975	5.516582	-1.444005
H	0.489360	5.464542	-2.464882
H	0.845403	6.563624	-1.120295
H	1.928010	5.198439	-1.471482
C	-1.438693	5.003615	-0.654742

H	-1.617541	6.054565	-0.402007
H	-1.759061	4.839829	-1.688886
H	-2.060886	4.381098	-0.003267
C	-0.172135	5.532924	1.928619
H	0.216087	5.395919	2.943721
H	0.006144	6.574680	1.636394
H	-1.250340	5.357823	1.957153
C	2.053029	4.709750	1.120761
H	2.388778	5.733220	0.919518
H	2.339016	4.448888	2.144946
H	2.580398	4.033174	0.440054

H	-1.064784	-2.980636	1.922702
H	-4.872028	0.400883	-1.319184
H	-5.490252	0.039502	0.285419
C	-5.397898	2.145904	-0.165990
C	-3.893274	2.606857	1.806720
H	-3.924247	0.536772	2.379887
H	-2.298596	1.162386	2.090726
H	-1.963695	-3.524351	-1.647971
H	-3.318734	-3.906868	-0.593450
C	-3.806918	-3.975156	-2.693130
C	-3.766980	-1.738065	-3.868481
H	-3.164997	-0.065580	-2.618787
H	-1.910844	-1.252376	-2.872455

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Ru	-0.062923	-0.805863	-0.148097
P	2.393486	-1.075070	-0.102789
P	-2.459344	-1.013410	0.103349
H	-0.040907	-2.476470	-0.056281
H	-0.001725	-1.185267	1.380601
H	-0.151830	-2.271781	-0.973143
C	3.681891	0.165662	-0.722685
C	2.892861	-1.283717	1.732600
C	2.868569	-2.727796	-0.916435
C	-2.981116	-2.000128	1.644586
C	-3.385914	0.639711	0.271050
C	-3.328983	-1.856656	-1.358044
H	4.646750	-0.220574	-0.363698
C	3.793282	0.300937	-2.256276
C	3.452427	1.559945	-0.099618
H	2.271817	-0.511822	2.207878
C	4.358720	-1.020865	2.148248
C	2.431677	-2.642622	2.305800
H	2.331136	-3.450686	-0.284832
C	4.362470	-3.121420	-0.893084
C	2.304944	-2.903132	-2.347847
H	-2.750642	-1.289685	2.450604
C	-4.484418	-2.345963	1.740642
C	-2.122805	-3.252791	1.935583
H	-2.762141	1.296947	-0.345597
C	-4.831621	0.717739	-0.272741
C	-3.327547	1.179142	1.717390
H	-4.407243	-1.749240	-1.175969
C	-3.041325	-3.366686	-1.502923
C	-2.986760	-1.142530	-2.685039
H	2.845586	0.669271	-2.664702
H	3.997351	-0.668999	-2.718329
C	4.929179	1.270379	-2.636085
C	4.586463	2.531470	-0.467841
H	3.372916	1.490459	0.990973
H	2.498065	1.956544	-0.456765
H	4.704572	-0.046961	1.790207
H	5.024068	-1.771482	1.701762
C	4.515637	-1.068800	3.680425
C	2.581493	-2.689976	3.835879
H	3.034902	-3.452106	1.870175
H	1.389269	-2.832996	2.031507
H	4.768042	-3.046360	0.120332
H	4.940341	-2.423092	-1.513475
C	4.576516	-4.554260	-1.418401
C	2.506142	-4.340840	-2.856070
H	2.806144	-2.215361	-3.038562
H	1.242780	-2.642254	-2.378033
H	-5.098738	-1.451718	1.599870
H	-4.758722	-3.042138	0.936073
C	-4.838228	-2.987455	3.095681
C	-2.483459	-3.876640	3.295263
H	-2.265374	-4.009256	1.153597

H	5.891141	0.841344	-2.315829
H	4.980254	1.365668	-3.728927
C	4.750469	2.650068	-1.989225
H	4.381831	3.517306	-0.030135
H	5.531725	2.180771	-0.025055
H	3.941290	-0.242447	4.123534
H	5.566585	-0.897010	3.948164
C	4.024632	-2.397899	4.268700
H	1.906325	-1.947493	4.285312
H	2.261783	-3.671857	4.209174
H	5.648502	-4.791408	-1.418439
H	4.100384	-5.263996	-0.725345
C	3.985900	-4.747099	-2.821491
H	1.923797	-5.033565	-2.229546
H	2.108951	-4.432405	-3.875390
H	-4.688173	-2.245540	3.894046
H	-5.904071	-3.250676	3.111464
C	-3.975628	-4.221836	3.386691
H	-2.225545	-3.168381	4.096725
H	-1.871995	-4.773037	3.462634
H	-4.825116	2.809656	-0.829818
H	-6.433433	2.158074	-0.531299
C	-5.327739	2.684727	1.268491
H	-3.254564	3.286054	1.225995
H	-3.857496	2.953175	2.848392
H	-4.886733	-3.922586	-2.488313
H	-3.559282	-5.041122	-2.782277
C	-3.507611	-3.243992	-4.008475
H	-3.490849	-1.215178	-4.793361
H	-4.844238	-1.566289	-3.722279
H	3.853903	3.126188	-2.406973
H	5.601064	3.299727	-2.234799
H	4.678646	-3.211682	3.920596
H	4.101969	-2.382201	5.363628
H	4.546128	-4.128822	-3.538685
H	4.107123	-5.788843	-3.145387
H	-4.211524	-5.010366	2.656200
H	-4.216348	-4.630561	4.376593
H	-5.991834	2.089632	1.913476
H	-5.697764	3.717582	1.306821
H	-2.453545	-3.404235	-4.280182
H	-4.108887	-3.666100	-4.824185
C	0.616098	4.070404	2.339492
C	0.677396	2.844206	3.348589
B	0.234571	2.079372	1.199498
O	0.178258	1.746060	2.563594
O	0.611720	3.429869	1.051505
O	-0.040362	1.283665	0.181204
C	-0.203820	2.989390	4.593436
H	-0.120665	2.084465	5.204792
H	0.110694	3.842076	5.206968
H	-1.256445	3.118939	4.330947
C	2.105891	2.486684	3.788665
H	2.538059	3.252385	4.442454

H	2.077947	1.541169	4.340299	H	-2.971378	1.986498	2.109225
H	2.767698	2.354970	2.927913	C	-3.631734	3.871310	1.268964
C	1.816767	5.019230	2.404407	C	-3.986082	3.841046	-1.235572
H	1.698882	5.806240	1.651748	H	-3.602707	1.940039	-2.188243
H	1.891074	5.500786	3.386574	H	-2.156162	2.705209	-1.515623
H	2.755317	4.499122	2.198813	H	-5.088261	0.146475	-1.670399
C	-0.677662	4.891817	2.454065	H	-5.062349	-1.500944	-1.046787
H	-0.726364	5.451217	3.394926	C	-5.024483	-1.392126	-3.199899
H	-0.715538	5.609189	1.627596	C	-2.891235	-2.758755	-3.243850
H	-1.562505	4.253955	2.384609	H	-2.872115	-2.873919	-1.087543
C	0.295685	3.270784	-3.137866	H	-1.415022	-2.154732	-1.761789
C	-1.248516	3.215599	-2.766548	H	-5.294040	-0.533601	0.843921
B	-0.204019	1.288355	-2.096694	H	-4.635684	0.385796	2.187300
H	-0.063452	0.086531	-2.002221	C	-5.230165	-1.618688	2.714814
O	-1.438667	1.826836	-2.374848	C	-2.908433	-2.101037	3.586752
O	0.841231	2.090969	-2.485553	H	-2.230946	-0.114799	3.056015
C	-1.628322	4.093936	-1.568704	H	-1.308420	-1.409440	2.296432
H	-1.552307	5.158259	-1.817960	H	5.377070	-0.145225	-0.710908
H	-2.669128	3.887239	-1.298094	H	4.902889	-1.835358	-0.775896
H	-0.998655	3.889231	-0.700768	C	5.573701	-1.039593	-2.669853
C	-2.200496	3.499521	-3.930985	C	3.385581	-1.678447	-3.765933
H	-3.234706	3.392361	-3.587260	H	2.653118	-2.505609	-1.910228
H	-2.073404	4.523118	-4.301708	H	1.619164	-1.258965	-2.569225
H	-2.049536	2.806041	-4.761601	H	4.652888	0.839606	2.101391
C	0.579091	3.098437	-4.636933	H	5.344292	1.363355	0.571728
H	0.239293	3.962731	-5.217802	C	4.884527	2.985170	1.913977
H	1.658616	2.990778	-4.782447	C	3.432512	4.071436	0.142377
H	0.096558	2.199913	-5.033926	H	3.843403	2.454520	-1.226073
C	1.030193	4.501502	-2.602503	H	2.115594	2.693009	-0.896984
H	2.078299	4.469997	-2.917800	H	1.553661	-2.839501	0.954164
H	0.590563	5.423971	-2.999717	H	3.043477	-3.022912	0.041318
H	1.003627	4.532209	-1.511198	C	3.194968	-3.715528	2.080181

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Ru	-0.005545	0.190460	-0.107995	H	2.722863	0.097875	3.043182
P	-2.415206	0.050034	-0.091755	H	1.384434	-1.011999	2.773090
P	2.397311	-0.037778	0.058022	H	-4.691017	3.668049	1.488089
H	-0.014266	-0.309689	-1.708815	H	-3.245363	4.457156	2.113390
H	0.003481	0.198969	1.653529	C	-3.527792	4.677691	-0.033110
H	-0.049429	-1.373132	0.287019	H	-3.854253	4.409091	-2.165779
H	-0.041768	1.026722	1.464845	H	-5.064094	3.636580	-1.144852
C	-3.352154	1.691020	-0.028306	H	-4.675151	-0.694750	-3.975806
C	-3.102343	-0.784247	-1.649612	H	-6.117890	-1.435373	-3.289386
C	-3.196506	-0.987812	1.310644	C	-4.413036	-2.778407	-3.447403
C	3.367596	-0.483918	-1.516676	H	-2.427879	-2.143634	-4.029951
C	3.177138	1.594116	0.655812	H	-2.478892	-3.769830	-3.357600
C	2.997125	-1.277633	1.355429	H	-6.248019	-1.313049	2.990577
H	-4.416513	1.464051	0.122474	H	-5.320662	-2.599871	2.225028
C	-2.867026	2.540834	1.167830	C	-4.354044	-1.754442	3.966827
C	-3.219320	2.509258	-1.332618	H	-2.882351	-3.109701	3.147386
H	-2.709683	-0.145288	-2.454484	H	-2.275323	-2.136766	4.483055
C	-4.636257	-0.841636	-1.814711	H	5.617018	-0.060695	-3.170046
C	-2.503004	-2.191075	-1.867187	H	6.613525	-1.346435	-2.496181
H	-3.232743	-1.994859	0.869321	C	4.864902	-2.046021	-3.585924
C	-4.639030	-0.606511	1.716970	H	3.311737	-0.730853	-4.320902
C	-2.319280	-1.100927	2.576507	H	2.875594	-2.436223	-4.374924
H	3.354572	0.465105	-2.073670	H	4.170210	3.194696	2.724233
C	4.847997	-0.882758	-1.320541	H	5.882314	2.976405	2.372343
C	2.666313	-1.530642	-2.413626	C	4.792202	4.093628	0.855276
H	2.455216	1.890902	1.431789	H	2.642080	4.352031	0.854116
C	4.573629	1.599424	1.316388	H	3.409673	4.822259	-0.658088
C	3.109754	2.683462	-0.438183	H	4.295101	-3.694585	2.054828
H	4.093053	-1.193135	1.370884	H	2.898155	-4.741502	1.826129
C	2.644632	-2.742878	1.021315	C	2.717862	-3.356824	3.493830
C	2.479027	-0.935557	2.770514	H	2.653081	-1.631850	4.818721
H	-1.796353	2.745127	1.039031	H	4.140170	-1.772658	3.885072
				H	-2.483107	4.984881	-0.184886
				H	-4.120728	5.598864	0.039502

H	-4.861485	-3.499400	-2.747387
H	-4.660447	-3.129641	-4.457532
H	-4.365923	-0.803239	4.519788
H	-4.766536	-2.514438	4.642985
H	4.935509	-3.050536	-3.142728
H	5.369707	-2.097492	-4.559221
H	5.591969	3.948945	0.113185
H	4.969069	5.074399	1.315859
H	1.629563	-3.503817	3.557116
H	3.169216	-4.031375	4.232913
C	0.074323	1.211058	-2.230809
O	0.032847	2.139025	-1.345767
H	-0.810729	1.046451	-2.869194
H	1.024498	1.014128	-2.754180

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Ru	0.000011	-0.008449	0.032063
P	2.430016	0.007331	0.015571
P	-2.389583	-0.083198	-0.124427
H	-1.605274	1.578813	2.537740
H	0.018196	-0.814020	-1.383282
H	-0.026715	-1.600226	-0.070540
H	-0.061468	0.758082	-1.358062
C	3.182761	1.671762	-0.463638
C	3.026930	-0.280507	1.779086
C	3.385609	-1.277115	-1.011262
C	-3.356431	-0.394577	1.482142
C	-3.081372	1.539165	-0.815739
C	-3.084527	-1.360704	-1.336373
H	4.274704	1.547811	-0.478255
C	2.731329	2.090757	-1.880632
C	2.847826	2.785458	0.553631
H	2.473721	0.504493	2.311017
C	4.533130	-0.126977	2.067249
C	2.513938	-1.627306	2.334422
H	3.466957	-2.126444	-0.316113
C	4.822317	-0.877851	-1.420909
C	2.615958	-1.792606	-2.246940
H	-3.447445	0.613756	1.913680
C	-4.784064	-0.973416	1.363683
C	-2.530054	-1.239545	2.479277
H	-2.582309	1.591839	-1.794265
C	-4.602044	1.636974	-1.054615
C	-2.593913	2.764765	-0.015023
H	-4.178033	-1.298866	-1.245320
C	-2.667677	-2.804962	-0.980625
C	-2.723461	-1.057463	-2.807573
H	1.636069	2.164579	-1.892567
H	2.995891	1.321210	-2.616084
C	3.339255	3.439412	-2.300821
C	3.450386	4.135768	0.126880
H	3.224553	2.520781	1.547814
H	1.759950	2.867996	0.656085
H	4.911506	0.830198	1.689380
H	5.093485	-0.916216	1.546700
C	4.820920	-0.239673	3.575794
C	2.806299	-1.754697	3.839712
H	2.997990	-2.463628	1.807541
H	1.437833	-1.717904	2.152239
H	5.396305	-0.526181	-0.558147
H	4.780957	-0.041521	-2.131610
C	5.563831	-2.049748	-2.088254
C	3.357270	-2.957006	-2.926315
H	2.481947	-0.974494	-2.969032
H	1.612194	-2.108961	-1.952974
H	-5.397442	-0.382469	0.676563

H	-4.739013	-1.988793	0.947927
C	-5.472076	-1.038506	2.740525
C	-3.213999	-1.313391	3.854694
H	-2.408554	-2.257280	2.082594
H	-1.521845	-0.826150	2.575906
H	-4.969554	0.782724	-1.635374
H	-5.126243	1.613541	-0.089620
C	-4.969217	2.946700	-1.777227
C	-2.961844	4.078616	-0.726517
H	-3.052432	2.761693	0.984332
H	-1.511181	2.705932	0.134479
H	-1.574999	-2.883090	-1.028718
H	-2.949777	-3.048048	0.049863
C	-3.297065	-3.830506	-1.939572
C	-3.344882	-2.087322	-3.767996
H	-3.062025	-0.055360	-3.093980
H	-1.631809	-1.063730	-2.918471
H	4.431963	3.339047	-2.385417
H	2.973591	3.714843	-3.298754
C	3.009032	4.541956	-1.285630
H	3.167438	4.909728	0.852329
H	4.548830	4.069470	0.155157
H	4.337818	0.599144	4.098044
H	5.899396	-0.143538	3.758462
C	4.298378	-1.564734	4.149387
H	2.223866	-0.994516	4.380088
H	2.462894	-2.731570	4.204858
H	6.572418	-1.729618	-2.381162
H	5.694243	-2.860288	-1.355693
C	4.796543	-2.583038	-3.305869
H	3.377647	-3.816983	-2.239844
H	2.800015	-3.281905	-3.814661
H	-5.611379	-0.016482	3.123334
H	-6.476001	-1.469606	2.631567
C	-4.648220	-1.851129	3.749273
H	-3.234272	-0.307205	4.299486
H	-2.620380	-1.941010	4.531981
H	-4.523388	2.941184	-2.782932
H	-6.056680	3.000604	-1.918452
C	-4.468677	4.175559	-1.004895
H	-2.412878	4.136497	-1.678160
H	-2.629956	4.933084	-0.122571
H	-4.390982	-3.820969	-1.818974
H	-2.962493	-4.840697	-1.670013
C	-2.946937	-3.523182	-3.401702
H	-3.043098	-1.857325	-4.798123
H	-4.441281	-1.997207	-3.736837
H	1.923746	4.721588	-1.288020
H	3.484731	5.487076	-1.578302
H	4.868468	-2.396941	3.709252
H	4.472252	-1.606392	5.232484
H	4.775838	-1.808134	-4.086777
H	5.316941	-3.447775	-3.737554
H	-4.616721	-2.901923	3.424608
H	-5.134907	-1.842639	4.733091
H	-5.009263	4.244335	-0.048982
H	-4.697818	5.094406	-1.559872
H	-1.863839	-3.647416	-3.547900
H	-3.438789	-4.239346	-4.072631
C	-0.523659	1.772199	2.632300
O	0.267565	1.092951	1.712590
H	-0.235742	1.500519	3.664013
H	-0.385464	2.865293	2.543222

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Ru	-0.006800	-0.097017	-0.174436
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P	2.412719	0.067382	-0.035169
P	-2.431622	-0.038683	0.093001
H	-0.019123	1.616025	-0.399197
H	0.035075	0.094269	1.389097
C	3.399529	-0.738210	-1.433060
C	2.991231	1.871807	-0.065870
C	3.215478	-0.607862	1.560274
C	-3.400799	1.532828	-0.377078
C	-3.214551	-1.419676	-0.953009
C	-3.021674	-0.449773	1.839951
H	4.459079	-0.663079	-1.154684
C	3.053376	-2.235850	-1.582723
C	3.224047	-0.028618	-2.793489
H	2.550514	2.246710	-0.999974
C	4.511030	2.135898	-0.125005
C	2.366270	2.701109	1.077680
H	3.201148	0.271613	2.220469
C	4.687862	-1.065077	1.433395
C	2.393487	-1.704765	2.269896
H	-3.443659	1.461591	-1.475059
C	-4.856736	1.607085	0.142925
C	-2.684236	2.861806	-0.043641
H	-2.596922	-2.281160	-0.662223
C	-4.685107	-1.826970	-0.715610
C	-2.974764	-1.197160	-2.462812
H	-4.119784	-0.436541	1.797595
C	-2.580882	0.595710	2.888356
C	-2.582385	-1.859863	2.289124
H	1.994237	-2.333448	-1.853057
H	3.177505	-2.764989	-0.630766
C	3.915884	-2.906978	-2.665603
C	4.087838	-0.692623	-3.881232
H	3.489395	1.032440	-2.720067
H	2.170459	-0.073007	-3.091606
H	4.987432	1.560998	-0.927629
H	4.977097	1.814031	0.816073
C	4.798583	3.635733	-0.328078
C	2.646640	4.201524	0.885964
H	2.789940	2.381670	2.041315
H	1.288875	2.519363	1.123480
H	5.304094	-0.300588	0.950930
H	4.740474	-1.957982	0.796374
C	5.289065	-1.410824	2.808233
C	2.994152	-2.060010	3.641210
H	2.359764	-2.609017	1.647112
H	1.359448	-1.372555	2.390924
H	-5.406869	0.685831	-0.063155
H	-4.846757	1.726446	1.235011
C	-5.610216	2.799875	-0.474643
C	-3.425715	4.061512	-0.658510
H	-2.635757	2.992523	1.045830
H	-1.652153	2.843209	-0.394612
H	-4.888964	-1.985712	0.349372
H	-5.355203	-1.026368	-1.052475
C	-5.026100	-3.105170	-1.504903
C	-3.330668	-2.455624	-3.274020
H	-3.596124	-0.359982	-2.814093
H	-1.934373	-0.917003	-2.649797
H	-1.484532	0.639158	2.909529
H	-2.926372	1.596289	2.607957
C	-3.112296	0.250696	4.291532
C	-3.121075	-2.203534	3.688730
H	-2.915129	-2.621609	1.575266
H	-1.487391	-1.903123	2.303942
H	4.970399	-2.894849	-2.351151
H	3.630958	-3.962473	-2.762246
C	3.779834	-2.190443	-4.016345

H	3.927963	-0.182395	-4.839814
H	5.151448	-0.561205	-3.631131
H	4.409268	3.946085	-1.308812
H	5.883082	3.804628	-0.354257
C	4.150400	4.490371	0.770560
H	2.135404	4.544746	-0.024829
H	2.213767	4.768444	1.720421
H	6.326978	-1.745267	2.680854
H	5.327936	-0.501171	3.425970
C	4.464898	-2.483041	3.532374
H	2.917391	-1.185676	4.305338
H	2.400408	-2.857312	4.106588
H	-5.698105	2.646676	-1.560569
H	-6.634478	2.831692	-0.080484
C	-4.890270	4.127305	-0.203982
H	-3.386442	3.983165	-1.755279
H	-2.901848	4.989489	-0.396211
H	-4.414153	-3.937454	-1.127172
H	-6.073694	-3.381754	-1.327931
C	-4.768991	-2.922100	-3.007696
H	-2.631197	-3.261089	-3.006294
H	-3.185632	-2.259245	-4.344138
H	-4.210719	0.319113	4.291511
H	-2.754487	0.997052	5.012624
C	-2.694341	-1.159175	4.728734
H	-2.770196	-3.201486	3.981418
H	-4.219810	-2.255877	3.655560
H	2.752263	-2.315153	-4.388344
H	4.441236	-2.650430	-4.761802
H	4.636276	4.267962	1.732554
H	4.322238	5.556368	0.573429
H	4.529309	-3.427679	2.972115
H	4.883769	-2.679863	4.527607
H	-4.925455	4.342546	0.874510
H	-5.412008	4.953388	-0.704173
H	-5.471458	-2.173048	-3.403162
H	-4.973835	-3.856459	-3.545935
H	-1.601175	-1.192437	4.846067
H	-3.123163	-1.397953	5.710510
C	0.033780	1.716003	-2.234816
O	-0.070878	0.577317	-2.602593
O	0.148662	2.884443	-2.376873
O	-0.023457	-3.140532	0.137347
C	-0.005831	-1.979023	0.034762

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C	-0.174952	1.157924	2.704423
H	-0.281940	2.203319	3.074674
O	-0.205868	1.075631	1.420179
O	-0.049329	0.248319	3.528354
Ru	0.034090	-0.750487	0.170611
C	0.173213	-2.403669	0.862044
P	-2.383842	-1.058925	-0.077817
P	2.488333	-0.568227	0.051177
H	0.163077	-1.513192	-1.232246
O	0.264049	-3.473851	1.326340
C	-2.979874	-2.726116	-0.782492
C	-3.107147	0.192671	-1.298768
C	-3.421469	-0.811303	1.484993
C	3.248557	-2.245065	-0.419943
C	3.039907	0.762536	-1.166646
C	3.408996	-0.124070	1.636096
H	-3.913426	-2.470960	-1.303842
C	-2.009316	-3.325642	-1.826528
C	-3.339149	-3.812308	0.257161
H	-2.864693	1.155467	-0.828850
C	-2.417680	0.179019	-2.681262

C	-4.639257	0.133954	-1.497449	H	6.212002	-4.076469	-0.200774
H	-4.405787	-1.260868	1.280817	H	4.612911	-4.583165	0.333544
C	-3.639491	0.682877	1.827010	H	4.563692	3.079275	-1.602450
C	-2.784168	-1.539573	2.695085	H	5.965359	2.283356	-2.314153
H	2.694559	-2.932257	0.234334	C	4.164061	2.181790	-3.531930
C	2.931817	-2.664495	-1.871835	H	2.168694	1.897880	-4.348170
C	4.750007	-2.474295	-0.128924	H	2.211912	2.831880	-2.851748
H	2.660349	1.671811	-0.676798	H	5.056285	1.546438	3.237812
C	4.564202	0.930210	-1.352671	H	3.797643	2.709492	3.643709
C	2.350390	0.696989	-2.548864	C	3.496073	0.726203	4.492290
H	4.474870	-0.302037	1.436772	H	3.335033	-1.406563	4.886747
C	3.264052	1.362391	2.033931	H	4.777884	-0.945695	3.982671
C	2.966936	-1.062832	2.782606	H	-2.110048	-6.026502	-1.014269
H	-1.079611	-3.617282	-1.324274	H	-3.497502	-6.482358	-2.000477
H	-1.726544	-2.581300	-2.576784	H	-4.730342	2.263582	-4.268136
C	-2.617996	-4.558595	-2.516991	H	-4.711735	0.502845	-4.304472
C	-3.946574	-5.052154	-0.424826	H	-2.848616	0.553615	4.537080
H	-2.437462	-4.110365	0.807438	H	-4.453154	0.226308	5.200837
H	-4.053119	-3.430126	0.993034	H	5.026427	-5.457161	-1.945252
H	-1.328300	0.194109	-2.571202	H	5.407748	-3.841493	-2.534029
H	-2.665897	-0.752114	-3.208654	H	4.359223	3.117017	-4.072482
C	-2.885348	1.370972	-3.534866	H	4.578955	1.371600	-4.150348
C	-5.125387	1.323043	-2.347213	H	2.427844	0.893619	4.683013
H	-4.911634	-0.797870	-2.012106	H	4.033115	0.951630	5.423056
H	-5.168523	0.126236	-0.538760	C	0.211059	5.047707	-0.460775
H	-2.665911	1.169559	1.937661	C	-1.324016	4.795027	-0.166295
H	-4.155181	1.201777	1.012341	B	-0.319169	2.861490	-0.832980
C	-4.457809	0.854476	3.119997	H	-0.190377	1.741349	-1.204267
C	-3.629742	-1.370251	3.968597	O	-1.540451	3.470831	-0.744881
H	-2.652752	-2.604975	2.486989	O	0.739464	3.692398	-0.591561
H	-1.785512	-1.128626	2.879466	C	-1.651518	4.680756	1.326725
H	1.872443	-2.501714	-2.094712	H	-1.555403	5.645792	1.835433
H	3.508161	-2.036278	-2.564025	H	-2.683952	4.335033	1.438535
C	3.305548	-4.134495	-2.123086	H	-1.000974	3.953568	1.819462
H	4.992534	-2.225753	0.908963	C	-2.284472	5.771998	-0.842638
H	5.362005	-1.819795	-0.763005	H	-3.316125	5.490549	-0.607995
C	5.138930	-3.942975	-0.389797	H	-2.122912	6.793510	-0.479729
H	5.079381	0.978677	-0.386714	H	-2.172717	5.766154	-1.929304
H	4.965507	0.054123	-1.879682	C	0.471709	5.745485	-1.802410
C	4.880205	2.194219	-2.173335	H	0.159133	6.794731	-1.779354
C	2.652420	1.965965	-3.364803	H	1.544379	5.711831	-2.017360
H	2.705390	-0.177573	-3.106288	H	-0.052292	5.245091	-2.622864
H	1.269235	0.572093	-2.433629	C	0.977651	5.754850	0.655493
H	2.205668	1.623789	2.106317	H	2.030598	5.851594	0.371561
H	3.690928	2.006862	1.256589	H	0.579901	6.761862	0.826221
C	3.969079	1.660005	3.369856	H	0.931352	5.196757	1.592980
C	3.701403	-0.741379	4.094877				
H	1.889177	-0.949077	2.946310	50			
H	3.146203	-2.110483	2.507924	C	0.097393	-1.211604	2.939077
H	-3.504608	-4.255691	-3.094506	H	0.175474	-2.220965	3.406496
H	-1.899462	-4.965568	-3.240268	O	0.175599	-1.245987	1.655049
C	-3.016719	-5.633678	-1.497093	O	-0.042934	-0.228955	3.670045
H	-4.174937	-5.810252	0.335335	Ru	0.020437	0.500390	0.220350
H	-4.906135	-4.774653	-0.886626	C	-0.046608	2.050269	1.170933
H	-2.567583	2.303322	-3.048501	P	2.450302	0.800704	-0.034978
H	-2.394356	1.338479	-4.516454	P	-2.441827	0.543389	0.026906
C	-4.411750	1.376294	-3.706013	H	-0.054236	1.390654	-1.112124
H	-6.212013	1.256215	-2.489017	O	-0.089312	3.058050	1.756352
H	-4.935733	2.256925	-1.798828	C	3.034859	2.518130	-0.632651
H	-4.558632	1.924784	3.344519	C	3.186923	-0.327671	-1.367438
H	-5.477911	0.474198	2.955339	C	3.506304	0.418027	1.486886
C	-3.827461	0.112569	4.305840	C	-3.059771	2.334532	-0.119346
H	-4.611061	-1.852545	3.835547	C	-3.059573	-0.475062	-1.442833
H	-3.134872	-1.887374	4.800095	C	-3.462651	-0.116089	1.467819
H	2.678788	-4.780627	-1.491174	H	3.929445	2.290642	-1.229139
H	3.080508	-4.400766	-3.164060	C	2.018782	3.209611	-1.569942
C	4.786156	-4.394361	-1.813623	C	3.481218	3.516032	0.458852

H	2.908018	-1.330627	-1.023801
C	2.541920	-0.134654	-2.758089
C	4.726017	-0.289748	-1.512377
H	4.514972	0.809369	1.281776
C	3.616827	-1.105648	1.733625
C	2.958036	1.112722	2.756639
H	-2.550204	2.807918	0.731272
C	-2.571556	3.067909	-1.387690
C	-4.572441	2.593572	0.070771
H	-2.736177	-1.483241	-1.150169
C	-4.587252	-0.526224	-1.666005
C	-2.349242	-0.161146	-2.779501
H	-4.518052	0.056926	1.214075
C	-3.277885	-1.637398	1.667560
C	-3.150702	0.662276	2.767540
H	1.125486	3.474078	-0.992926
H	1.678011	2.526768	-2.353373
C	2.612266	4.480050	-2.202036
C	4.072508	4.794267	-0.164591
H	2.623556	3.787217	1.087940
H	4.231968	3.065776	1.115699
H	1.449666	-0.137992	-2.681348
H	2.824242	0.846109	-3.164428
C	3.009564	-1.228303	-3.734165
C	5.211213	-1.379823	-2.486920
H	5.042744	0.689401	-1.897668
H	5.222128	-0.419478	-0.545007
H	2.607902	-1.515588	1.846674
H	4.064418	-1.612081	0.872016
C	4.459313	-1.420843	2.983104
C	3.828567	0.805670	3.987091
H	2.899788	2.194864	2.617228
H	1.937232	0.769074	2.951488
H	-1.505689	2.883047	-1.549970
H	-3.103285	2.673492	-2.264172
C	-2.842767	4.579024	-1.290020
H	-4.952214	2.100862	0.970833
H	-5.133177	2.179640	-0.776772
C	-4.857208	4.104720	0.169130
H	-5.117211	-0.754361	-0.734683
H	-4.944596	0.456281	-2.000509
C	-4.949870	-1.575645	-2.733403
C	-2.703876	-1.209755	-3.848351
H	-2.653578	0.828345	-3.142245
H	-1.264903	-0.116194	-2.638941
H	-2.214326	-1.861492	1.792424
H	-3.602730	-2.180615	0.772178
C	-4.072681	-2.150390	2.882172
C	-3.971914	0.131068	3.954694
H	-2.085354	0.571721	3.006204
H	-3.360769	1.730795	2.635192
H	3.457437	4.206077	-2.851796
H	1.862271	4.952072	-2.849953
C	3.092117	5.469531	-1.132183
H	4.362049	5.488915	0.634362
H	4.996478	4.537154	-0.704301
H	2.655271	-2.202934	-3.369360
H	2.548870	-1.070970	-4.718304
C	4.539735	-1.253562	-3.861735
H	6.302894	-1.324922	-2.589403
H	4.985907	-2.368144	-2.060483
H	4.479576	-2.507465	3.142327
H	5.501446	-1.114404	2.803296
C	3.931329	-0.704683	4.232662
H	4.837509	1.224285	3.845825
H	3.400220	1.305470	4.864693
H	-2.250886	4.998061	-0.463320

H	-2.498376	5.076763	-2.205963
C	-4.331539	4.869698	-1.053507
H	-5.936225	4.268652	0.287659
H	-4.379603	4.499356	1.077945
H	-4.678658	-2.574516	-2.360966
H	-6.036452	-1.585005	-2.890027
C	-4.221328	-1.312330	-4.059302
H	-2.204944	-0.958760	-4.793639
H	-2.311877	-2.188483	-3.535504
H	-5.150400	-2.059271	2.676203
H	-3.873662	-3.221627	3.020969
C	-3.739524	-1.370817	4.161711
H	-3.699626	0.687577	4.860099
H	-5.043746	0.314965	3.780052
H	2.223775	5.838873	-0.567261
H	3.558960	6.346131	-1.599650
H	4.856085	-2.075528	-4.516887
H	4.876534	-0.323269	-4.343251
H	2.933572	-1.090423	4.482868
H	4.580071	-0.913519	5.093485
H	-4.497665	5.947393	-0.928486
H	-4.903528	4.565791	-1.943202
H	-4.455554	-2.100836	-4.786155
H	-4.589719	-0.369754	-4.491086
H	-2.686238	-1.531048	4.428698
H	-4.343672	-1.741931	5.000067
C	-0.572409	-4.469516	-0.678732
C	0.975442	-4.397503	-0.347179
B	0.143133	-2.308012	-0.670146
H	0.117649	-1.136766	-0.967749
O	1.307281	-3.015578	-0.698289
O	-0.985685	-3.067696	-0.603598
C	1.296372	-4.564234	1.142118
H	1.098203	-5.586310	1.481654
H	2.357717	-4.349862	1.301319
H	0.719930	-3.862940	1.749278
C	1.860134	-5.320510	-1.183198
H	2.909395	-5.153996	-0.919658
H	1.625034	-6.371709	-0.981416
H	1.747660	-5.137385	-2.254268
C	-0.874799	-4.930041	-2.110326
H	-0.640279	-5.990432	-2.250051
H	-1.940560	-4.785026	-2.312906
H	-0.309101	-4.349208	-2.845653
C	-1.410066	-5.267018	0.318760
H	-2.464129	-5.226923	0.025935
H	-1.102361	-6.318857	0.332114
H	-1.324511	-4.864189	1.329846

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C	0.126665	-1.471818	2.789597
H	0.196218	-2.528316	3.132308
O	0.222279	-1.342886	1.507998
O	-0.018709	-0.579363	3.623414
Ru	0.010709	0.514463	0.209487
C	-0.087686	2.035468	1.208833
P	2.430211	0.861629	-0.031474
P	-2.450970	0.501387	0.029891
H	-0.089518	1.448057	-1.084824
O	-0.154814	3.017967	1.834110
C	2.983785	2.611090	-0.554699
C	3.191133	-0.214225	-1.390456
C	3.482464	0.455105	1.488561
C	-3.109437	2.282176	-0.076295
C	-3.046978	-0.499437	-1.458401
C	-3.452440	-0.204196	1.464125
H	3.910024	2.432999	-1.118572

C	1.982404	3.299104	-1.509978	H	3.272001	1.184660	4.900686
C	3.350722	3.585690	0.586985	H	-2.366488	4.965255	-0.420218
H	2.961345	-1.231009	-1.050096	H	-2.664368	5.052794	-2.154639
C	2.510908	-0.045133	-2.767253	C	-4.459658	4.799404	-0.952630
C	4.723657	-0.105348	-1.563514	H	-6.010231	4.156297	0.431988
H	4.472435	0.906348	1.318050	H	-4.435590	4.415321	1.176075
C	3.671249	-1.069599	1.670501	H	-4.664423	-2.576070	-2.436904
C	2.878723	1.063829	2.777791	H	-6.013942	-1.570201	-2.956208
H	-2.583012	2.756973	0.763050	C	-4.186986	-1.278249	-4.102428
C	-2.674121	3.036468	-1.351769	H	-2.161764	-0.920001	-4.809775
C	-4.619913	2.511245	0.164421	H	-2.287405	-2.175910	-3.580161
H	-2.723328	-1.510815	-1.175054	H	-5.156135	-2.148253	2.642906
C	-4.572119	-0.543716	-1.696764	H	-3.898166	-3.346905	2.926343
C	-2.320019	-0.164707	-2.781013	C	-3.703578	-1.536927	4.122525
H	-4.509292	-0.006677	1.236510	H	-3.605390	0.496781	4.884741
C	-3.294385	-1.733634	1.612247	H	-4.979181	0.187607	3.822475
C	-3.100477	0.526159	2.781170	H	2.049393	5.896272	-0.410338
H	1.057915	3.511224	-0.961005	H	3.404536	6.487643	-1.369354
H	1.698349	2.632874	-2.329765	H	4.873820	-1.882350	-4.571866
C	2.553391	4.611587	-2.073486	H	4.819836	-0.130944	-4.397820
C	3.918792	4.904985	0.031218	H	2.933365	-1.211827	4.402122
H	2.460887	3.804074	1.190984	H	4.556671	-0.981962	5.056509
H	4.092384	3.139958	1.256916	H	-4.644034	5.872566	-0.814991
H	1.421765	-0.097633	-2.668326	H	-5.051137	4.489629	-1.827388
H	2.742697	0.947070	-3.177736	H	-4.417875	-2.048900	-4.849166
C	3.007346	-1.117431	-3.752572	H	-4.547012	-0.324289	-4.515994
C	5.239345	-1.171082	-2.549296	H	-2.648874	-1.726434	4.363273
H	4.986766	0.887422	-1.954036	H	-4.299459	-1.922562	4.960202
H	5.243864	-0.211176	-0.605442	C	-0.451588	-4.442943	-0.704594
H	2.685786	-1.541032	1.740887	C	1.104465	-4.343862	-0.418247
H	4.164037	-1.509947	0.797763	B	0.188407	-2.258388	-0.506064
C	4.504606	-1.395921	2.923223	H	0.109772	-1.112961	-0.916461
C	3.741347	0.746461	4.011190	O	1.376094	-2.929926	-0.649563
H	2.766275	2.146963	2.684796	O	-0.913088	-3.077490	-0.485314
H	1.874184	0.658595	2.937501	C	1.487380	-4.652332	1.034036
H	-1.609470	2.876270	-1.546029	H	1.362776	-5.715759	1.264451
H	-3.222262	2.638122	-2.216349	H	2.539052	-4.389756	1.185450
C	-2.972883	4.540994	-1.233706	H	0.891942	-4.066985	1.737593
H	-4.958751	2.010308	1.076220	C	1.988203	-5.153640	-1.367317
H	-5.201453	2.087215	-0.663883	H	3.040766	-4.982963	-1.119150
C	-4.932165	4.015892	0.279574	H	1.788849	-6.226662	-1.266463
H	-5.110489	-0.789569	-0.774628	H	1.837070	-4.868026	-2.410906
H	-4.923459	0.447278	-2.012868	C	-0.785578	-4.783071	-2.163398
C	-4.928810	-1.568315	-2.789714	H	-0.519869	-5.816398	-2.410212
C	-2.671094	-1.188368	-3.874894	H	-1.862160	-4.660279	-2.318149
H	-2.610415	0.834801	-3.127026	H	-0.266634	-4.114961	-2.857813
H	-1.237227	-0.134171	-2.626052	C	-1.223129	-5.368207	0.235823
H	-2.235273	-1.987089	1.708595	H	-2.287650	-5.343263	-0.018835
H	-3.647048	-2.241970	0.707402	H	-0.876233	-6.403406	0.138154
C	-4.077054	-2.268012	2.825625	H	-1.119482	-5.061598	1.278680
C	-3.908390	-0.024707	3.968311				
H	-2.032761	0.403681	2.993594				
H	-3.288001	1.602872	2.685430				
H	3.433506	4.391220	-2.696565				
H	1.813012	5.079255	-2.735464				
C	2.952737	5.578728	-0.951494				
H	4.152088	5.580794	0.863965				
H	4.871377	4.699130	-0.480117				
H	2.702930	-2.106062	-3.380562				
H	2.521423	-0.981570	-4.727729				
C	4.534361	-1.075101	-3.910026				
H	6.324915	-1.065188	-2.674270				
H	5.069429	-2.169112	-2.119708				
H	4.581015	-2.486055	3.033817				
H	5.531560	-1.025966	2.779929				
C	3.915331	-0.766455	4.191825				
H	4.730120	1.220873	3.909192				

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C	0.089448	1.255387	2.290046
H	-0.116294	1.468267	3.360610
O	0.424527	2.190419	1.547830
O	-0.049048	0.018680	1.982004
Ru	0.125153	-0.552261	-0.117609
P	-2.245992	-1.266310	-0.027619
P	2.582078	-0.354974	0.053765
C	-2.655484	-2.912497	-0.912846
C	-3.507625	-0.077227	-0.804375
C	-2.954559	-1.522095	1.713994
C	3.564320	-1.677427	-0.917002
C	3.209039	1.371543	-0.397956
C	3.294553	-0.749614	1.769261
H	-3.716931	-2.813505	-1.179573
C	-1.858718	-3.108804	-2.220847

C	-2.533403	-4.189080	-0.052567	H	3.551328	-4.214639	-2.157181
H	-3.339305	0.854723	-0.247822	H	3.232924	-3.634237	-3.788867
C	-3.219618	0.238596	-2.289045	C	5.186152	-3.084565	-3.003589
C	-4.995220	-0.472463	-0.650339	H	6.869748	-2.366820	-1.825058
H	-3.870135	-2.115594	1.564497	H	5.771048	-3.427780	-0.947463
C	-3.360099	-0.204089	2.415415	H	4.234951	3.861037	0.332526
C	-2.012455	-2.312456	2.656093	H	5.922726	3.536596	-0.061379
H	3.497796	-2.536084	-0.233542	C	4.600000	3.614833	-1.788645
C	2.937587	-2.141844	-2.245224	H	3.021052	3.365596	-3.261809
C	5.067354	-1.384210	-1.123649	H	2.439905	3.783300	-1.654436
H	2.531365	1.993047	0.204655	H	5.065211	-0.161132	3.839635
C	4.661925	1.769214	-0.048711	H	3.934890	0.724757	4.859379
C	2.922128	1.697449	-1.883073	C	3.490848	-1.396074	4.677591
H	4.365097	-0.920017	1.578902	H	3.017459	-3.412124	4.014325
C	3.196080	0.343693	2.854634	H	4.503145	-2.757455	3.332959
C	2.705981	-2.059935	2.344659	H	-1.184256	-5.833973	-1.926084
H	-0.797560	-3.224273	-1.968880	H	-2.630985	-6.484590	-2.693764
H	-1.927612	-2.229976	-2.865938	H	-6.253732	1.853873	-2.935931
C	-2.331621	-4.349290	-2.998230	H	-5.881151	0.163675	-3.261633
C	-3.001128	-5.437394	-0.823887	H	-2.280837	-0.743881	4.985422
H	-1.486928	-4.326193	0.253313	H	-3.704818	-1.565584	5.621262
H	-3.126997	-4.103162	0.862104	H	5.697930	-3.984203	-3.368742
H	-2.175004	0.528318	-2.427641	H	5.330550	-2.308335	-3.769680
H	-3.384862	-0.659906	-2.899116	H	4.732481	4.691157	-1.959675
C	-4.137942	1.360438	-2.804181	H	5.335385	3.104347	-2.429163
C	-5.922049	0.649047	-1.155707	H	2.471084	-1.249692	5.062409
H	-5.199626	-1.380870	-1.234025	H	4.106708	-1.706230	-5.531790
H	-5.245153	-0.708242	0.388958	C	-0.637998	5.068970	-0.293082
H	-2.460720	0.397668	2.575666	C	-2.094507	4.573613	0.117059
H	-4.033761	0.393804	1.795370	B	-0.813819	2.811022	-0.586188
C	-4.045633	-0.483783	3.765561	H	-0.557618	1.703424	-0.954727
C	-2.705469	-2.616506	3.995734	O	-1.990330	3.122642	0.042013
H	-1.676033	-3.245599	2.198847	O	-0.068658	3.898002	-0.947071
H	-1.121521	-1.704138	2.832003	C	-2.519117	4.938094	1.540464
H	1.894033	-2.415394	-2.082317	H	-2.584666	6.024819	1.667841
H	2.942784	-1.322744	-2.976009	H	-3.507739	4.513388	1.744395
C	3.686314	-3.353781	-2.829600	H	-1.819606	4.538359	2.277179
H	5.543498	-1.066157	-0.189798	C	-3.191148	4.983481	-0.874501
H	5.181297	-0.556812	-1.835372	H	-4.126835	4.488101	-0.595566
C	5.808865	-2.611509	-1.684164	H	-3.361789	6.065300	-0.866015
H	4.900065	1.546181	0.995730	H	-2.940972	4.678982	-1.895208
H	5.369022	1.197808	-0.658593	C	-0.611929	6.222479	-1.298296
C	4.890291	3.267978	-0.321695	H	-1.060173	7.126621	-0.870377
C	3.184053	3.182422	-2.191565	H	0.426652	6.451746	-1.557400
H	3.559827	1.074259	-2.526882	H	-1.140490	5.974048	-2.221656
H	1.885449	1.456398	-2.135770	C	0.268723	5.398026	0.900496
H	2.150378	0.461382	3.142714	H	1.273272	5.622495	0.526017
H	3.535098	1.317229	2.490559	H	-0.092351	6.276055	1.447390
C	4.000401	-0.066642	4.101497	H	0.346633	4.545089	1.577819
C	3.469560	-2.497897	3.607955	C	0.171632	-0.688936	-1.954325
H	1.650204	-1.887204	2.582607	O	0.176379	-0.630994	-3.120872
H	2.731926	-2.873601	1.610496	H	0.420261	-2.091572	0.016196
H	-3.372574	-4.202020	-3.323465				
H	-1.732591	-4.457310	-3.911412				
C	-2.241001	-5.618859	-2.143229				
H	-2.883956	-6.323887	-0.187136				
H	-4.077101	-5.345650	-1.035303				
H	-3.903877	2.284796	-2.259011				
H	-3.923599	1.554269	-3.863197				
C	-5.621566	1.015696	-2.615375				
H	-6.969711	0.339373	-1.046302				
H	-5.789795	1.537641	-0.521167				
H	-4.306356	0.467630	4.247451				
H	-4.994702	-1.011740	3.585529				
C	-3.164985	-1.329524	4.694795				
H	-3.575815	-3.268821	3.823635				
H	-2.020407	-3.177518	4.644913				
				51			
				C	-0.255369	1.325496	2.506390
				H	-0.405856	1.490992	3.583439
				O	-0.125603	2.406374	1.838387
				O	-0.235605	0.146130	2.101746
				Ru	-0.182201	-0.417543	-0.046897
				P	-2.639746	-0.499016	0.020924
				P	2.243932	-0.941340	0.060302
				C	-3.506336	-1.773054	-1.105824
				C	-3.548259	1.125497	-0.318555
				C	-3.360058	-1.045653	1.710923
				C	2.542405	-2.773462	-0.366222
				C	3.379318	0.162529	-0.983944
				C	3.047887	-0.847764	1.774250

H	-4.536814	-1.800021	-0.719741	H	-4.133702	-3.178523	3.376114
C	-3.591317	-1.389029	-2.601485	H	-2.580423	-3.397609	4.177007
C	-2.920306	-3.197131	-0.970973	H	1.327924	-5.235959	-0.973610
H	-3.283358	1.723662	0.565442	H	1.477376	-5.116415	-2.724231
C	-3.001962	1.913058	-1.531743	C	3.371218	-5.331733	-1.676697
C	-5.090227	1.032443	-0.381291	H	5.102965	-5.151559	-0.370370
H	-4.320617	-1.516466	1.449753	H	3.562521	-5.250263	0.478336
C	-3.674082	0.099844	2.701623	H	5.347602	2.157958	-1.128054
C	-2.496331	-2.103965	2.438950	H	6.734791	1.084438	-1.294271
H	1.992834	-3.262001	0.451345	C	5.388675	1.078547	-3.003625
C	1.878243	-3.263614	-1.671020	H	3.696052	0.979320	-4.367268
C	4.001310	-3.281797	-0.313065	H	3.483188	2.101002	-3.026471
H	3.034106	1.161438	-0.681774	H	4.969730	0.274270	3.505027
C	4.900973	0.079520	-0.715122	H	3.997605	1.647277	4.025291
C	3.120773	0.035240	-2.501804	C	3.255147	-0.284709	4.698557
H	4.066843	-1.234558	1.634467	H	2.564491	-2.338867	4.897294
C	3.185787	0.593853	2.313349	H	4.095731	-2.165519	4.045766
C	2.355776	-1.751927	2.819529	H	-2.809567	-3.859141	-3.718702
H	-2.585930	-1.310697	-3.026575	H	-4.423426	-4.561281	-3.819976
H	-4.061537	-0.411158	-2.724698	H	-5.605107	4.253834	-1.629670
C	-4.396241	-2.424971	-3.408170	H	-5.504058	2.768027	-2.569989
C	-3.715422	-4.229502	-1.790029	H	-2.655031	-1.093331	5.069273
H	-1.875753	-3.187415	-1.305770	H	-4.141256	-1.926903	5.517587
H	-2.906607	-3.515553	0.074367	H	3.375299	-6.429132	-1.697326
H	-1.918971	2.023201	-1.449889	H	3.945428	-4.999906	-2.554620
H	-3.208328	1.374654	-2.464163	H	5.899767	1.892651	-3.533591
C	-3.643204	3.309274	-1.603026	H	5.811643	0.139030	-3.390423
C	-5.722149	2.434740	-0.446218	H	2.262074	0.124147	4.937684
H	-5.391647	0.469714	-1.274236	H	3.826513	-0.285726	5.635862
H	-5.493067	0.483878	0.478153	C	1.706826	4.344226	-0.012964
H	-2.739300	0.587358	3.000934	C	0.357695	4.596455	-0.787194
H	-4.299390	0.870550	2.243569	B	0.274784	2.562698	0.329844
C	-4.388229	-0.431042	3.959460	H	0.043726	1.439341	-0.222136
C	-3.217066	-2.652100	3.683062	O	-0.520123	3.620199	-0.201753
H	-2.232145	-2.929438	1.774219	O	1.656485	2.921583	0.215969
H	-1.552269	-1.638359	2.736799	C	-0.253620	5.984669	-0.582428
H	0.836954	-2.940576	-1.706846	H	0.419276	6.771432	-0.944750
H	2.382395	-2.824271	-2.541316	H	-1.191980	6.059877	-1.142526
C	1.936137	-4.797987	-1.779266	H	-0.475778	6.171483	0.470923
H	4.509752	-2.953949	0.599823	C	0.471718	4.298682	-2.292111
H	4.565702	-2.862506	-1.155894	H	-0.532614	4.293347	-2.728454
C	4.057557	-4.818115	-0.403972	H	1.068087	5.053054	-2.818069
H	5.126189	0.183807	0.350322	H	0.920440	3.315630	-2.466063
H	5.283908	-0.901410	-1.021464	C	2.976706	4.669030	-0.801074
C	5.658779	1.169582	-1.495875	H	3.020211	5.734640	-1.056377
C	3.882682	1.112502	-3.293818	H	3.858425	4.433327	-0.194296
H	3.445400	-0.954507	-2.851727	H	3.037351	4.088206	-1.724419
H	2.054388	0.113671	-2.722725	C	1.756147	5.057285	1.350874
H	2.197330	1.037532	2.446081	H	2.605608	4.665988	1.921064
H	3.698329	1.239266	1.595078	H	1.886898	6.140104	1.241570
C	3.934206	0.615127	3.657292	H	0.847120	4.870484	1.928395
C	3.098469	-1.716228	4.167619	C	-0.211145	-0.695928	-1.857151
H	1.322185	-1.417449	2.956265	O	-0.245792	-0.818198	-3.018426
H	2.310033	-2.788760	2.467718	H	-0.337741	-1.993244	0.229754
H	-5.440039	-2.427710	-3.059096				
H	-4.420967	-2.121786	-4.462687				
C	-3.812515	-3.835307	-3.268097				
H	-3.245898	-5.216089	-1.684017				
H	-4.729533	-4.320441	-1.372371				
H	-3.307367	3.891656	-0.734938				
H	-3.269863	3.835386	-2.491353				
C	-5.176945	3.243036	-1.632504				
H	-6.814682	2.345992	-0.511051				
H	-5.506240	2.971204	0.489696				
H	-4.584322	0.401988	4.647029				
H	-5.370728	-0.832953	3.669683				
C	-3.579824	-1.528672	4.662613				

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C	-1.131924	2.706956	2.710509
H	-2.015077	2.984145	3.309313
O	-1.384337	2.925049	1.420107
O	-0.127206	2.252444	3.204790
Ru	-0.120717	-0.575544	-0.088133
P	-2.534129	-0.782872	-0.037251
P	2.299794	-0.863357	0.133619
C	-3.241579	-2.399717	-0.727457
C	-3.581637	0.573518	-0.835903
C	-3.143610	-0.879301	1.766559
C	2.801750	-2.666024	-0.185218

C	3.463456	0.284396	-0.829518
C	2.833154	-0.598052	1.924922
H	-4.330076	-2.310105	-0.592190
C	-2.956811	-2.584202	-2.232511
C	-2.778349	-3.652136	0.048051
H	-3.519201	1.383594	-0.096536
C	-2.966667	1.136248	-2.135815
C	-5.072555	0.234678	-1.056681
H	-3.855492	-1.716071	1.800325
C	-3.883000	0.364842	2.300366
C	-1.949318	-1.226219	2.684285
H	2.209954	-3.177461	0.587985
C	2.310221	-3.237015	-1.533873
C	4.282414	-3.042754	0.033569
H	2.996478	1.261900	-0.645005
C	4.932865	0.372201	-0.351212
C	3.431825	0.034465	-2.354573
H	3.889744	-0.894031	1.990226
C	2.719010	0.884797	2.342623
C	2.038645	-1.490207	2.903609
H	-1.872231	-2.634736	-2.385978
H	-3.313513	-1.722146	-2.805326
C	-3.608031	-3.864615	-2.784173
C	-3.430901	-4.932896	-0.502573
H	-1.686848	-3.729732	-0.026560
H	-3.015307	-3.564435	1.114860
H	-1.926957	1.416795	-1.957503
H	-2.972056	0.370346	-2.922453
C	-3.749829	2.367773	-2.622366
C	-5.853654	1.476178	-1.525521
H	-5.161365	-0.545758	-1.824383
H	-5.531842	-0.172075	-0.147404
H	-3.240259	1.246131	2.204783
H	-4.776957	0.569960	1.703265
C	-4.297853	0.184989	3.772906
C	-2.369779	-1.402879	4.152718
H	-1.446344	-2.130813	2.325934
H	-1.216499	-0.405138	2.628377
H	1.254368	-2.993618	-1.674113
H	2.863236	-2.779341	-2.363705
C	2.504390	-4.762768	-1.588496
H	4.658688	-2.652477	0.985801
H	4.896005	-2.592696	-0.757346
C	4.474496	-4.570234	-0.009112
H	4.989395	0.575653	0.722023
H	5.438509	-0.586465	-0.515313
C	5.698893	1.469055	-1.114109
C	4.203669	1.120697	-3.124727
H	3.895082	-0.936997	-2.571781
H	2.403629	-0.018379	-2.722878
H	1.684460	1.224540	2.244787
H	3.311787	1.523706	1.679871
C	3.178343	1.094850	3.795269
C	2.489964	-1.272889	4.358402
H	0.968976	-1.254027	2.821658
H	2.143832	-2.549470	2.642475
H	-4.702935	-3.771053	-2.724724
H	-3.361556	-3.971599	-3.848322
C	-3.163223	-5.107767	-2.003080
H	-3.058850	-5.801542	0.056204
H	-4.517217	-4.893422	-0.330477
H	-3.614651	3.178034	-1.893207
H	-3.318900	2.725241	-3.567066
C	-5.245333	2.070733	-2.803436
H	-6.906869	1.212035	-1.688679
H	-5.839628	2.233268	-0.727624
H	-4.793270	1.098640	4.126586

H	-5.046094	-0.619043	3.838804
C	-3.106067	-0.162421	4.675510
H	-3.025584	-2.282513	4.236765
H	-1.485202	-1.612248	4.767524
H	1.857171	-5.233077	-0.833127
H	2.172468	-5.141918	-2.563744
C	3.962951	-5.165210	-1.328408
H	5.535063	-4.814605	0.135159
H	3.931027	-5.025646	0.832034
H	5.261091	2.449091	-0.874848
H	6.739240	1.499858	-0.764784
C	5.651405	1.246489	-2.631696
H	4.183006	0.892411	-4.198116
H	3.690783	2.085150	-3.002586
H	4.254214	0.874137	3.880454
H	3.048968	2.150266	4.063453
C	2.396741	0.203175	4.769261
H	1.884921	-1.899224	5.027377
H	3.529868	-1.617076	4.465968
H	-2.086892	-5.268843	-2.162239
H	-3.674722	-6.002024	-2.381969
H	-5.785393	2.982203	-3.091046
H	-5.377907	1.355641	-3.629368
H	-2.404428	0.683317	4.702767
H	-3.444741	-0.323706	5.706823
H	4.064090	-6.258163	-1.318465
H	4.591308	-4.800562	-2.154858
H	6.164825	2.063981	-3.154141
H	6.199211	0.324655	-2.878640
H	1.345424	0.520293	4.770192
H	2.770436	0.333990	5.793390
C	1.126285	4.571949	-0.379511
C	0.125639	4.192802	-1.543019
B	-0.424287	3.098943	0.382043
H	-0.113128	1.177944	0.046431
O	-0.949463	3.545588	-0.816774
O	0.866111	3.542177	0.612335
C	-0.462567	5.386960	-2.295755
H	0.326159	5.956053	-2.801785
H	-1.163780	5.030952	-3.057516
H	-1.005664	6.059915	-1.627916
C	0.702900	3.180068	-2.539170
H	-0.093273	2.846385	-3.211784
H	1.498751	3.624263	-3.147020
H	1.091534	2.299323	-2.022901
C	2.605667	4.536528	-0.754360
H	2.832393	5.288263	-1.519551
H	3.213627	4.758893	0.129012
H	2.903073	3.556750	-1.132597
C	0.795200	5.916352	0.288611
H	1.390240	6.011276	1.202364
H	1.026929	6.764666	-0.364502
H	-0.262267	5.971761	0.566144
C	-0.070288	-0.613816	-1.880516
O	-0.038639	-0.637463	-3.051759
H	-0.132172	-2.240339	0.019161

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Ru	0.890680	0.093850	0.286107
P	1.376160	-2.269219	-0.023176
P	0.588150	2.488182	0.084920
H	-0.749112	-0.170227	-0.313501
C	0.473741	-3.178225	-1.423480
C	3.223036	-2.618109	-0.357411
C	1.201616	-3.377196	1.517068
C	0.340415	3.457114	1.691190
C	-0.924415	2.986755	-0.939371

C	2.140909	3.309534	-0.646546	C	0.327057	-4.114251	4.280138
H	0.713399	-4.244373	-1.287280	H	-1.215829	-5.227122	3.223963
C	0.973938	-2.744858	-2.821542	H	0.429630	-5.736612	2.855943
C	-1.060934	-3.012820	-1.381743	H	2.193345	3.854458	4.629640
H	3.648610	-2.464448	0.645663	H	1.403146	5.127812	3.703140
C	3.962145	-1.630705	-1.289225	C	0.019950	3.758570	4.650053
C	3.565878	-4.068807	-0.773673	H	-2.102248	3.680741	4.179612
H	1.872472	-4.231071	1.345945	H	-1.241832	5.020407	3.425456
C	1.709011	-2.619952	2.767167	H	-3.334259	4.429046	-1.062193
C	-0.200474	-3.958856	1.788475	H	-2.701857	5.821409	-1.935764
H	0.320006	4.523129	1.424437	C	-2.729753	3.976641	-3.090855
C	1.515812	3.226209	2.667533	H	-2.506953	1.959847	-3.872048
C	-0.988599	3.124248	2.402729	H	-3.199732	2.033089	-2.252190
H	-1.745071	2.607753	-0.311952	H	3.828416	6.363686	-0.757792
C	-1.172633	4.496643	-1.142953	H	4.477213	4.811230	-0.238960
C	-1.049573	2.243554	-2.288576	C	4.016123	4.893317	-2.350326
H	2.935932	2.812814	-0.072687	H	4.542456	2.818611	-2.016264
C	2.323279	4.831418	-0.443650	H	3.934941	3.140990	-3.637883
C	2.385757	2.955969	-2.129704	H	-1.541315	-2.391358	-4.091031
H	0.779374	-1.671342	-2.949127	H	-1.704723	-4.053022	-4.657198
H	2.053784	-2.878031	-2.913914	H	6.933257	-3.467806	-1.497604
C	0.285853	-3.536284	-3.948604	H	5.605092	-3.492700	-2.654092
C	-1.749687	-3.827333	-2.489958	H	0.356918	-4.791299	5.144136
H	-1.471515	-3.293810	-0.411945	H	-0.365439	-3.300463	4.538899
H	-1.293674	-1.948856	-1.513664	H	-0.099715	4.395736	5.535892
H	3.621318	-1.758126	-2.324001	H	0.024979	2.718661	5.007139
H	3.732580	-0.599543	-1.016779	H	-3.743042	4.125916	-3.486143
C	5.482489	-1.865027	-1.234924	H	-2.038210	4.388651	-3.841014
C	5.085676	-4.313920	-0.723184	H	3.348821	5.463237	-3.014394
H	3.062499	-4.802100	-0.134026	H	5.041708	5.174255	-2.622405
H	3.212853	-4.255485	-1.796227	C	2.594270	0.364831	1.028548
H	1.052087	-1.761781	2.941857	O	3.648055	0.536692	1.500568
H	2.717143	-2.220706	2.602156	H	1.471966	0.212473	-1.196956
C	1.717719	-3.524651	4.010834	C	-5.641647	-1.606258	-0.348650
C	-0.199725	-4.852792	3.042937	C	-5.579229	-0.057495	-0.037816
H	-0.919798	-3.142753	1.916648	B	-3.608071	-1.052553	0.495568
H	-0.536080	-4.558365	0.935278	O	-4.146874	0.162999	0.135865
H	1.553697	2.161113	2.927944	O	-4.462758	-2.111271	0.339112
H	2.475718	3.465464	2.195736	C	-6.079271	0.852457	-1.157007
C	1.353680	4.056957	3.952551	H	-7.142785	0.676412	-1.355043
C	-1.159655	3.954695	3.688077	H	-5.960959	1.899579	-0.859685
H	-1.844132	3.310024	1.741965	H	-5.521993	0.699847	-2.083900
H	-0.992195	2.057929	2.656532	C	-6.246712	0.322077	1.290883
H	-1.100449	5.043706	-0.195780	H	-5.990146	1.357635	1.535222
H	-0.400874	4.909131	-1.806407	H	-7.337175	0.242207	1.231643
C	-2.556078	4.745467	-1.772671	H	-5.897384	-0.315101	2.109727
C	-2.437636	2.479915	-2.907397	C	-6.867233	-2.329523	0.206256
H	-0.283636	2.602281	-2.987267	H	-7.788137	-1.934713	-0.237947
H	-0.870951	1.174591	-2.142455	H	-6.804054	-3.395150	-0.036173
H	1.569364	5.381442	-1.021023	H	-6.933954	-2.235944	1.292377
H	2.184425	5.114554	0.604051	C	-5.465594	-1.931500	-1.837669
C	3.726951	5.278924	-0.893463	H	-5.319154	-3.010132	-1.949548
C	3.790929	3.391691	-2.578826	H	-6.345673	-1.641501	-2.421244
H	2.252804	1.881602	-2.289275	H	-4.589525	-1.425638	-2.255778
H	1.643744	3.470750	-2.754890	O	-2.347203	-1.232928	1.000986
H	0.653357	-3.182093	-4.920815	C	-1.487000	-0.157557	1.197272
H	0.577209	-4.594927	-3.873007	H	-1.978995	0.798381	0.994245
C	-1.242131	-3.429107	-3.881125	O	-0.600513	-0.265587	2.075996
H	-1.564224	-4.899941	-2.326883				
H	-2.835978	-3.687060	-2.421752				
H	5.988343	-1.163254	-1.910913	52			
H	5.844014	-1.637310	-0.221416	Ru	0.119409	-0.771931	-0.441536
C	5.851358	-3.310777	-1.597128	P	2.548589	-0.716607	0.020465
H	5.428380	-4.225825	0.318318	P	-2.323673	-0.964788	-0.240518
H	5.305608	-5.342375	-1.038724	H	-0.793493	2.022334	-2.655931
H	2.439327	-4.343617	3.867253	C	2.998906	-0.033607	1.739771
H	2.065293	-2.950829	4.879801	C	3.337152	-2.438891	-0.164480
				C	3.679746	0.313479	-1.100127

C	-4.386993	0.390173	1.102386	H	-7.193541	0.185795	1.168440
C	-3.493743	-2.225614	0.435153	H	-7.370573	0.236577	2.920206
C	1.859038	1.673162	-2.553687	H	-5.544114	-3.408841	-1.090259
C	1.769957	2.779118	0.197542	H	-4.679409	-3.405441	-2.626355
C	-0.262760	3.629327	-1.982381	C	-3.824168	-4.732012	-1.130394
H	-2.986387	-1.436286	3.273305	H	-2.990905	-5.662393	0.649602
C	-2.090339	0.507853	3.580850	H	-4.502071	-4.799784	0.927214
C	-0.857092	-1.567606	2.900312	H	1.545296	0.503256	-5.823746
H	-4.866584	0.094523	0.157539	H	2.506251	1.878225	-5.282792
C	-4.300334	1.932132	1.076965	C	3.229942	-0.035802	-4.559865
C	-5.330918	-0.063294	2.244063	H	4.714552	-0.265055	-2.990066
H	-4.475021	-2.256577	0.929458	H	4.472600	1.402079	-3.510292
C	-3.739428	-2.200950	-1.091358	H	4.346835	3.430241	1.117072
C	-2.753645	-3.516904	0.836327	H	4.299940	5.138825	0.686365
H	2.363060	2.607658	-2.837865	C	2.928133	4.576799	2.281863
C	1.112035	1.134135	-3.795556	H	1.434691	3.655002	3.565607
C	2.959289	0.676514	-2.133628	H	2.607305	2.524404	2.887616
H	2.406484	1.905379	0.388477	H	0.199660	6.214930	-4.282823
C	2.689720	3.963685	-0.170254	H	-1.083071	5.009336	-4.290153
C	1.024687	3.061162	1.522722	C	-1.206000	6.392444	-2.631975
H	-1.012183	3.122163	-2.605528	H	-2.748553	4.930109	-2.218982
C	0.537830	4.554214	-2.929490	H	-2.505828	6.088400	-0.913539
C	-1.044232	4.485933	-0.960967	H	0.448148	0.079068	4.780974
H	-1.335857	1.142618	3.096133	H	-0.159467	-0.737377	6.220680
H	-3.028444	1.067248	3.552667	H	-7.658296	2.517089	1.879292
C	-1.689793	0.268317	5.048126	H	-6.308553	2.474215	3.009899
C	-0.465973	-1.833298	4.363723	H	-4.419068	-5.607345	-1.423124
H	-0.880771	-2.508716	2.347875	H	-2.868718	-4.788143	-1.663717
H	-0.079941	-0.951087	2.432392	H	3.945161	-0.145230	-5.385923
H	-3.828434	2.302437	1.996499	H	2.807039	-1.025199	-4.352322
H	-3.668083	2.263978	0.250865	H	3.644649	4.771669	3.090521
C	-5.698405	2.561956	0.935922	H	2.334307	5.495823	2.163035
C	-6.728885	0.562535	2.091334	H	-0.523107	7.036558	-2.057787
H	-5.427690	-1.154087	2.275195	H	-1.894595	7.061968	-3.163038
H	-4.915804	0.239039	3.213762	C	-2.189549	1.005547	-1.557855
H	-2.774909	-2.186511	-1.609355	O	-2.963611	1.289915	-2.385389
H	-4.277818	-1.292442	-1.390366	H	-1.489425	1.806013	0.481208
C	-4.538488	-3.437068	-1.538392	C	4.822395	-0.224387	2.961594
C	-3.547980	-4.756010	0.378696	C	4.701212	-1.798710	2.898815
H	-1.760885	-3.537795	0.372934	B	2.999924	-0.826753	1.739743
H	-2.630318	-3.564545	1.924527	O	3.732584	-1.989145	1.831146
H	0.630858	0.183992	-3.536957	O	3.510024	0.205472	2.499369
H	0.317833	1.822024	-4.111863	C	5.985238	-2.536010	2.523834
C	2.090040	0.910117	-4.962131	H	6.766431	-2.366962	3.273927
C	3.947171	0.458298	-3.295062	H	5.789327	-3.611985	2.475977
H	3.505545	1.043232	-1.256464	H	6.361889	-2.219708	1.548596
H	2.502217	-0.280271	-1.868016	C	4.089818	-2.410256	4.166860
H	3.248178	3.755239	-1.090129	H	3.844549	-3.458709	3.971350
H	2.080091	4.855192	-0.366115	H	4.784329	-2.370350	5.012552
C	3.670727	4.285224	0.970860	H	3.167289	-1.893578	4.451692
C	2.003178	3.410748	2.658236	C	5.059055	0.352150	4.355863
H	0.311714	3.884036	1.391249	H	6.007544	-0.008050	4.770581
H	0.434950	2.182506	1.806429	H	5.109252	1.444443	4.299922
H	1.300972	5.105702	-2.366753	H	4.253762	0.086742	5.044556
H	1.065714	3.977177	-3.693913	C	5.851902	0.340757	1.973266
C	-0.394337	5.559836	-3.632431	H	5.741773	1.428851	1.927574
C	-1.978470	5.485954	-1.664598	H	6.877245	0.113251	2.282887
H	-1.622465	3.846212	-0.286776	H	5.698394	-0.057843	0.965184
H	-0.335246	5.046426	-0.336834	O	1.881643	-0.680333	0.979913
H	-1.598069	1.232853	5.564073	C	1.413756	-1.822989	0.234015
H	-2.497313	-0.280813	5.555047	H	1.084947	-2.583983	0.954043
C	-0.383573	-0.528978	5.166557	O	0.378982	-1.398732	-0.576231
H	-1.206845	-2.503496	4.824897	C	0.492153	-4.509365	-2.191039
H	0.494583	-2.364095	4.395473	C	1.327018	-3.650780	-3.222199
H	-5.609807	3.655933	0.945198	B	0.098443	-2.183651	-1.871959
H	-6.113912	2.291394	-0.045939	H	-0.746237	-1.471450	-2.415221
C	-6.658067	2.094392	2.038178	O	1.346789	-2.360388	-2.614852

O	-0.390661	-3.544825	-1.615985
C	2.768519	-4.126224	-3.431678
H	2.797381	-5.152622	-3.817678
H	3.271146	-3.480904	-4.160900
H	3.340697	-4.088319	-2.500825
C	0.626562	-3.534360	-4.591182
H	1.156342	-2.792382	-5.198414
H	0.623438	-4.483224	-5.139987
H	-0.407241	-3.195962	-4.473321
C	-0.333363	-5.634193	-2.831834
H	0.308500	-6.341052	-3.372849
H	-0.864272	-6.195754	-2.054561
H	-1.078227	-5.239313	-3.527191
C	1.357112	-5.128854	-1.075158
H	0.693963	-5.510142	-0.290471
H	1.965058	-5.965022	-1.441286
H	2.029109	-4.396827	-0.619795

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Ru	-0.052536	-0.634919	-0.102153
P	2.419176	-0.753795	-0.027109
P	-2.560322	-0.697628	0.068118
H	-1.231556	1.101788	-2.753157
H	-0.020550	-0.185568	1.417769
C	3.524921	0.119926	-1.291792
C	2.966034	0.006420	1.627274
C	3.033024	-2.546982	-0.002834
C	-3.740719	0.515213	-0.811424
C	-3.065600	-2.377856	-0.652931
C	-3.193692	-0.724084	1.844883
H	4.550857	-0.062930	-0.938497
C	3.414026	-0.451364	-2.723559
C	3.299469	1.646834	-1.319521
H	2.332938	0.905194	1.661224
C	4.432795	0.462960	1.803680
C	2.559114	-0.878347	2.827399
H	2.605459	-2.920564	0.938191
C	4.560413	-2.764238	0.069213
C	2.440540	-3.431960	-1.128463
H	-3.728740	0.136598	-1.843733
C	-5.209763	0.493697	-0.322778
C	-3.263797	1.981899	-0.874738
H	-2.357600	-3.056521	-0.161448
C	-4.474646	-2.950444	-0.385320
C	-2.759937	-2.440239	-2.167873
H	-4.282600	-0.854399	1.780144
C	-2.912422	0.614624	2.563378
C	-2.633851	-1.894972	2.680197
H	2.373797	-0.380565	-3.061937
H	3.668618	-1.514268	-2.729295
C	4.362366	0.271486	-3.698503
C	4.282997	2.349228	-2.269863
H	3.384271	2.074567	-0.315055
H	2.280079	1.846745	-1.656445
H	4.758763	1.101573	0.977226
H	5.102031	-0.406267	1.808106
C	4.609754	1.226132	3.130225
C	2.735829	-0.129627	4.159469
H	3.184662	-1.782608	2.845528
H	1.520621	-1.206657	2.724299
H	5.006377	-2.172347	0.874107
H	5.027937	-2.425927	-0.866008
C	4.897638	-4.250836	0.296775
C	2.750329	-4.915905	-0.871801
H	2.872433	-3.149044	-2.094387
H	1.362891	-3.280151	-1.222365
H	-5.594759	-0.525087	-0.239796

H	-5.263031	0.931041	0.683328
C	-6.117948	1.309394	-1.261596
C	-4.158005	2.809886	-1.815157
H	-3.292084	2.424731	0.130415
H	-2.227684	2.031075	-1.205115
H	-4.733516	-2.903887	0.679280
H	-5.228933	-2.363166	-0.924067
C	-4.554981	-4.409203	-0.877234
C	-2.844719	-3.887791	-2.681653
H	-3.499802	-1.833966	-2.712013
H	-1.776635	-2.010825	-2.387733
H	-1.828358	0.785408	2.585370
H	-3.346555	1.451838	2.006680
C	-3.471824	0.618817	3.997050
C	-3.214194	-1.893785	4.105631
H	-2.843319	-2.857327	2.199640
H	-1.543686	-1.805119	2.740299
H	5.403505	0.047628	-3.419677
H	4.218668	-0.131054	-4.709547
C	4.163442	1.792012	-3.694315
H	4.089607	3.430105	-2.264841
H	5.313134	2.212605	-1.906981
H	4.012490	2.149486	3.095112
H	5.657241	1.535907	3.240735
C	4.171627	0.383388	4.335959
H	2.036795	0.718835	4.187883
H	2.461964	-0.789469	4.993004
H	5.987522	-4.383020	0.311676
H	4.533700	-4.548601	1.291294
C	4.262830	-5.159418	-0.765169
H	2.256365	-5.232704	0.057842
H	2.323270	-5.526534	-1.677764
H	-6.131219	0.833698	-2.253378
H	-7.150560	1.283691	-0.889496
C	-5.633801	2.758886	-1.397949
H	-4.054741	2.420985	-2.839499
H	-3.805167	3.848177	-1.842058
H	-3.857525	-5.025011	-0.290677
H	-5.559945	-4.809132	-0.688593
C	-4.207779	-4.523445	-2.369450
H	-2.046904	-4.481803	-2.212219
H	-2.654017	-3.909223	-3.762340
H	-4.570671	0.568939	3.958045
H	-3.220614	1.568854	4.486338
C	-2.942680	-0.563178	4.820101
H	-2.786629	-2.728661	4.675572
H	-4.299733	-2.069101	4.060513
H	3.165582	2.031083	-4.090064
H	4.890561	2.274853	-4.360051
H	4.851922	-0.475134	4.440884
H	4.260051	0.966633	5.261644
H	4.729773	-4.956423	-1.740565
H	4.468401	-6.212497	-0.533685
H	-5.754038	3.270646	-0.431325
H	-6.256493	3.303794	-2.119148
H	-4.985524	-4.013788	-2.958066
H	-4.221041	-5.575772	-2.681585
H	-1.858502	-0.446892	4.964486
H	-3.394948	-0.565292	5.820315
C	0.100938	4.987836	-0.665931
C	0.566111	4.514368	0.774851
B	0.146961	2.694415	-0.565164
O	0.266283	3.099148	0.759828
O	0.181502	3.771775	-1.443951
O	0.015879	1.419029	-0.958872
C	-0.196744	0.744668	-2.621561
H	0.538407	1.371990	-3.154078

O	0.030877	-0.494041	-2.468027
C	-0.188714	5.153882	1.942094
H	0.179854	4.737471	2.885455
H	-0.031979	6.238637	1.967320
H	-1.261841	4.957158	1.886837
C	2.077465	4.664596	1.003139
H	2.371515	5.716174	1.091467
H	2.348824	4.153476	1.932849
H	2.651990	4.213442	0.189315
C	0.992997	6.042059	-1.323869
H	0.608521	6.272511	-2.322965
H	1.001716	6.971211	-0.742271
H	2.021303	5.690009	-1.434427
C	-1.360877	5.456897	-0.705830
H	-1.495991	6.413571	-0.189792
H	-1.662992	5.583223	-1.750460
H	-2.027371	4.719474	-0.248781
C	-0.079124	-2.332402	0.566125
O	-0.082746	-3.405413	1.036356

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Ru	-0.001202	0.214034	-0.148468
P	-2.421774	-0.017977	-0.147864
P	2.420793	-0.052798	0.023694
H	-0.019271	-0.790145	-1.544601
H	-0.040177	-1.119515	0.737652
C	-3.407981	1.524646	-0.617177
C	-3.014117	-1.316912	-1.394596
C	-3.225211	-0.624711	1.475543
C	3.357506	-0.843156	-1.433934
C	3.250597	1.642266	0.264587
C	3.000511	-1.027041	1.535761
H	-4.464652	1.303628	-0.416334
C	-2.992776	2.728029	0.257355
C	-3.278992	1.901803	-2.109783
H	-2.602377	-0.945071	-2.344036
C	-4.539695	-1.471525	-1.577159
C	-2.378532	-2.703205	-1.148285
H	-3.245883	-1.715559	1.336604
C	-4.681267	-0.163674	1.721438
C	-2.383047	-0.361329	2.741258
H	3.386408	-0.022174	-2.166089
C	4.821141	-1.262842	-1.158270
C	2.616701	-2.019036	-2.111634
H	2.595543	2.089988	1.025000
C	4.691247	1.731848	0.813935
C	3.113904	2.518559	-1.001431
H	4.098690	-0.988600	1.507956
C	2.581244	-2.512751	1.507250
C	2.538726	-0.384091	2.861790
H	-1.933776	2.945166	0.073369
H	-3.083900	2.487374	1.323572
C	-3.834483	3.974225	-0.066220
C	-4.122635	3.146448	-2.440655
H	-3.597984	1.072989	-2.752792
H	-2.224959	2.105689	-2.326550
H	-5.020682	-0.502587	-1.752944
H	-4.979627	-1.881533	-0.658129
C	-4.861017	-2.428760	-2.740018
C	-2.700285	-3.675972	-2.296514
H	-2.765859	-3.125767	-0.209385
H	-1.296472	-2.602074	-1.027637
H	-5.313301	-0.351342	0.848404
H	-4.696026	0.920916	1.892057
C	-5.290761	-0.864345	2.949486
C	-2.988328	-1.055810	3.973400
H	-2.324409	0.718891	2.930550

H	-1.358846	-0.708508	2.582845
H	5.385200	-0.455002	-0.686087
H	4.833639	-2.105700	-0.454340
C	5.533739	-1.689985	-2.455481
C	3.316961	-2.442568	-3.414384
H	2.586019	-2.879723	-1.431234
H	1.575189	-1.754949	-2.307890
H	4.817222	1.119533	1.714032
H	5.404012	1.353549	0.070674
C	5.057782	3.194505	1.131264
C	3.497624	3.979456	-0.705976
H	3.781257	2.132316	-1.787072
H	2.089830	2.473384	-1.386451
H	1.485943	-2.572809	1.481217
H	2.942691	-3.000703	0.596588
C	3.116841	-3.278989	2.730417
C	3.090561	-1.143489	4.080801
H	2.842378	0.667068	2.919198
H	1.443431	-0.395449	2.897584
H	-4.885710	3.784550	0.199190
H	-3.502036	4.815567	0.555417
C	-3.744059	4.341179	-1.554132
H	-3.997401	3.404239	-3.500485
H	-5.189159	2.912967	-2.299820
H	-4.494866	-1.989778	-3.680051
H	-5.948806	-2.531535	-2.846724
C	-4.211880	-3.804654	-2.532892
H	-2.217456	-3.316075	-3.217456
H	-2.263563	-4.659792	-2.080957
H	-6.316419	-0.505085	3.105598
H	-5.365402	-1.943776	2.749304
C	-4.445713	-0.638106	4.209819
H	-2.942123	-2.146241	3.830914
H	-2.378643	-0.831664	4.858237
H	5.610403	-0.820796	-3.125569
H	6.562330	-1.997705	-2.226073
C	4.784898	-2.820606	-3.173038
H	3.269280	-1.613826	-4.137246
H	2.776114	-3.283082	-3.868371
H	4.404278	3.563651	1.935392
H	6.085048	3.243607	1.515760
C	4.905253	4.094013	-0.103958
H	2.764973	4.404991	-0.004902
H	3.427619	4.573099	-1.626614
H	4.215884	-3.314196	2.684289
H	2.771153	-4.320205	2.690156
C	2.688922	-2.624157	4.050175
H	2.730827	-0.668216	5.002432
H	4.188079	-1.063872	4.095785
H	-2.714833	4.650096	-1.786412
H	-4.389815	5.200878	-1.775909
H	-4.673670	-4.292198	-1.661202
H	-4.411435	-4.453990	-3.395087
H	-4.477292	0.428245	4.478369
H	-4.871426	-1.187845	5.059154
H	4.826761	-3.730396	-2.555675
H	5.280456	-3.064217	-4.121613
H	5.647889	3.795003	-0.859221
H	5.127523	5.137173	0.155675
H	1.597044	-2.703892	4.156918
H	3.127802	-3.158795	4.902505
C	0.093435	0.720891	-2.494902
O	-0.021545	1.806304	-1.841833
H	-0.757845	0.352482	-3.088629
H	1.077537	0.415481	-2.879492
C	0.016105	1.333974	1.384287
O	0.051262	2.073847	2.282216

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Ru	0.016616	-0.157804	-0.029000
P	2.458397	0.029970	-0.058963
P	-2.409187	-0.037366	0.100092
H	-1.520428	0.531624	-3.014386
H	0.018698	0.668511	1.332484
C	3.324134	-1.276506	-1.106563
C	2.898150	1.668709	-0.870518
C	3.397334	0.067138	1.592812
C	-3.215725	1.397820	-0.843808
C	-3.189067	-1.621358	-0.580410
C	-3.156269	0.091544	1.834933
H	4.406941	-1.126360	-0.993429
C	2.979850	-2.694214	-0.597483
C	2.981130	-1.155429	-2.608752
H	2.353081	1.583316	-1.818795
C	4.389540	1.936562	-1.155052
C	2.276234	2.862895	-0.113571
H	3.394367	1.138939	1.841857
C	4.874720	-0.388176	1.544701
C	2.664925	-0.654356	2.744226
H	-3.256528	1.018618	-1.875220
C	-4.655148	1.789762	-0.439250
C	-2.321734	2.660835	-0.863062
H	-2.748006	-2.383838	0.078984
C	-4.722168	-1.772559	-0.507578
C	-2.696125	-1.942232	-2.008093
H	-4.237551	0.210519	1.678268
C	-2.655129	1.335748	2.600981
C	-2.954656	-1.169031	2.703668
H	1.893907	-2.839592	-0.665875
H	3.238809	-2.804170	0.462275
C	3.686929	-3.783553	-1.420291
C	3.677996	-2.252736	-3.432737
H	3.278523	-0.172628	-2.991038
H	1.894117	-1.211878	-2.734947
H	4.842450	1.104661	-1.707460
H	4.938440	2.022531	-0.206884
C	4.572946	3.243124	-1.949332
C	2.461973	4.172515	-0.899318
H	2.747838	2.973704	0.874508
H	1.211897	2.676856	0.062652
H	5.423388	0.125671	0.748903
H	4.920584	-1.461034	1.314823
C	5.578077	-0.143859	2.892355
C	3.368901	-0.420779	4.091572
H	2.623036	-1.733131	2.541504
H	1.629503	-0.308110	2.799390
H	-5.317564	0.919137	-0.418115
H	-4.652575	2.205756	0.576986
C	-5.226872	2.848428	-1.400717
C	-2.887069	3.725598	-1.818080
H	-2.264960	3.085209	0.148588
H	-1.299872	2.394886	-1.144262
H	-5.095465	-1.557130	0.500266
H	-5.194168	-1.047158	-1.183601
C	-5.156837	-3.189166	-0.925566
C	-3.128868	-3.354626	-2.438081
H	-3.112808	-1.211032	-2.715464
H	-1.605937	-1.845646	-2.061203
H	-1.570801	1.250207	2.744306
H	-2.818745	2.246556	2.015721
C	-3.348757	1.479114	3.966828
C	-3.658384	-1.027304	4.065628
H	-3.333869	-2.062196	2.195035
H	-1.884961	-1.334250	2.870080

H	4.775455	-3.698729	-1.282783
H	3.400705	-4.773963	-1.043437
C	3.351605	-3.659639	-2.912526
H	3.387578	-2.158799	-4.487306
H	4.767445	-2.099641	-3.395339
H	4.107173	3.129692	-2.939289
H	5.641372	3.425429	-2.124795
C	3.938940	4.438814	-1.223968
H	1.889491	4.109612	-1.836184
H	2.040343	5.011089	-0.329704
H	6.617823	-0.491524	2.833533
H	5.621085	0.938439	3.085889
C	4.845180	-0.838359	4.047972
H	3.302429	0.646527	4.351994
H	2.840355	-0.967666	4.882976
H	-5.316821	2.411248	-2.406292
H	-6.243134	3.120980	-1.087160
C	-4.335082	4.096275	-1.465945
H	-2.849559	3.340134	-2.847721
H	-2.249104	4.618632	-1.796875
H	-4.761136	-3.915674	-0.200559
H	-6.250863	-3.269734	-0.882880
C	-4.649285	-3.543294	-2.331045
H	-2.624591	-4.093449	-1.797979
H	-2.792351	-3.548944	-3.464565
H	-4.421156	1.672250	3.812312
H	-2.947285	2.355517	4.491899
C	-3.180512	0.217918	4.824348
H	-3.481880	-1.930648	4.663330
H	-4.745935	-0.962723	3.909733
H	2.279841	-3.860037	-3.058115
H	3.894673	-4.417453	-3.492040
H	4.487746	4.625464	-0.288389
H	4.039220	5.348345	-1.830373
H	4.909280	-1.928328	3.912289
H	5.337347	-0.612476	5.002733
H	-4.351687	4.601146	-0.488480
H	-4.735979	4.813006	-2.194201
H	-5.146781	-2.894216	-3.067269
H	-4.925539	-4.574148	-2.587078
H	-2.118851	0.096447	5.084920
H	-3.726279	0.322505	5.770915
C	-0.461141	0.834003	-3.074275
O	0.285339	0.539800	-1.941468
H	-0.448688	1.916062	-3.305094
H	-0.037883	0.321514	-3.958036
C	0.012191	-1.624108	1.073153
O	0.011413	-2.635198	1.667666

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C	-0.132353	-0.609886	2.430084
O	-0.215504	-0.761249	3.584671
Ru	-0.116981	-0.553242	0.512042
P	2.170705	-1.168430	0.046751
P	-2.472295	-0.237493	0.184444
B	0.549597	2.477559	0.188435
H	-0.210168	-0.773714	-1.147868
H	0.088585	1.420836	0.505287
H	-0.422267	-2.101275	0.536602
C	2.397412	-3.004471	-0.390399
C	2.983378	-0.265452	-1.426186
C	3.559665	-0.986019	1.366491
C	-3.489238	0.441694	1.633367
C	-3.411475	-1.832755	-0.222810
C	-2.828993	1.053453	-1.179295

O	-0.258612	3.498881	-0.216603
O	1.871432	2.801946	0.267639
H	3.464857	-3.117815	-0.630382
C	1.581060	-3.429768	-1.628709
C	2.088783	-3.945544	0.795072
H	3.246846	0.701477	-0.978615
C	2.057371	0.073668	-2.612835
C	4.282343	-0.922249	-1.947107
H	4.260812	-1.808171	1.154284
C	4.364120	0.334031	1.317965
C	3.021828	-1.170390	2.801488
H	-4.484577	0.680737	1.235832
C	-2.871598	1.751180	2.173614
C	-3.693021	-0.565303	2.786980
H	-3.290700	-2.393459	0.716035
C	-4.925910	-1.687229	-0.488469
C	-2.764187	-2.705710	-1.319597
H	-2.062577	1.811594	-0.967982
C	-4.192708	1.783318	-1.161295
C	-2.548942	0.523217	-2.602542
C	0.610266	4.601358	-0.631963
C	1.966878	4.254032	0.101307
H	0.518245	-3.252553	-1.429973
H	1.838934	-2.808041	-2.491668
C	1.802166	-4.909489	-1.987882
C	2.299577	-5.425630	0.428315
H	2.724147	-3.705017	1.653338
H	1.050262	-3.789134	1.114959
H	1.724635	-0.841948	-3.117103
H	1.148096	0.557996	-2.248228
C	2.776440	0.974232	-3.633665
C	5.003865	-0.019516	-2.964169
H	4.964038	-1.167233	-1.124228
H	4.037485	-1.873032	-2.439127
H	3.685859	1.181070	1.487173
H	4.817834	0.489276	0.335431
C	5.492883	0.349973	2.367549
C	4.153707	-1.196886	3.842389
H	2.353723	-0.333600	3.030822
H	2.413742	-2.074236	2.890643
H	-1.869360	1.536841	2.564305
H	-2.738463	2.484013	1.368573
C	-3.725676	2.360241	3.298564
C	-4.539483	0.047092	3.918907
H	-4.189496	-1.472711	2.425007
H	-2.721683	-0.873860	3.188377
H	-5.412451	-1.091389	0.292168
H	-5.079323	-1.150741	-1.434231
C	-5.611669	-3.063311	-0.578088
C	-3.444799	-4.083089	-1.399062
H	-2.848655	-2.211650	-2.294961
H	-1.696731	-2.816822	-1.116615
H	-5.005700	1.076497	-1.373248
H	-4.399001	2.214045	-0.177086
C	-4.223760	2.918079	-2.203832
C	-2.566695	1.659650	-3.638962
H	-1.587791	0.000988	-2.626725
H	-3.320943	-0.207827	-2.878474
C	-0.044219	5.912704	-0.202280
C	0.702086	4.531866	-2.161039
C	2.067419	4.842885	1.514164
C	3.233948	4.565895	-0.691123
H	1.184226	-5.171932	-2.856792
H	2.848933	-5.061168	-2.293021
C	1.484117	-5.832331	-0.805033
H	3.367507	-5.601250	0.227638
H	2.036985	-6.055874	1.288092

H	2.106465	1.187096	-4.477254
H	3.004122	1.943188	-3.161920
C	4.084558	0.347695	-4.136687
H	5.337312	0.900452	-2.460644
H	5.909700	-0.520609	-3.330255
H	6.229992	-0.424684	2.107109
H	6.023719	1.310325	2.318322
C	4.979403	0.094108	3.789488
H	3.728176	-1.338608	4.844100
H	4.809672	-2.060523	3.654690
H	-3.246534	3.273931	3.674571
H	-4.703398	2.663784	2.894301
C	-3.936409	1.358068	4.441848
H	-4.639764	-0.678967	4.736031
H	-5.556882	0.240945	3.546213
H	-5.550074	-3.557900	0.402847
H	-6.680265	-2.932280	-0.794231
C	-4.956425	-3.959267	-1.638502
H	-2.981273	-4.679326	-2.196046
H	-3.269722	-4.628521	-0.459393
H	-5.206738	3.407330	-2.186139
H	-3.488162	3.683214	-1.914262
C	-3.901096	2.417268	-3.617684
H	-1.745525	2.358990	-3.422509
H	-2.374662	1.251762	-4.640229
H	-0.990994	6.041431	-0.736385
H	0.599779	6.765709	-0.445002
H	-0.256977	5.929239	0.868860
H	1.147610	3.589545	-2.494166
H	1.294593	5.359274	-2.565279
H	-0.306343	4.594676	-2.581542
H	1.176429	4.614174	2.107317
H	2.197898	5.929714	1.488099
H	2.931798	4.404315	2.021911
H	4.111591	4.253092	-0.116643
H	3.318837	5.642340	-0.878782
H	3.253270	4.042273	-1.649461
H	0.411609	-5.764605	-0.570285
H	1.683346	-6.879282	-1.068847
H	4.597864	1.030177	-4.826679
H	3.851908	-0.561469	-4.710825
H	5.818321	0.049243	4.496312
H	4.346702	0.936989	4.104748
H	-4.581360	1.791190	5.217609
H	-2.968249	1.145322	4.917578
H	-5.428471	-4.950416	-1.643081
H	-5.130299	-3.525447	-2.634841
H	-4.703057	1.743611	-3.955088
H	-3.881051	3.256970	-4.324904

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C	0.096034	2.007661	1.026642
O	0.186853	3.004430	1.628383
Ru	-0.010944	0.376849	0.008086
P	-2.447827	0.648535	-0.040564
P	2.436511	0.361981	0.064185
B	-0.175070	-1.848718	0.026897
H	0.016617	0.053872	-1.703674
H	-0.093968	-0.951933	1.114418
H	0.057691	0.987225	-1.623165
C	-3.063326	2.390037	-0.534187
C	-3.428903	-0.455967	-1.237403
C	-3.347367	0.333635	1.608256
C	3.200055	-0.094557	1.738670
C	3.142696	2.109807	-0.195562
C	3.308124	-0.818461	-1.141947
O	0.903230	-2.726787	-0.148834

O	-1.368153	-2.582814	-0.035298	H	-3.327953	-2.553397	-3.104774
H	-4.072876	2.217325	-0.930025	C	-5.097624	-1.386660	-3.531263
C	-2.217846	3.007885	-1.670228	H	-5.523264	-2.290780	-1.609935
C	-3.215593	3.418861	0.608457	H	-6.740014	-1.127157	-2.128405
H	-3.240104	-1.452225	-0.823623	H	-5.425845	-0.854017	3.105979
C	-2.873552	-0.482893	-2.676487	H	-4.627272	-2.399537	3.373253
C	-4.956701	-0.225527	-1.275460	C	-3.697256	-0.720731	4.397094
H	-4.305357	0.870680	1.532784	H	-2.752821	1.157424	4.956269
C	-3.662396	-1.154060	1.883068	H	-4.268807	1.342128	4.079817
C	-2.563140	0.905745	2.811740	H	3.316519	-2.936571	3.768622
H	4.287712	-0.033707	1.596436	H	4.673400	-1.910930	3.312676
C	2.864318	-1.537242	2.173503	C	3.244261	-0.932110	4.610510
C	2.826615	0.884370	2.873607	H	3.227074	1.211886	4.979274
H	2.754068	2.631154	0.689708	H	4.620851	0.643908	4.065423
C	4.679763	2.262433	-0.170365	H	4.741994	4.188258	0.817342
C	2.564821	2.868747	-1.411133	H	6.182705	3.830571	-0.130473
H	2.708141	-1.727207	-1.014784	C	4.490237	4.533024	-1.304714
C	4.781816	-1.195088	-0.859813	H	2.562981	4.868151	-2.254922
C	3.156474	-0.376740	-2.614334	H	2.503741	4.827459	-0.495227
C	0.406250	-4.020949	-0.566864	H	6.309782	-2.538014	-1.620590
C	-1.061708	-3.998149	-0.011956	H	4.684041	-3.214735	-1.634516
H	-1.206569	3.201074	-1.293875	C	5.083431	-1.886164	-3.294815
H	-2.103526	2.303126	-2.500254	H	2.978260	-2.349821	-3.487915
C	-2.833339	4.320067	-2.186784	H	3.535977	-1.120366	-4.618497
C	-3.832975	4.733526	0.095308	H	2.310494	-5.030301	-0.410162
H	-3.851364	3.023078	1.406880	H	0.918576	-6.105197	-0.199745
H	-2.236709	3.633587	1.052191	H	1.403606	-5.003031	1.108345
H	-3.023017	0.491788	-3.161462	H	-0.164559	-3.299790	-2.549097
H	-1.796016	-0.670567	-2.655364	H	0.157341	-5.048134	-2.487856
C	-3.572816	-1.564629	-3.519522	H	1.499078	-3.891955	-2.423265
C	-5.658894	-1.317346	-2.104123	H	-0.437102	-3.938489	2.080982
H	-5.383614	-0.197317	-0.266395	H	-0.989354	-5.541793	1.546542
H	-5.179576	0.747254	-1.734765	H	-2.163437	-4.242531	1.827136
H	-2.723271	-1.716379	1.921875	H	-3.086089	-4.633493	-0.409446
H	-4.246696	-1.593242	1.068987	H	-1.862871	-5.812863	-0.909969
C	-4.438483	-1.331425	3.200889	H	-2.141328	-4.349157	-1.878296
C	-3.343824	0.747184	4.127110	H	-2.030711	5.642386	-0.677134
H	-1.607346	0.372451	2.885227	H	-3.504059	6.248547	-1.431281
H	-2.310721	1.957805	2.659879	H	-5.574176	-2.202719	-4.089870
H	1.781183	-1.618718	2.322489	H	-5.348916	-0.456161	-4.062310
H	3.114595	-2.255291	1.387344	H	-4.302383	-0.811202	5.308680
C	3.585326	-1.911897	3.479627	H	-2.771340	-1.286876	4.576996
C	3.534978	0.514445	4.189483	H	3.803359	-1.184911	5.520896
H	3.085128	1.915373	2.609393	H	2.177236	-1.028070	4.860204
H	1.740384	0.862524	3.024386	H	4.748159	5.596757	-1.221541
H	5.119079	1.742207	0.688423	H	4.939680	4.175074	-2.243411
H	5.109541	1.804316	-1.070755	H	5.751169	-1.039745	-3.515248
C	5.087856	3.747141	-0.129152	H	5.388548	-2.705085	-3.959185
C	2.966890	4.353498	-1.373210				
H	2.932455	2.424032	-2.344474				
H	1.475417	2.777277	-1.424450	54			
H	5.432158	-0.319469	-0.974459	Ru	0.008988	0.474998	0.471239
H	4.909226	-1.548385	0.168042	P	-2.378081	0.636814	0.067756
C	5.258645	-2.296259	-1.826314	P	2.415801	0.338419	0.159375
C	3.633857	-1.472462	-3.583129	B	-0.201970	-1.665248	0.010438
H	2.114475	-0.117634	-2.831324	H	0.063052	0.797601	-1.096075
H	3.754129	0.526805	-2.793903	H	0.339239	-0.198161	2.182488
C	1.307984	-5.104964	0.024826	C	-3.112814	2.394787	0.070822
C	0.468544	-4.071454	-2.101115	C	-2.978498	-0.052461	-1.605206
C	-1.160313	-4.463907	1.449480	C	-3.603588	-0.190248	1.291144
C	-2.093726	-4.742085	-0.860004	C	3.416480	-0.127473	1.701172
H	-2.197110	4.738232	-2.977809	C	3.156192	2.042211	-0.253407
H	-3.809436	4.109685	-2.649808	C	3.025431	-0.910673	-1.130448
C	-3.018092	5.339033	-1.054770	O	0.033444	-2.360573	-1.182059
H	-4.859818	4.540086	-0.250454	O	-0.588277	-2.591874	0.995401
H	-3.913036	5.447591	0.925239	H	-4.159679	2.257565	-0.233512
H	-3.179573	-1.548570	-4.544556	C	-2.442739	3.328148	-0.960921
				C	-3.143733	3.053815	1.468592

H	-2.988729	-1.133656	-1.418725	H	-6.032647	-1.513061	1.843201
C	-2.018095	0.152631	-2.796728	H	-5.425466	-3.152690	1.642308
C	-4.413208	0.371549	-1.996313	C	-4.621093	-2.104643	3.369890
H	-4.490131	0.462394	1.280454	H	-3.677084	-0.714135	4.750438
C	-4.076289	-1.613365	0.921892	H	-4.947164	0.001307	3.761306
C	-3.049004	-0.224024	2.732636	H	3.627451	-2.951356	3.756703
H	4.473668	-0.110770	1.404025	H	4.979140	-1.997543	3.152507
C	3.090488	-1.555374	2.185966	C	3.736651	-0.933723	4.565752
C	3.242429	0.883604	2.855613	H	3.896038	1.211389	4.896863
H	2.876476	2.608801	0.645226	H	5.140735	0.544120	3.845034
C	4.691459	2.147954	-0.387129	H	4.893390	4.091487	0.545697
C	2.489184	2.776461	-1.439061	H	6.226715	3.679221	-0.529150
H	2.448033	-1.804544	-0.865800	C	4.444578	4.400046	-1.549490
C	4.522190	-1.295951	-1.115839	H	2.446521	4.754855	-2.329763
C	2.592650	-0.532741	-2.563693	H	2.543239	4.757588	-0.571255
C	-0.349978	-3.754929	-1.043898	H	5.870948	-2.692343	-2.088785
C	-0.392144	-3.947218	0.518610	H	4.269126	-3.347544	-1.763753
H	-1.375984	3.422502	-0.731052	C	4.349505	-2.097871	-3.527779
H	-2.503445	2.893429	-1.963800	H	2.237956	-2.531485	-3.294265
C	-3.081808	4.728340	-0.980004	H	2.585611	-1.364341	-4.566061
C	-3.777621	4.456542	1.426451	H	0.649470	-4.403115	-2.846591
H	-3.713858	2.434906	2.168929	H	0.447936	-5.690599	-1.647621
H	-2.127552	3.132868	1.869770	H	1.692875	-4.445844	-1.419551
H	-1.908494	1.221015	-3.022222	H	-2.491021	-3.334224	-1.233824
H	-1.026850	-0.217498	-2.529435	H	-2.036663	-4.977513	-1.724569
C	-2.523786	-0.577195	-4.055009	H	-1.639402	-3.594914	-2.762804
C	-4.908110	-0.386450	-3.240983	H	1.779269	-3.857679	0.771008
H	-5.115103	0.218090	-1.167477	H	1.117592	-5.503434	0.850907
H	-4.429584	1.446265	-2.221174	H	0.882568	-4.377387	2.202710
H	-3.207491	-2.281599	0.918514	H	-1.509614	-4.844529	2.132796
H	-4.514536	-1.642356	-0.080090	H	-1.423084	-5.859852	0.683548
C	-5.127114	-2.133549	1.922105	H	-2.512680	-4.460743	0.728231
C	-4.105789	-0.707868	3.739816	H	-2.041775	5.542624	0.731969
H	-2.198293	-0.915618	2.753268	H	-3.569080	6.352699	0.382680
H	-2.666449	0.755861	3.036541	H	-4.302190	-0.757878	-5.297238
H	2.020562	-1.628095	2.419465	H	-3.979522	0.877535	-4.726998
H	3.277325	-2.280644	1.386146	H	-5.416350	-2.418896	4.058333
C	3.914467	-1.944907	3.425535	H	-3.801845	-2.829619	3.481444
C	4.069793	0.486689	4.091018	H	4.365549	-1.208377	5.422415
H	3.533868	1.890816	2.537736	H	2.695023	-0.963727	4.918659
H	2.182204	0.939504	3.135265	H	4.731617	5.458946	-1.512911
H	5.204649	1.633152	0.432849	H	4.796579	4.014232	-2.518115
H	5.015148	1.661972	-1.316551	H	4.970048	-1.273103	-3.909815
C	5.135602	3.623026	-0.419794	H	4.517197	-2.950451	-4.198807
C	2.917616	4.253646	-1.474016	H	-0.432188	0.026404	2.238799
H	2.783180	2.301996	-2.382880	C	0.224635	2.331279	1.003904
H	1.401304	2.697143	-1.375929	O	0.406816	3.420288	1.375301
H	5.139007	-0.433662	-1.395960				
H	4.847724	-1.599662	-0.115014	55			
C	4.800981	-2.445945	-2.102665	Ru	-0.044531	0.553717	0.121625
C	2.873776	-1.675206	-3.553116	P	-2.447325	0.544128	0.008705
H	1.529402	-0.276150	-2.576010	P	2.373978	0.468569	0.074292
H	3.148470	0.355293	-2.890992	B	-0.098428	-1.630519	-0.188621
C	0.675588	-4.625356	-1.774637	H	0.000446	0.781883	-1.425536
C	-1.715917	-3.929591	-1.723588	C	-3.353055	2.217971	0.016357
C	0.930513	-4.455713	1.111737	C	-3.236426	-0.348543	-1.468374
C	-1.532020	-4.827691	1.037841	C	-3.256619	-0.255247	1.537912
H	-2.546757	5.363615	-1.697816	C	3.092794	0.242937	1.812421
H	-4.118503	4.653139	-1.342254	C	3.131332	2.133315	-0.442233
C	-3.079466	5.370571	0.412304	C	3.214825	-0.896840	-0.932839
H	-4.841441	4.366148	1.158916	O	0.041165	-2.386952	-1.356660
H	-3.745550	4.900396	2.429987	O	-0.257597	-2.513598	0.897791
H	-1.842175	-0.375710	-4.891734	H	-4.417015	1.962187	-0.088064
H	-2.485760	-1.661910	-3.878923	C	-2.961553	3.113700	-1.179355
C	-3.958535	-0.181378	-4.428469	C	-3.213668	2.997654	1.343985
H	-4.979561	-1.460052	-3.011012	H	-3.123595	-1.405373	-1.194201
H	-5.922659	-0.053826	-3.497247	C	-2.457585	-0.166993	-2.791226

C	-4.742418	-0.079604	-1.680333
H	-4.162719	0.330710	1.752121
C	-3.684737	-1.728120	1.381016
C	-2.291602	-0.126162	2.741296
H	4.186615	0.319827	1.734046
C	2.755412	-1.146983	2.394022
C	2.610130	1.346525	2.780491
H	2.729418	2.788881	0.341804
C	4.667105	2.291328	-0.402458
C	2.595091	2.699426	-1.778036
H	2.644131	-1.783917	-0.631660
C	4.706208	-1.188363	-0.652498
C	2.974659	-0.722409	-2.448504
C	-0.216151	-3.790711	-1.088789
C	-0.039465	-3.886249	0.474269
H	-1.887543	3.327642	-1.137178
H	-3.134734	2.588323	-2.124078
C	-3.744111	4.438837	-1.191467
C	-4.006318	4.317180	1.313775
H	-3.568521	2.392019	2.184847
H	-2.159513	3.223184	1.536959
H	-2.472081	0.886348	-3.099474
H	-1.410484	-0.437346	-2.635149
C	-3.057695	-1.025510	-3.918972
C	-5.322508	-0.965846	-2.796887
H	-5.303925	-0.237250	-0.750759
H	-4.895595	0.970864	-1.961192
H	-2.803309	-2.325853	1.125148
H	-4.407573	-1.841522	0.565841
C	-4.308754	-2.274611	2.678657
C	-2.912764	-0.666125	4.040213
H	-1.383456	-0.701353	2.511908
H	-1.985074	0.916169	2.882114
H	1.666242	-1.280160	2.416345
H	3.140911	-1.939404	1.744107
C	3.332359	-1.330518	3.808616
C	3.194582	1.163331	4.191251
H	2.875515	2.341645	2.406285
H	1.512677	1.319680	2.838135
H	5.089012	1.887579	0.524961
H	5.119258	1.726718	-1.228001
C	5.062105	3.773794	-0.544676
C	2.973652	4.182767	-1.928050
H	3.022813	2.139887	-2.619204
H	1.510484	2.577248	-1.840186
H	5.321040	-0.328210	-0.940587
H	4.883663	-1.354134	0.415922
C	5.183644	-2.420924	-1.443454
C	3.471369	-1.939789	-3.245643
H	1.908907	-0.559054	-2.637164
H	3.511997	0.166210	-2.802880
C	0.763678	-4.637291	-1.904891
C	-1.643162	-4.098369	-1.566417
C	1.375314	-4.291501	0.914054
C	-1.046048	-4.791329	1.190503
H	-3.403639	5.057117	-2.032272
H	-4.810421	4.231164	-1.368883
C	-3.592676	5.201308	0.130813
H	-5.081739	4.094253	1.242158
H	-3.861010	4.851586	2.261655
H	-2.513406	-0.834517	-4.853044
H	-2.903224	-2.087873	-3.681883
C	-4.558592	-0.770748	-4.113819
H	-5.262608	-2.021747	-2.493410
H	-6.388261	-0.739545	-2.932941
H	-5.245677	-1.735138	2.884594
H	-4.582300	-3.328873	2.538748

C	-3.363600	-2.123828	3.878504
H	-2.190232	-0.577515	4.862031
H	-3.778159	-0.044674	4.316591
H	3.044998	-2.316117	4.197708
H	4.431618	-1.325182	3.755545
C	2.868855	-0.222723	4.763707
H	2.812357	1.951287	4.852998
H	4.286578	1.292311	4.150425
H	4.686096	4.330352	0.326490
H	6.155833	3.869700	-0.527789
C	4.492317	4.392916	-1.829499
H	2.600275	4.565435	-2.886959
H	2.468660	4.761333	-1.141428
H	6.247858	-2.599986	-1.241199
H	4.644734	-3.311516	-1.086387
C	4.944822	-2.253787	-2.950503
H	2.851872	-2.809564	-2.992069
H	3.328689	-1.758567	-4.319065
H	0.603744	-4.452539	-2.972354
H	0.606860	-5.706985	-1.720484
H	1.803945	-4.397932	-1.675745
H	-2.387472	-3.515282	-1.017580
H	-1.888378	-5.160767	-1.456243
H	-1.725258	-3.836510	-2.625824
H	2.141299	-3.675475	0.436024
H	1.584548	-5.341853	0.682527
H	1.464231	-4.155608	1.996544
H	-0.885026	-4.730812	2.272253
H	-0.914736	-5.837646	0.889248
H	-2.079856	-4.503993	0.988957
H	-2.544141	5.506991	0.256334
H	-4.191141	6.121483	0.113136
H	-4.962215	-1.432852	-4.890895
H	-4.711807	0.259212	-4.469727
H	-3.851765	-2.479089	4.795364
H	-2.479356	-2.758274	3.722980
H	3.332990	-0.348590	5.750397
H	1.782271	-0.305742	4.914690
H	4.735697	5.462326	-1.875295
H	4.978377	3.924874	-2.698819
H	5.574361	-1.432348	-3.324751
H	5.259366	-3.157340	-3.488857
C	0.075359	2.458299	0.418769
O	0.204140	3.607199	0.581080

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C	-0.030148	-2.216351	0.760976
O	-0.060437	-3.214900	1.367067
Ru	0.018222	-0.421995	0.034476
P	2.452352	-0.478764	0.160112
P	-2.412604	-0.313760	0.267173
B	0.088585	1.731702	-0.362401
H	0.073182	0.130660	1.498222
C	3.299750	-2.112825	-0.385459
C	3.481158	0.772485	-0.841375
C	3.115703	-0.188968	1.919343
C	-2.953876	0.215679	2.003373
C	-3.217104	-2.035428	0.147354
C	-3.396002	0.870113	-0.843857
O	-0.709992	2.429277	-1.284962
O	0.929408	2.660329	0.269844
H	4.288901	-1.803380	-0.747801
C	2.560803	-2.767370	-1.573993
C	3.550263	-3.174839	0.707800
H	3.070309	1.733538	-0.510626
C	3.222528	0.669564	-2.360603
C	5.003313	0.774738	-0.570767

H	4.164098	-0.523851	1.902260
C	3.095637	1.301822	2.329954
C	2.372037	-1.007792	2.999962
H	-4.052296	0.178618	2.010245
C	-2.527092	1.665126	2.319521
C	-2.453391	-0.733060	3.114473
H	-2.759075	-2.541631	1.007895
C	-4.746810	-2.133782	0.326541
C	-2.787907	-2.853336	-1.091367
H	-2.779015	1.773016	-0.787609
C	-4.833764	1.254944	-0.427894
C	-3.367774	0.438686	-2.326574
C	-0.282762	3.809658	-1.401292
C	0.573124	4.015469	-0.093585
H	1.566224	-3.085362	-1.236754
H	2.405989	-2.037449	-2.375272
C	3.320941	-3.983125	-2.133101
C	4.325529	-4.382771	0.148030
H	4.116379	-2.746239	1.541030
H	2.594348	-3.526441	1.114424
H	3.585559	-0.297495	-2.735825
H	2.145751	0.706522	-2.562362
C	3.943765	1.784404	-3.140224
C	5.715137	1.899889	-1.344625
H	5.215528	0.882217	0.497612
H	5.443722	-0.183099	-0.880614
H	2.060326	1.659082	2.323717
H	3.629782	1.922930	1.605155
C	3.723186	1.508868	3.720377
C	3.012689	-0.821229	4.386124
H	1.329798	-0.670740	3.034651
H	2.340523	-2.070469	2.750633
H	-1.433226	1.727876	2.275334
H	-2.910075	2.355553	1.558490
C	-3.014723	2.113904	3.707857
C	-2.939261	-0.283127	4.503470
H	-2.792236	-1.759639	2.935885
H	-1.357069	-0.757415	3.098473
H	-5.082060	-1.566119	1.201945
H	-5.248731	-1.694839	-0.545335
C	-5.195075	-3.601060	0.462408
C	-3.235015	-4.321438	-0.971281
H	-3.224037	-2.419642	-2.000629
H	-1.699480	-2.812926	-1.200406
H	-5.497718	0.384847	-0.482890
H	-4.864448	1.605252	0.609265
C	-5.391574	2.360590	-1.344739
C	-3.936083	1.536121	-3.242481
H	-2.340446	0.210082	-2.625705
H	-3.963346	-0.474699	-2.462400
C	-1.519708	4.706052	-1.506327
C	0.524056	3.917960	-2.703082
C	-0.223073	4.603608	1.081888
C	1.858192	4.826418	-0.279789
H	2.745291	-4.431349	-2.953490
H	4.274252	-3.646286	-2.567517
C	3.600613	-5.023819	-1.041804
H	5.327013	-4.055288	-0.169740
H	4.477734	-5.121159	0.945943
H	3.759273	1.663493	-4.215843
H	3.519059	2.758350	-2.858988
C	5.450692	1.800232	-2.852389
H	5.361561	2.873990	-0.975514
H	6.793421	1.862198	-1.141370
H	4.791638	1.246523	3.678922
H	3.675772	2.572708	3.988493
C	3.038275	0.656686	4.796553

H	2.462415	-1.415083	5.127631
H	4.040848	-1.214254	4.372705
H	-2.670737	3.137535	3.905863
H	-4.114862	2.146934	3.716277
C	-2.529186	1.163483	4.810312
H	-2.543198	-0.963676	5.268331
H	-4.035750	-0.365875	4.550252
H	-4.765608	-4.026234	1.381562
H	-6.286080	-3.647050	0.576635
C	-4.748653	-4.439719	-0.743365
H	-2.940793	-4.873467	-1.873430
H	-2.701331	-4.786735	-0.130011
H	-6.418165	2.607329	-1.043025
H	-4.796546	3.275557	-1.208894
C	-5.353318	1.948833	-2.822851
H	-3.270715	2.409203	-3.199205
H	-3.933274	1.188804	-4.284417
H	-2.067674	4.473995	-2.425803
H	-1.235654	5.764608	-1.544719
H	-2.200643	4.563314	-0.663719
H	1.400056	3.265202	-2.682262
H	0.856875	4.943931	-2.897110
H	-0.108516	3.599253	-3.538071
H	-1.140992	4.038604	1.264001
H	-0.487214	5.653632	0.912705
H	0.389842	4.546318	1.987290
H	2.406273	4.865347	0.667630
H	1.635060	5.856451	-0.582758
H	2.516560	4.381534	-1.029838
H	2.648147	-5.452254	-0.696979
H	4.190737	-5.855549	-1.447658
H	5.932632	2.631762	-3.382603
H	5.905612	0.876059	-3.239556
H	3.542984	0.781050	5.763645
H	2.005080	1.009402	4.932818
H	-2.923599	1.474846	5.786288
H	-1.432888	1.221666	4.880297
H	-5.032546	-5.490703	-0.603652
H	-5.279008	-4.089571	-1.641824
H	-6.039724	1.102988	-2.979964
H	-5.717843	2.767703	-3.456739
C	-0.195324	-1.860021	-3.280246
O	-0.312903	-2.785567	-3.982101
O	-0.076262	-0.924019	-2.587011

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C	0.098415	1.796740	1.461380
O	0.180381	2.551202	2.337681
Ru	-0.002406	0.445823	0.097172
P	-2.506113	0.570587	0.075743
P	2.484659	0.306627	0.127113
B	-0.165050	-1.730785	-0.146483
H	-0.007525	-0.665903	1.284097
C	-3.327016	2.277938	-0.159269
C	-3.354973	-0.491552	-1.245733
C	-3.389832	0.047896	1.697592
C	3.190915	-0.419072	1.731312
C	3.277626	2.046145	0.072008
C	3.320396	-0.757991	-1.192089
O	0.858033	-2.550218	-0.619157
O	-1.288021	-2.518492	0.118745
H	-4.396068	2.057970	-0.017482
C	-3.174731	2.913032	-1.559455
C	-2.925659	3.312383	0.914659
H	-3.245381	-1.496885	-0.825199
C	-2.614647	-0.519861	-2.601479
C	-4.861359	-0.218033	-1.457275

H	-4.267878	0.709787	1.751721	H	-2.660169	0.223586	5.115255
C	-3.908021	-1.408091	1.741296	H	-4.146461	0.746412	4.329439
C	-2.528441	0.309170	2.954053	H	3.554100	-3.546745	3.239959
H	4.268933	-0.214203	1.687222	H	4.795827	-2.311812	3.067537
C	3.025803	-1.946279	1.873717	C	3.197439	-1.748344	4.410984
C	2.630991	0.276781	2.991335	H	2.895704	0.277868	5.143334
H	2.522276	2.660678	0.578712	H	4.390444	0.050428	4.240544
C	4.614804	2.259542	0.821402	H	4.241669	4.299021	1.434820
C	3.415898	2.608141	-1.363244	H	5.950960	3.880007	1.368240
H	2.964912	-1.754589	-0.910545	C	5.067611	4.359183	-0.562377
C	4.864747	-0.775182	-1.169600	H	3.864270	4.473325	-2.370248
C	2.790299	-0.524323	-2.624503	H	2.940151	4.658691	-0.883883
C	0.343823	-3.885254	-0.879765	H	6.516446	-1.801541	-2.136795
C	-0.936676	-3.925184	0.028086	H	5.125048	-2.829683	-1.804427
H	-2.129338	3.180154	-1.736663	C	4.891872	-1.607263	-3.573910
H	-3.463276	2.211794	-2.346353	H	2.974148	-2.568713	-3.315218
C	-4.029745	4.188617	-1.681665	H	2.993022	-1.374403	-4.609801
C	-3.764920	4.598350	0.796652	H	2.287513	-4.776008	-1.187661
H	-3.045285	2.902167	1.922484	H	1.055918	-5.929253	-0.652921
H	-1.866669	3.565346	0.792906	H	1.773320	-4.789474	0.505494
H	-2.641284	0.465382	-3.080527	H	-0.727947	-3.237061	-2.671897
H	-1.556834	-0.747765	-2.442670	H	-0.316820	-4.966266	-2.666268
C	-3.247709	-1.554088	-3.549155	H	0.941486	-3.748560	-2.948603
C	-5.483985	-1.266138	-2.397873	H	0.174222	-3.869852	1.912905
H	-5.401285	-0.211528	-0.502987	H	-0.431819	-5.484610	1.484770
H	-5.005693	0.774359	-1.901327	H	-1.548362	-4.238851	2.074256
H	-3.055921	-2.090502	1.661401	H	-2.975917	-4.628253	0.133258
H	-4.561413	-1.621141	0.890176	H	-1.877565	-5.755914	-0.678276
C	-4.690008	-1.690207	3.037485	H	-2.436065	-4.294501	-1.518376
C	-3.309785	0.035748	4.250582	H	-2.634622	5.563306	-0.771823
H	-1.645920	-0.341167	2.914548	H	-4.312305	6.099488	-0.679150
H	-2.151753	1.334875	2.971844	H	-5.183171	-2.091671	-4.388166
H	1.957996	-2.192695	1.899655	H	-4.899326	-0.357322	-4.270559
H	3.442943	-2.469408	1.007828	H	-4.453462	-1.557301	5.196324
C	3.709270	-2.463171	3.153090	H	-3.013244	-2.102686	4.338693
C	3.325612	-0.225998	4.268242	H	3.741507	-2.099000	5.297394
H	2.727836	1.365492	2.923363	H	2.139805	-2.006686	4.569056
H	1.557461	0.066930	3.061562	H	5.275383	5.435251	-0.501638
H	4.557719	1.900020	1.852784	H	5.911456	3.908200	-1.106197
H	5.415943	1.689733	0.332012	H	5.279602	-0.652545	-3.959847
C	4.993624	3.753993	0.845549	H	5.269345	-2.390827	-4.243751
C	3.770651	4.103990	-1.340909	C	0.114908	2.200082	-1.267539
H	4.212100	2.065557	-1.888665	O	0.006823	1.267677	-2.071844
H	2.501391	2.464088	-1.941361	O	0.223253	3.399012	-1.190869
H	5.258175	0.209228	-1.453040				
H	5.242636	-0.985003	-0.161742				
C	5.418851	-1.826835	-2.149065	57			
C	3.357264	-1.575946	-3.594076	C	0.675158	-2.412116	0.888577
H	1.698308	-0.560472	-2.625540	O	0.849487	-3.454517	1.396960
H	3.072881	0.471210	-2.983982	Ru	0.334239	-0.878984	-0.056037
C	1.426210	-4.905282	-0.523721	P	2.699386	-0.192575	0.029511
C	0.031982	-3.967683	-2.380985	P	-2.052371	-1.362740	0.104518
C	-0.659901	-4.413376	1.459015	B	-0.725136	3.240732	0.181664
C	-2.123873	-4.695071	-0.551396	H	-0.199430	2.190728	0.364791
H	-3.898248	4.620795	-2.681977	C	3.969590	-1.308637	-0.825007
H	-5.095093	3.926125	-1.590948	C	3.090317	1.595244	-0.493402
C	-3.664009	5.216777	-0.603424	C	3.265857	-0.082859	1.841132
H	-4.817825	4.366554	1.018375	C	-2.676702	-0.940370	1.839917
H	-3.436868	5.318071	1.557644	C	-2.530069	-3.176795	-0.094955
H	-2.728529	-1.534857	-4.516185	C	-3.104400	-0.268229	-1.031136
H	-3.100213	-2.562995	-3.134994	O	-2.034789	3.365389	-0.193454
C	-4.751105	-1.313093	-3.746196	O	-0.078057	4.434141	0.341731
H	-5.434228	-2.256684	-1.921626	H	4.933373	-1.105071	-0.332316
H	-6.548644	-1.043921	-2.547736	C	4.132947	-1.022547	-2.337471
H	-5.599002	-1.069828	3.055059	C	3.620217	-2.806390	-0.646461
H	-5.028582	-2.734856	3.038364	H	2.582449	2.171051	0.295845
C	-3.855563	-1.396506	4.289857	C	2.452350	2.036027	-1.830196
				C	4.584620	1.996142	-0.452614

H	4.140468	0.581830	1.844222
C	2.162795	0.587386	2.693094
C	3.711701	-1.406044	2.497151
H	-3.773887	-0.993883	1.811285
C	-2.274823	0.503986	2.213151
C	-2.201243	-1.923419	2.932627
H	-2.005755	-3.634139	0.756904
C	-4.030549	-3.505049	0.052569
C	-1.943571	-3.846075	-1.358821
H	-2.531717	0.669197	-1.029554
C	-4.539401	0.065395	-0.563889
C	-3.134469	-0.770029	-2.493600
C	-2.257657	4.772322	-0.527195
C	-1.083979	5.490207	0.248256
H	3.174721	-1.196675	-2.841960
H	4.406468	0.019986	-2.516275
C	5.210659	-1.927044	-2.963910
C	4.704036	-3.713108	-1.254216
H	3.478220	-3.064199	0.405388
H	2.666209	-2.998456	-1.150962
H	2.913475	1.492440	-2.663513
H	1.393833	1.769975	-1.852492
C	2.635726	3.547590	-2.056126
C	4.759018	3.509359	-0.680314
H	5.048559	1.721770	0.501550
H	5.137443	1.456360	-1.231446
H	1.270175	-0.054721	2.679208
H	1.861127	1.547973	2.258049
C	2.611305	0.801758	4.148816
C	4.164154	-1.182899	3.952292
H	2.886989	-2.128883	2.486448
H	4.535730	-1.854162	1.931614
H	-1.177360	0.576240	2.207040
H	-2.631456	1.218126	1.463000
C	-2.799615	0.904563	3.602218
C	-2.732329	-1.518735	4.319697
H	-2.531675	-2.943355	2.708124
H	-1.104387	-1.949811	2.959531
H	-4.444931	-3.052989	0.961822
H	-4.585095	-3.075749	-0.792411
C	-4.261875	-5.027309	0.079063
C	-2.175927	-5.366622	-1.321348
H	-2.420991	-3.436608	-2.256701
H	-0.876224	-3.628552	-1.452220
H	-5.153757	-0.844732	-0.552593
H	-4.542797	0.460475	0.456936
C	-5.187162	1.107908	-1.494482
C	-3.774018	0.276830	-3.421281
H	-2.126212	-0.999790	-2.843539
H	-3.723895	-1.694903	-2.551368
C	-3.664982	5.158909	-0.077369
C	-2.139916	4.880404	-2.053038
C	-1.444705	5.871697	1.690152
C	-0.463148	6.685203	-0.472129
H	5.289668	-1.706484	-4.036285
H	6.188683	-1.682918	-2.521225
C	4.911810	-3.415254	-2.744478
H	5.652642	-3.568511	-0.714118
H	4.420335	-4.763543	-1.110403
H	2.204116	3.823966	-3.027445
H	2.069033	4.097809	-1.291574
C	4.112179	3.962995	-1.996367
H	4.300235	4.055165	0.157401
H	5.827646	3.761681	-0.670235
H	3.437827	1.527663	4.170763
H	1.790480	1.247057	4.726236
C	3.070739	-0.512277	4.794427

H	4.452767	-2.144122	4.396244
H	5.065473	-0.551709	3.960121
H	-2.466411	1.922571	3.843520
H	-3.899424	0.933648	3.579784
C	-2.340602	-0.080872	4.685309
H	-2.357080	-2.221431	5.074614
H	-3.828960	-1.608307	4.327589
H	-3.798735	-5.444844	0.985500
H	-5.336935	-5.237864	0.152475
C	-3.663135	-5.712867	-1.157741
H	-1.777401	-5.820042	-2.237584
H	-1.606316	-5.799048	-0.485413
H	-6.210701	1.317934	-1.156439
H	-4.624346	2.048285	-1.405621
C	-5.188493	0.653059	-2.960204
H	-3.137758	1.173153	-3.437750
H	-3.796811	-0.109017	-4.448493
H	-4.403950	4.589214	-0.649883
H	-3.849920	6.224712	-0.254087
H	-3.824604	4.948767	0.982613
H	-1.141204	4.596194	-2.398478
H	-2.353804	5.896207	-2.402009
H	-2.860920	4.198999	-2.514861
H	-1.882027	5.025730	2.230009
H	-2.152326	6.706712	1.721232
H	-0.533420	6.172539	2.216085
H	0.361490	7.085052	0.126522
H	-1.200784	7.484386	-0.608554
H	-0.065478	6.406865	-1.450464
H	3.999865	-3.684914	-3.295090
H	5.723913	-4.031877	-3.151493
H	4.211354	5.050261	-2.112218
H	4.652756	3.507798	-2.839730
H	3.430625	-0.331776	5.815448
H	2.210918	-1.193133	4.879241
H	-2.764698	0.194745	5.659338
H	-1.247056	-0.019484	4.790191
H	-3.799444	-6.799967	-1.090689
H	-4.211255	-5.383239	-2.053117
H	-5.849280	-0.220416	-3.067463
H	-5.606401	1.439693	-3.602115
C	0.422675	-1.205626	-2.042052
O	0.027624	-0.004029	-2.136660
O	0.733409	-2.114382	-2.785017

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Ru	-0.056168	-0.221467	-0.059035
O	0.018954	-3.291154	0.154120
C	-0.009964	-2.141245	-0.050100
C	0.153414	-1.062760	-3.149982
O	-0.110946	0.007989	-2.747480
O	0.414971	-2.110761	-3.591765
P	-2.442983	0.042004	0.107070
P	2.311686	0.144461	0.131565
C	-3.633218	-0.979417	-0.986176
C	-3.071984	-0.334897	1.857523
C	-3.053691	1.824559	-0.156470
C	2.855445	1.928898	-0.190363
C	3.384971	-0.816385	-1.121806
C	2.969769	-0.171483	1.876334
H	-4.583110	-1.001504	-0.433758
C	-3.144588	-2.434676	-1.152492
C	-3.944523	-0.381960	-2.375689
H	-2.514905	0.401857	2.452096
C	-2.662624	-1.722325	2.397911
C	-4.579687	-0.112516	2.112909
H	-4.141795	1.762837	-0.314773

C	-2.800798	2.742687	1.061582
C	-2.408644	2.469735	-1.406276
H	3.953983	1.930229	-0.194138
C	2.400156	2.930743	0.891569
C	2.365385	2.389594	-1.580923
H	2.790566	-0.712518	-2.043493
C	4.799344	-0.285790	-1.451840
C	3.460988	-2.328152	-0.813213
H	2.420025	0.596299	2.440636
C	4.477292	0.066811	2.112558
C	2.547533	-1.526411	2.487100
H	-2.192534	-2.430923	-1.698917
H	-2.928400	-2.892432	-0.183531
C	-4.158573	-3.300557	-1.918683
C	-4.955367	-1.246588	-3.151882
H	-4.349161	0.630477	-2.281708
H	-3.016731	-0.299287	-2.960190
H	-3.212874	-2.508466	1.863087
H	-1.598569	-1.900079	2.222373
C	-2.976008	-1.839496	3.899684
C	-4.905581	-0.220173	3.614462
H	-4.913572	0.859209	1.732654
H	-5.160963	-0.874142	1.574831
H	-1.721722	2.770134	1.261273
H	-3.280096	2.348674	1.962940
C	-3.320015	4.171815	0.818312
C	-2.940240	3.890677	-1.660793
H	-1.324928	2.507495	-1.242858
H	-2.564802	1.856978	-2.297861
H	1.307431	2.892606	0.974579
H	2.804087	2.651421	1.871640
C	2.849067	4.366001	0.559111
C	2.818237	3.822561	-1.907904
H	2.718515	1.707317	-2.364526
H	1.269108	2.340979	-1.594028
H	4.773473	0.775748	-1.716336
H	5.445881	-0.374332	-0.569649
C	5.426931	-1.069313	-2.621093
C	4.071956	-3.110674	-1.988238
H	4.090165	-2.481166	0.073835
H	2.473006	-2.730566	-0.574771
H	5.056803	-0.709187	1.594382
H	4.798240	1.028450	1.695760
C	4.816135	0.017099	3.614136
C	2.881513	-1.575965	3.987967
H	1.477054	-1.687571	2.336362
H	3.067142	-2.348995	1.980419
H	-3.762277	-4.317899	-2.029463
H	-5.083995	-3.387890	-1.329593
C	-4.485181	-2.699757	-3.291748
H	-5.920400	-1.228473	-2.623582
H	-5.134112	-0.803295	-4.140276
H	-2.691915	-2.836467	4.260558
H	-2.355844	-1.118403	4.452713
C	-4.458340	-1.569295	4.195730
H	-4.397685	0.594756	4.151296
H	-5.982278	-0.074393	3.772319
H	-4.416131	4.146657	0.721560
H	-3.100712	4.793891	1.696086
C	-2.717319	4.798473	-0.444858
H	-2.450014	4.312576	-2.548093
H	-4.015962	3.847404	-1.890651
H	2.479950	5.052716	1.332071
H	3.947800	4.422224	0.592298
C	2.365149	4.812458	-0.826754
H	2.425301	4.119458	-2.889142
H	3.915489	3.851093	-1.989093

H	4.840577	-0.878780	-3.532572
H	6.438025	-0.689300	-2.817569
C	5.464870	-2.579862	-2.352966
H	4.123321	-4.177128	-1.734212
H	3.405496	-3.029632	-2.859524
H	5.894426	0.166787	3.756818
H	4.314332	0.853919	4.122442
C	4.369888	-1.306063	4.252840
H	2.276100	-0.824064	4.516083
H	2.593233	-2.552311	4.398440
H	-3.584436	-2.731323	-3.923077
H	-5.247229	-3.300284	-3.804865
H	-4.645931	-1.598579	5.276863
H	-5.066354	-2.371459	3.751144
H	-3.146898	5.793234	-0.621463
H	-1.636910	4.943806	-0.296833
H	2.731913	5.822066	-1.052946
H	1.266438	4.869019	-0.826332
H	5.862852	-3.111343	-3.226948
H	6.157118	-2.782553	-1.522021
H	4.966657	-2.128940	3.831449
H	4.572208	-1.294616	5.331653
H	-0.065131	-0.274508	1.508537
H	-0.101533	1.413367	0.281765

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Ru	-0.062997	-0.154199	-0.008965
O	-0.049079	-3.208565	0.189832
C	-0.048991	-2.053785	0.085517
C	0.044469	-0.250648	-2.150199
O	-0.038465	0.989927	-1.998387
O	0.137421	-1.063695	-3.042989
P	-2.499372	0.013048	0.076959
P	2.376174	0.100798	0.113481
C	-3.522148	-0.750880	-1.323845
C	-3.260150	-0.709745	1.660734
C	-3.123790	1.812057	0.134228
C	2.961860	1.894394	-0.048895
C	3.369607	-0.774169	-1.238857
C	3.018317	-0.398350	1.829314
H	-4.554757	-0.773703	-0.947401
C	-3.080755	-2.202496	-1.619184
C	-3.536162	0.072889	-2.631294
H	-2.892725	-0.008945	2.422210
C	-2.739735	-2.096840	2.090887
C	-4.805134	-0.689910	1.702203
H	-4.162206	1.768800	-0.229239
C	-3.147990	2.440490	1.546634
C	-2.313099	2.735322	-0.806051
H	4.033596	1.877391	0.193161
C	2.264235	2.817033	0.974372
C	2.819925	2.473486	-1.475205
H	3.040367	-0.223834	-2.132208
C	4.905525	-0.639976	-1.146803
C	2.974591	-2.246789	-1.487652
H	2.248003	0.041611	2.478700
C	4.381567	0.167432	2.289178
C	2.979276	-1.924511	2.063561
H	-2.044336	-2.194539	-1.974998
H	-3.098001	-2.807484	-0.706598
C	-3.969741	-2.861503	-2.687882
C	-4.416925	-0.595447	-3.703143
H	-3.914556	1.083250	-2.445366
H	-2.515268	0.177860	-3.016711
H	-3.054052	-2.865345	1.373409
H	-1.647968	-2.098434	2.102510
C	-3.267714	-2.471947	3.487808

C	-5.331842	-1.059809	3.100954
H	-5.198914	0.289532	1.405425
H	-5.198826	-1.416536	0.978780
H	-2.126022	2.457016	1.951096
H	-3.754054	1.848867	2.238951
C	-3.712988	3.873797	1.519273
C	-2.899433	4.155731	-0.851924
H	-1.280729	2.780622	-0.439105
H	-2.248065	2.323756	-1.814237
H	1.185790	2.815260	0.774443
H	2.387151	2.432705	1.994486
C	2.797802	4.257614	0.897446
C	3.345071	3.918990	-1.544964
H	3.376615	1.864004	-2.195702
H	1.769792	2.438970	-1.783859
H	5.205682	0.401951	-0.986723
H	5.268369	-1.210161	-0.281142
C	5.588467	-1.182442	-2.415687
C	3.664899	-2.791243	-2.750999
H	3.254300	-2.867952	-0.627376
H	1.894624	-2.328318	-1.616312
H	5.188452	-0.245999	1.671771
H	4.418663	1.254739	2.168610
C	4.651176	-0.179164	3.766025
C	3.241165	-2.267920	3.540150
H	2.017385	-2.341144	1.751573
H	3.749972	-2.408099	1.448669
H	-3.609393	-3.879470	-2.882952
H	-4.997112	-2.959541	-2.304989
C	-3.983941	-2.040195	-3.983337
H	-5.464557	-0.589279	-3.365090
H	-4.382489	0.001154	-4.623690
H	-2.902991	-3.470058	3.761745
H	-2.850383	-1.772669	4.227912
C	-4.800144	-2.425433	3.556439
H	-5.021613	-0.288101	3.821129
H	-6.429486	-1.058005	3.095102
H	-4.772221	3.833112	1.224016
H	-3.690198	4.292071	2.534092
C	-2.953518	4.783382	0.546103
H	-2.297976	4.776913	-1.527880
H	-3.913747	4.123727	-1.278367
H	2.261923	4.886328	1.620435
H	3.857278	4.273930	1.194969
C	2.659496	4.830714	-0.519085
H	3.200887	4.309264	-2.560487
H	4.430302	3.921723	-1.360732
H	5.301389	-0.557319	-3.273971
H	6.678091	-1.093169	-2.314557
C	5.190696	-2.639008	-2.690665
H	3.390886	-3.844776	-2.889232
H	3.274967	-2.251322	-3.625454
H	5.632901	0.212981	4.061533
H	3.908359	0.333043	4.395501
C	4.577724	-1.690097	4.024754
H	2.423259	-1.863431	4.154640
H	3.223762	-3.357012	3.674051
H	-2.975257	-2.037756	-4.419410
H	-4.650627	-2.501241	-4.723498
H	-5.144788	-2.648316	4.574260
H	-5.216134	-3.209212	2.906181
H	-3.420984	5.775860	0.509190
H	-1.927717	4.932132	0.914238
H	3.080384	5.843377	-0.565379
H	1.592473	4.920453	-0.770237
H	5.648371	-2.988099	-3.625153
H	5.589415	-3.278787	-1.888802

H	5.401188	-2.189285	3.492533
H	4.722600	-1.900906	5.091990
H	-0.071900	-0.165651	1.642250
H	-0.136311	0.991111	1.258058

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Ru	-0.038524	-0.027441	0.146618
O	0.086163	-2.996056	0.634140
C	0.020050	-1.833560	0.513027
C	0.001436	0.257023	-1.849589
O	0.028545	1.491437	-1.520457
O	-0.004834	-0.363584	-2.897106
P	-2.530052	-0.000583	0.082776
P	2.429121	0.117698	0.142319
C	-3.412660	-1.071234	-1.221816
C	-3.326482	-0.631465	1.698828
C	-3.272647	1.746921	-0.029526
C	3.066417	1.899201	0.092401
C	3.258733	-0.674003	-1.353788
C	3.189901	-0.569116	1.752698
H	-4.343166	-1.391441	-0.730405
C	-2.587224	-2.335871	-1.558987
C	-3.817206	-0.352703	-2.527096
H	-2.807847	-0.057293	2.480090
C	-3.042468	-2.122292	1.981137
C	-4.842898	-0.361249	1.846065
H	-4.360556	1.602229	-0.106541
C	-2.982342	2.557420	1.257736
C	-2.817072	2.588269	-1.245140
H	4.123289	1.847007	0.385882
C	2.324220	2.766070	1.134310
C	3.013865	2.572098	-1.298268
H	2.907002	-0.015077	-2.160352
C	4.802593	-0.640156	-1.358935
C	2.730945	-2.081849	-1.710937
H	2.428485	-0.296028	2.498698
C	4.526342	0.047143	2.228861
C	3.291575	-2.111888	1.762897
H	-1.653392	-2.028155	-2.042227
H	-2.309549	-2.878375	-0.651076
C	-3.362865	-3.278618	-2.495326
C	-4.589287	-1.298249	-3.465872
H	-4.443838	0.519244	-2.311093
H	-2.916174	0.005723	-3.040745
H	-3.540362	-2.741602	1.223028
H	-1.974281	-2.332160	1.908082
C	-3.551236	-2.541979	3.371223
C	-5.360371	-0.786017	3.233699
H	-5.076501	0.696034	1.688778
H	-5.393743	-0.920758	1.077082
H	-1.896752	2.710153	1.337128
H	-3.289591	2.015330	2.157781
C	-3.686142	3.926883	1.238324
C	-3.547478	3.941780	-1.282922
H	-1.737615	2.747174	-1.187768
H	-2.987090	2.058788	-2.183557
H	1.260553	2.803445	0.864886
H	2.381667	2.311784	2.132701
C	2.883175	4.198092	1.187523
C	3.574167	4.004934	-1.236649
H	3.598581	1.997897	-2.025538
H	1.980651	2.585155	-1.658668
H	5.175702	0.367877	-1.140589
H	5.188829	-1.296709	-0.567847
C	5.361849	-1.112747	-2.713189
C	3.302592	-2.544689	-3.062298
H	3.007776	-2.805583	-0.934802

H	1.640806	-2.059119	-1.770736
H	5.322208	-0.176912	1.506525
H	4.454395	1.137135	2.291781
C	4.929679	-0.494488	3.613757
C	3.683039	-2.641279	3.153445
H	2.350847	-2.569993	1.450788
H	4.054495	-2.428759	1.040203
H	-2.739550	-4.151402	-2.727799
H	-4.256236	-3.661246	-1.977549
C	-3.788565	-2.566437	-3.785502
H	-5.542498	-1.578676	-2.991936
H	-4.845797	-0.762311	-4.388816
H	-3.343228	-3.607701	3.529516
H	-2.987439	-1.995886	4.142356
C	-5.048842	-2.256960	3.537581
H	-4.893081	-0.150394	4.000627
H	-6.440748	-0.601368	3.293242
H	-4.775159	3.769542	1.253216
H	-3.439735	4.477595	2.155667
C	-3.308634	4.748685	-0.000421
H	-3.210880	4.511253	-2.158558
H	-4.628208	3.777432	-1.414552
H	2.313007	4.789675	1.915627
H	3.921394	4.171283	1.551466
C	2.845322	4.863810	-0.194505
H	3.499740	4.466605	-2.229462
H	4.646221	3.969251	-0.988855
H	5.069052	-0.394130	-3.492694
H	6.459306	-1.109669	-2.680852
C	4.837148	-2.506514	-3.086107
H	2.943107	-3.557971	-3.281988
H	2.905255	-1.894470	-3.854356
H	5.892927	-0.058892	3.909074
H	4.193309	-0.154669	4.357407
C	5.000978	-2.026308	3.640079
H	2.881729	-2.405428	3.869434
H	3.758456	-3.735489	3.119998
H	-2.891659	-2.293106	-4.358630
H	-4.378946	-3.239745	-4.420556
H	-5.380499	-2.515284	4.551320
H	-5.617999	-2.898422	2.848448
H	-3.875728	5.688320	-0.021017
H	-2.245313	5.023646	0.058384
H	3.289416	5.866480	-0.146703
H	1.798421	4.996402	-0.503478
H	5.212434	-2.799625	-4.075027
H	5.231707	-3.244092	-2.370742
H	5.820227	-2.363776	2.987962
H	5.240607	-2.378878	4.651341
H	-0.482473	0.663961	2.092116
H	0.286419	0.698533	2.104325

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C	0.016257	-0.047376	1.889828
O	-0.013033	-0.091029	3.060441
Ru	0.041947	-0.112006	0.051771
P	2.481459	0.025117	-0.039723
P	-2.382026	0.056691	-0.034069
C	3.549114	-0.722832	1.339011
C	3.287943	-0.705524	-1.592948
C	2.906640	1.866906	-0.159453
C	-2.872102	1.876682	0.082349
C	-3.289433	-0.744327	1.407697
C	-3.124872	-0.512314	-1.683156
H	4.498398	-0.976406	0.845357
C	2.921279	-2.035270	1.867363
C	3.896744	0.198825	2.526301

H	2.622993	-0.372726	-2.401006
C	3.279432	-2.252094	-1.615362
C	4.721145	-0.205959	-1.890835
H	3.996607	1.976646	-0.058528
C	2.482898	2.445487	-1.531998
C	2.229308	2.699621	0.954910
H	-3.947373	1.947703	-0.130194
C	-2.112279	2.694728	-0.986800
C	-2.635962	2.486517	1.481900
H	-2.882610	-0.176878	2.257671
C	-4.823937	-0.583743	1.433413
C	-2.892642	-2.218278	1.654692
H	-2.326314	-0.245802	-2.389555
C	-4.424828	0.179599	-2.153474
C	-3.294292	-2.047199	-1.775683
H	1.985214	-1.797425	2.384449
H	2.648652	-2.705433	1.047563
C	3.869744	-2.749465	2.844978
C	4.842287	-0.510382	3.514373
H	4.371432	1.123446	2.177875
H	2.976990	0.483239	3.054403
H	3.951923	-2.632557	-0.833935
H	2.285888	-2.648905	-1.401124
C	3.760412	-2.783295	-2.976336
C	5.221064	-0.733651	-3.248903
H	4.777491	0.887179	-1.887812
H	5.403152	-0.553689	-1.101388
H	1.395728	2.323480	-1.647859
H	2.941423	1.893860	-2.357827
C	2.846479	3.935788	-1.654212
C	2.599044	4.188927	0.851672
H	1.139534	2.586316	0.865709
H	2.491712	2.326976	1.947412
H	-1.032019	2.594653	-0.802443
H	-2.289696	2.289209	-1.989941
C	-2.496001	4.183272	-0.950756
C	-3.018093	3.977223	1.517061
H	-3.217419	1.951514	2.240829
H	-1.579582	2.372146	1.760527
H	-5.115074	0.463479	1.284431
H	-5.266051	-1.154180	0.605496
C	-5.407469	-1.093642	2.764456
C	-3.467742	-2.711883	2.993088
H	-3.279914	-2.852121	0.848989
H	-1.805150	-2.331829	1.637826
H	-5.250925	-0.075682	-1.476049
H	-4.327637	1.269901	-2.131084
C	-4.788271	-0.252485	-3.587241
C	-3.634409	-2.473983	-3.213206
H	-2.395099	-2.568758	-1.439561
H	-4.113662	-2.361078	-1.114689
H	3.392047	-3.665081	3.215499
H	4.778924	-3.065260	2.310962
C	4.256597	-1.837116	4.017015
H	5.803335	-0.703431	3.014312
H	5.058361	0.157679	4.358130
H	3.750941	-3.880469	-2.964799
H	3.046826	-2.472939	-3.752882
C	5.162444	-2.265343	-3.325130
H	4.598470	-0.305488	-4.048355
H	6.244854	-0.379432	-3.427403
H	3.941573	4.039913	-1.633694
H	2.516768	4.315840	-2.629735
C	2.235957	4.771171	-0.520889
H	2.095778	4.749450	1.650025
H	3.679574	4.305356	1.023374
H	-1.915374	4.733734	-1.702269

H	-3.553762	4.291792	-1.233180
C	-2.277376	4.786282	0.443762
H	-2.811288	4.385285	2.514577
H	-4.102466	4.074596	1.358575
H	-5.051684	-0.447600	3.580810
H	-6.501428	-1.002413	2.748638
C	-4.993776	-2.544727	3.050714
H	-3.194242	-3.763708	3.144195
H	-3.006102	-2.146984	3.816324
H	-5.725901	0.231943	-3.889934
H	-4.011461	0.113261	-4.274968
C	-4.903611	-1.776852	-3.721751
H	-2.786497	-2.228780	-3.868212
H	-3.755283	-3.563931	-3.253360
H	3.362396	-1.630939	4.622852
H	4.973810	-2.341750	4.677119
H	5.462368	-2.607251	-4.324088
H	5.890887	-2.689420	-2.617704
H	2.566743	5.814959	-0.595047
H	1.141171	4.782039	-0.629841
H	-2.603879	5.833805	0.462513
H	-1.200935	4.789823	0.671715
H	-5.378154	-2.861043	4.028907
H	-5.457888	-3.205904	2.303622
H	-5.767521	-2.127200	-3.137053
H	-5.101809	-2.050945	-4.765926
C	-0.000376	-1.953433	-0.755564
O	0.037331	-1.297846	-1.845368
O	-0.041655	-3.110346	-0.398272

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C	1.148079	-2.303895	0.806371
O	1.525554	-3.314847	1.264951
Ru	0.507033	-0.817295	-0.058450
P	2.712360	0.290262	0.017981
P	-1.746361	-1.728752	0.112700
B	-1.366165	3.220491	0.386927
H	-0.619367	2.341763	0.673685
C	4.130015	-0.528466	-0.934583
C	2.766448	2.145562	-0.402848
C	3.309110	0.407930	1.819642
C	-2.396442	-1.480742	1.869546
C	-1.886010	-3.592405	-0.140529
C	-3.015440	-0.817387	-0.962416
O	-2.665407	3.005368	0.016559
O	-1.006455	4.538524	0.410198
H	5.060863	-0.166761	-0.470340
C	4.163255	-0.156666	-2.436642
C	4.072588	-2.070948	-0.814975
H	2.208991	2.578089	0.442509
C	1.999836	2.550686	-1.681888
C	4.174537	2.788444	-0.390885
H	4.025228	1.240441	1.843568
C	2.124951	0.782744	2.740429
C	4.046443	-0.826709	2.377174
H	-3.458380	-1.760353	1.860213
C	-2.289772	0.006865	2.275076
C	-1.694709	-2.365628	2.922886
H	-1.269889	-3.970938	0.687899
C	-3.295698	-4.201878	0.012393
C	-1.209656	-4.099837	-1.435154
H	-2.641553	0.215449	-0.925569
C	-4.478931	-0.798567	-0.463827
C	-2.976550	-1.255174	-2.444924
C	-3.198057	4.282194	-0.459307
C	-2.220298	5.326681	0.211758
H	3.231414	-0.489509	-2.909522

H	4.227109	0.925324	-2.574749
C	5.357929	-0.817808	-3.149150
C	5.273080	-2.735239	-1.510127
H	4.032911	-2.393887	0.227681
H	3.145764	-2.414645	-1.288194
H	2.497637	2.135268	-2.566262
H	0.997312	2.118513	-1.674744
C	1.925912	4.081979	-1.824322
C	4.084237	4.319598	-0.526678
H	4.722146	2.540957	0.525890
H	4.771352	2.394995	-1.223273
H	1.382766	-0.027697	2.706349
H	1.618220	1.685080	2.375816
C	2.573416	0.999223	4.196127
C	4.500279	-0.595593	3.830210
H	3.389823	-1.704157	2.342907
H	4.922724	-1.058658	1.762484
H	-1.229882	0.300531	2.258226
H	-2.796861	0.653625	1.550769
C	-2.856477	0.255347	3.682876
C	-2.258739	-2.114841	4.332957
H	-1.805658	-3.427531	2.677669
H	-0.617195	-2.155825	2.919989
H	-3.772191	-3.866942	0.942095
H	-3.934575	-3.856261	-0.811166
C	-3.238197	-5.740857	-0.011678
C	-1.147934	-5.636820	-1.442966
H	-1.775784	-3.763304	-2.311785
H	-0.206211	-3.678982	-1.539205
H	-4.899978	-1.812273	-0.491970
H	-4.541545	-0.459202	0.574716
C	-5.339171	0.133442	-1.337308
C	-3.830714	-0.319891	-3.317486
H	-1.951204	-1.265902	-2.819840
H	-3.370730	-2.276240	-2.533520
C	-4.658116	4.388554	-0.023773
C	-3.101086	4.249093	-1.989957
C	-2.670939	5.782560	1.605917
C	-1.872104	6.538238	-0.650553
H	5.342040	-0.543498	-4.211887
H	6.294788	-0.413399	-2.735789
C	5.349129	-2.343673	-2.990916
H	6.204076	-2.437888	-1.003042
H	5.195139	-3.825049	-1.405999
H	1.414177	4.333204	-2.763067
H	1.309522	4.493196	-1.012614
C	3.316658	4.730737	-1.790336
H	3.574536	4.730080	0.357626
H	5.094812	4.748943	-0.533526
H	3.228224	1.881875	4.246740
H	1.699269	1.224125	4.821269
C	3.324500	-0.222948	4.742511
H	5.003073	-1.496660	4.203843
H	5.247319	0.211995	3.853391
H	-2.741227	1.314865	3.946194
H	-3.937701	0.050376	3.680026
C	-2.173488	-0.634758	4.729972
H	-1.720269	-2.737555	5.058763
H	-3.310200	-2.437435	4.364479
H	-2.692996	-6.093176	0.876596
H	-4.254102	-6.150546	0.063112
C	-2.539597	-6.263491	-1.275624
H	-0.685389	-5.980338	-2.376736
H	-0.493515	-5.976482	-0.626521
H	-6.376785	0.121426	-0.977887
H	-4.972486	1.162489	-1.210456
C	-5.281405	-0.249762	-2.822176

H	-3.384639	0.684942	-3.302065
H	-3.798566	-0.659832	-4.360471
H	-5.245595	3.604076	-0.511363
H	-5.080550	5.356938	-0.315574
H	-4.769643	4.271002	1.056490
H	-2.062938	4.152073	-2.322041
H	-3.529288	5.150707	-2.440402
H	-3.654229	3.382146	-2.363880
H	-2.910449	4.928320	2.247069
H	-3.548794	6.434826	1.552902
H	-1.855721	6.339853	2.077534
H	-1.161694	7.176011	-0.114899
H	-2.766808	7.133854	-0.865096
H	-1.413158	6.243871	-1.596867
H	4.476402	-2.755335	-3.516659
H	6.239730	-2.781340	-3.460703
H	3.232338	5.824044	-1.843797
H	3.887725	4.417203	-2.677155
H	3.678297	-0.028883	5.763162
H	2.632397	-1.075484	4.805951
H	-2.623385	-0.478326	5.718819
H	-1.115994	-0.343300	4.817095
H	-2.466826	-7.358212	-1.241708
H	-3.154234	-6.017916	-2.154656
H	-5.759781	-1.231088	-2.960818
H	-5.859470	0.465208	-3.422339
C	0.580143	-1.007277	-2.060588
O	-0.027096	0.107026	-2.059436
O	1.015229	-1.797658	-2.872747

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Ru	-0.074188	-0.525004	-0.314001
P	-2.533832	-0.639802	0.044595
P	2.401185	-0.667987	-0.151522
B	-0.013544	2.411412	0.564352
H	-0.108278	1.270119	0.950154
C	-3.398652	-2.293747	-0.300645
C	-2.795290	-0.344690	1.897116
C	-3.784029	0.535841	-0.791094
C	3.419119	-0.246804	-1.683748
C	2.893419	-2.465253	0.189776
C	3.125467	0.464649	1.179870
O	-1.097862	3.248226	0.566268
O	1.191615	3.066398	0.537602
H	-4.427819	-2.142242	0.059947
C	-2.811938	-3.494734	0.473236
C	-3.481635	-2.603246	-1.814232
H	-2.709424	0.748818	1.974938
C	-1.662520	-0.931638	2.769898
C	-4.169744	-0.750880	2.472815
H	-4.697783	-0.070833	-0.887773
C	-4.161263	1.809173	-0.002224
C	-3.320751	0.945719	-2.207558
H	4.466607	-0.463347	-1.427795
C	3.327203	1.253163	-2.048824
C	3.035157	-1.138494	-2.887218
H	2.503737	-2.963856	-0.708159
C	4.397431	-2.802694	0.270350
C	2.153241	-3.102889	1.387639
H	2.748146	1.444409	0.860497
C	4.664820	0.573420	1.266949
C	2.542714	0.209736	2.587307
C	-0.622139	4.579396	0.200234
C	0.925890	4.498768	0.541262
H	-1.761805	-3.637733	0.200158
H	-2.834540	-3.303652	1.550706
C	-3.584702	-4.793961	0.180699

C	-4.241927	-3.913295	-2.087833
H	-3.982429	-1.787458	-2.344727
H	-2.471776	-2.676597	-2.233336
H	-1.680808	-2.027848	2.731981
H	-0.685219	-0.628787	2.372987
C	-1.798627	-0.475615	4.232422
C	-4.311763	-0.294082	3.936389
H	-4.987304	-0.334547	1.873523
H	-4.279508	-1.842568	2.431217
H	-3.273797	2.439725	0.123068
H	-4.524904	1.565541	1.001077
C	-5.264660	2.595621	-0.738003
C	-4.430798	1.701104	-2.954985
H	-2.443710	1.592861	-2.107162
H	-2.994778	0.081206	-2.792208
H	2.282785	1.532324	-2.217746
H	3.676971	1.872272	-1.214687
C	4.157117	1.575233	-3.303831
C	3.872910	-0.791955	-4.130539
H	3.179625	-2.197604	-2.641312
H	1.973608	-1.001959	-3.119125
H	4.949714	-2.363214	-0.567430
H	4.825146	-2.379695	1.188097
C	4.611537	-4.328217	0.283025
C	2.355513	-4.628524	1.403447
H	2.535814	-2.685380	2.327808
H	1.084285	-2.864188	1.347757
H	5.090971	-0.372875	1.621633
H	5.104674	0.767687	0.283420
C	5.074713	1.697236	2.237342
C	2.946204	1.329352	3.562420
H	1.450577	0.132634	2.542911
H	2.910939	-0.748048	2.977153
C	-1.409762	5.597882	1.025555
C	-0.916006	4.779449	-1.292589
C	1.273153	5.001921	1.949181
C	1.845682	5.154752	-0.488613
H	-3.117430	-5.624851	0.724918
H	-4.610615	-4.703549	0.568966
C	-3.636537	-5.095806	-1.321948
H	-5.295282	-3.791366	-1.792749
H	-4.241135	-4.113125	-3.166767
H	-0.999678	-0.923086	4.837619
H	-1.658790	0.614326	4.283965
C	-3.173993	-0.839085	4.812505
H	-4.305917	0.805272	3.973463
H	-5.284102	-0.614543	4.332274
H	-6.185256	1.992356	-0.752577
H	-5.501391	3.506569	-0.172124
C	-4.872729	2.949473	-2.179222
H	-4.075936	1.978961	-3.955311
H	-5.295985	1.036420	-3.102702
H	4.038288	2.637299	-3.554781
H	5.225929	1.422670	-3.087167
C	3.751748	0.694074	-4.492682
H	3.549235	-1.418896	-4.970930
H	4.930354	-1.036343	-3.944202
H	4.272083	-4.746791	-0.675615
H	5.683869	-4.550580	0.358651
C	3.845555	-4.999449	1.432332
H	1.839244	-5.062527	2.269683
H	1.885365	-5.059813	0.508111
H	6.169511	1.750934	2.298885
H	4.735632	2.661948	1.832547
C	4.471681	1.491336	3.633980
H	2.492174	2.271584	3.226562
H	2.538761	1.117892	4.559791

H	-2.468183	5.547027	0.750824
H	-1.059718	6.617196	0.826093
H	-1.330982	5.405520	2.098127
H	-0.434882	4.009973	-1.899685
H	-0.594135	5.770443	-1.630967
H	-1.996479	4.703593	-1.452387
H	0.660354	4.510619	2.711462
H	1.134623	6.084725	2.036966
H	2.322672	4.773746	2.161163
H	2.889179	5.020046	-0.184770
H	1.651920	6.231279	-0.559816
H	1.720154	4.707913	-1.476687
H	-2.617864	-5.283458	-1.689815
H	-4.215358	-6.009554	-1.508429
H	-3.267842	-0.458434	5.837512
H	-3.260840	-1.933977	4.876546
H	-5.709048	3.446343	-2.688352
H	-4.042654	3.670215	-2.162321
H	4.371462	0.926250	-5.368722
H	2.710770	0.912786	-4.768016
H	3.968928	-6.088980	1.386278
H	4.278639	-4.675918	2.390883
H	4.910527	0.589609	4.087064
H	4.736194	2.330013	4.290866
C	-0.107862	0.503021	-2.093535
O	-0.166419	0.011520	-3.208765
O	-0.056318	1.683604	-1.645392
O	0.018084	-3.230201	-1.573525
C	-0.042478	-2.186816	-1.045294

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Ru	0.011987	0.545725	0.300171
P	-2.424433	0.807624	0.004922
P	2.470042	0.434566	0.090187
B	-0.205518	-2.242241	0.229525
H	-0.102955	-1.121424	-0.501124
C	-2.879047	2.495154	-0.755559
C	-3.133165	-0.390392	-1.270210
C	-3.548444	0.580676	1.504914
C	3.523386	-0.170699	1.531320
C	3.115078	2.197813	-0.173217
C	2.961439	-0.676257	-1.352809
O	-1.428341	-2.892582	-0.148313
O	0.880272	-3.126188	-0.079467
H	-3.715037	2.269612	-1.431635
C	-1.727020	3.062844	-1.616009
C	-3.375951	3.591812	0.210025
H	-2.885411	-1.371935	-0.848850
C	-2.408293	-0.301938	-2.631071
C	-4.661600	-0.310677	-1.482052
H	-4.534356	0.968932	1.205479
C	-3.716500	-0.912189	1.883469
C	-3.063458	1.373739	2.742645
H	4.566803	-0.050811	1.204689
C	3.305682	-1.667185	1.851167
C	3.326393	0.688823	2.801866
H	2.823851	2.664767	0.778597
C	4.637882	2.406869	-0.326048
C	2.374923	2.985126	-1.277576
H	2.455401	-1.614405	-1.084765
C	4.464881	-0.980266	-1.532280
C	2.356530	-0.197540	-2.692052
C	-1.156369	-4.304747	-0.193661
C	0.352642	-4.333573	-0.655091
H	-0.899304	3.342199	-0.952659
H	-1.335831	2.306319	-2.305652
C	-2.172460	4.307059	-2.403954

C	-3.828344	4.843156	-0.565751
H	-4.209767	3.227979	0.819148
H	-2.569437	3.869954	0.900987
H	-2.602602	0.671854	-3.102966
H	-1.324491	-0.381494	-2.484393
C	-2.886003	-1.413112	-3.581513
C	-5.144850	-1.418163	-2.437490
H	-5.197546	-0.394872	-0.530723
H	-4.935937	0.664285	-1.910230
H	-2.741968	-1.338628	2.145276
H	-4.085811	-1.497654	1.036354
C	-4.682037	-1.076185	3.070756
C	-4.036839	1.211665	3.923629
H	-2.076056	1.005377	3.037713
H	-2.948450	2.436529	2.515081
H	2.267393	-1.838280	2.148814
H	3.468171	-2.287525	0.964170
C	4.240311	-2.124744	2.984183
C	4.250569	0.216334	3.938742
H	3.531020	1.746015	2.593660
H	2.282642	0.620474	3.128995
H	5.194285	1.865481	0.446734
H	4.970218	2.009152	-1.293798
C	4.988551	3.905375	-0.251077
C	2.705827	4.484933	-1.195166
H	2.672772	2.613859	-2.265445
H	1.292204	2.835698	-1.200639
H	5.007832	-0.063038	-1.794577
H	4.903655	-1.351106	-0.600341
C	4.682909	-2.020686	-2.646763
C	2.580815	-1.224857	-3.814502
H	1.283285	0.001065	-2.575452
H	2.825867	0.747549	-2.991669
C	-2.142456	-4.965426	-1.158927
C	-1.361081	-4.885250	1.218027
C	0.506080	-4.256477	-2.182299
C	1.164892	-5.516572	-0.120180
H	-1.330325	4.693572	-2.992318
H	-2.952326	4.019810	-3.124738
C	-2.715549	5.395252	-1.467329
H	-4.702428	4.586163	-1.182661
H	-4.161934	5.612144	0.142467
H	-2.370977	-1.323599	-4.546952
H	-2.600333	-2.384831	-3.156928
C	-4.407157	-1.370233	-3.782638
H	-4.977745	-2.396681	-1.965113
H	-6.227814	-1.325047	-2.591590
H	-5.689214	-0.750215	2.767859
H	-4.762548	-2.140416	3.326610
C	-4.231629	-0.264581	4.292165
H	-3.655858	1.773729	4.785650
H	-5.010231	1.656353	3.664056
H	4.051520	-3.182985	3.204612
H	5.287119	-2.056617	2.649051
C	4.054020	-1.273949	4.247638
H	4.061978	0.821512	4.834509
H	5.299416	0.394221	3.655132
H	4.748083	4.277803	0.755440
H	6.069924	4.038938	-0.383019
C	4.219202	4.728426	-1.294745
H	2.180532	5.025880	-1.992983
H	2.329594	4.885097	-0.242559
H	5.757131	-2.211975	-2.767099
H	4.226731	-2.973623	-2.342224
C	4.069394	-1.564072	-3.978034
H	2.020062	-2.139306	-3.584256
H	2.173643	-0.834631	-4.756560

H	-3.161358	-4.867056	-0.768090
H	-1.928515	-6.035158	-1.270485
H	-2.114554	-4.501412	-2.147989
H	-0.665133	-4.442306	1.935233
H	-1.240236	-5.974605	1.233428
H	-2.377577	-4.648617	1.549663
H	-0.059238	-3.413777	-2.592657
H	0.170458	-5.175113	-2.676821
H	1.563744	-4.111009	-2.425912
H	2.199106	-5.444682	-0.475278
H	0.754285	-6.471565	-0.470083
H	1.185576	-5.522912	0.971873
H	-1.894932	5.772316	-0.839551
H	-3.084302	6.250356	-2.047861
H	-4.730932	-2.200229	-4.423613
H	-4.677253	-0.443398	-4.311273
H	-4.961130	-0.364267	5.106465
H	-3.280495	-0.669592	4.664980
H	4.751709	-1.595120	5.031991
H	3.039379	-1.429615	4.639926
H	4.442570	5.796154	-1.175646
H	4.563606	4.447738	-2.301398
H	4.607683	-0.673781	-4.336970
H	4.201441	-2.338477	-4.744397
C	-0.077257	-0.545330	1.982123
O	-0.039236	-0.140000	3.128573
O	-0.174572	-1.834988	1.670172
C	0.120983	2.155334	1.243512
O	0.197683	3.144956	1.848590

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Ru	-0.049223	-0.567348	0.324489
P	2.361351	-0.867020	0.014284
P	-2.480160	-0.351988	0.083625
B	0.358505	2.493904	0.570149
H	0.108783	0.963519	-0.488217
C	2.778729	-2.586133	-0.707484
C	3.099155	0.264900	-1.310144
C	3.520535	-0.635349	1.489403
C	-3.537765	0.324666	1.492843
C	-3.209779	-2.090431	-0.145931
C	-2.939891	0.739082	-1.390880
O	1.599070	2.968682	0.133284
O	-0.676851	3.331784	0.164576
H	3.600787	-2.392874	-1.410180
C	1.600104	-3.165854	-1.523191
C	3.284473	-3.662937	0.275445
H	2.856417	1.267831	-0.938445
C	2.384742	0.097468	-2.669645
C	4.628758	0.161628	-1.504530
H	4.491061	-1.052706	1.178859
C	3.732425	0.857720	1.840941
C	3.044304	-1.392158	2.752846
H	-4.577492	0.259545	1.140460
C	-3.244080	1.810223	1.800608
C	-3.424028	-0.525020	2.779727
H	-2.967767	-2.535440	0.829996
C	-4.734916	-2.232411	-0.338694
C	-2.478956	-2.956657	-1.195948
H	-2.380471	1.655663	-1.159491
C	-4.427203	1.116788	-1.562463
C	-2.375983	0.183603	-2.717579
C	1.404258	4.346700	-0.269632
C	-0.117228	4.361176	-0.685814
H	0.787392	-3.422365	-0.832538
H	1.197124	-2.424587	-2.222725
C	2.015517	-4.433515	-2.290243

C	3.706654	-4.939886	-0.475608
H	4.135045	-3.293534	0.857355
H	2.489532	-3.913783	0.989851
H	2.565391	-0.911277	-3.066399
H	1.302210	0.205696	-2.532646
C	2.888769	1.116346	-3.706128
C	5.131312	1.188789	-2.536408
H	5.158187	0.311399	-0.558035
H	4.898497	-0.844370	-1.856654
H	2.775839	1.305653	2.129487
H	4.083088	1.427210	0.975375
C	4.738640	1.016394	2.994607
C	4.054957	-1.239904	3.903565
H	2.075642	-0.991422	3.067386
H	2.890279	-2.454171	2.547342
H	-2.207501	1.922921	2.129722
H	-3.343483	2.426499	0.901087
C	-4.180217	2.340159	2.900158
C	-4.346908	0.017985	3.885921
H	-3.687558	-1.570475	2.580372
H	-2.386415	-0.516619	3.131578
H	-5.288338	-1.630178	0.390014
H	-5.016328	-1.864035	-1.333866
C	-5.163054	-3.707351	-0.211777
C	-2.885156	-4.434353	-1.063005
H	-2.729609	-2.613774	-2.206950
H	-1.393062	-2.857102	-1.090556
H	-5.023890	0.219116	-1.767328
H	-4.826786	1.557184	-0.643393
C	-4.616181	2.111377	-2.723097
C	-2.577153	1.164797	-3.885306
H	-1.310279	-0.049940	-2.601780
H	-2.886594	-0.754036	-2.969558
C	2.387941	4.689602	-1.386584
C	1.699572	5.216199	0.963676
C	-0.344240	3.955257	-2.147307
C	-0.853067	5.669824	-0.392787
H	1.156670	-4.826699	-2.849436
H	2.781726	-4.172345	-3.035356
C	2.569134	-5.503200	-1.338801
H	4.570634	-4.709867	-1.116945
H	4.046357	-5.693801	0.245965
H	2.383135	0.948199	-4.666113
H	2.613081	2.128571	-3.380113
C	4.411384	1.038755	-3.883595
H	4.964394	2.202773	-2.145171
H	6.215642	1.078890	-2.668203
H	5.727786	0.660485	2.666792
H	4.853696	2.082052	3.231436
C	4.305495	0.235462	4.242042
H	3.683181	-1.776021	4.785937
H	5.006908	-1.717710	3.623838
H	-3.936577	3.389352	3.110511
H	-5.220153	2.326215	2.538213
C	-4.075097	1.499549	4.179759
H	-4.215511	-0.582451	4.795055
H	-5.396937	-0.104717	3.578313
H	-4.970485	-4.047148	0.816411
H	-6.245584	-3.794274	-0.371491
C	-4.405453	-4.610639	-1.196299
H	-2.365399	-5.033089	-1.822342
H	-2.554614	-4.811479	-0.084428
H	-5.681892	2.350410	-2.833482
H	-4.108771	3.055163	-2.474720
C	-4.052077	1.561828	-4.040529
H	-1.972903	2.064681	-3.712979
H	-2.204985	0.711354	-4.813466

H	3.413762	4.606221	-1.011798
H	2.239623	5.718715	-1.734393
H	2.283836	4.017557	-2.240965
H	1.003077	4.997729	1.778861
H	1.643204	6.285439	0.731957
H	2.710896	4.992741	1.317515
H	0.146630	3.004993	-2.376525
H	0.022752	4.719291	-2.841286
H	-1.418344	3.833156	-2.317096
H	-1.903463	5.573962	-0.687490
H	-0.417934	6.501006	-0.960207
H	-0.824864	5.918582	0.670440
H	1.759006	-5.855643	-0.683799
H	2.916736	-6.376658	-1.905098
H	4.754340	1.807783	-4.587692
H	4.675255	0.067470	-4.328601
H	5.063615	0.325114	5.031109
H	3.379516	0.674324	4.639453
H	-4.773951	1.870922	4.940686
H	-3.064008	1.604428	4.597429
H	-4.683300	-5.660568	-1.038774
H	-4.708698	-4.358396	-2.223627
H	-4.635875	0.679093	-4.342239
H	-4.166425	2.301115	-4.843668
C	0.060668	0.501358	2.003859
O	-0.034173	0.089695	3.144331
O	0.258252	1.837946	1.813953
C	-0.209303	-2.184864	1.342821
O	-0.306029	-3.146784	1.986067

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Ru	-0.370757	-0.723237	0.332152
P	1.850201	-1.653486	-0.078382
P	-2.609047	0.200141	0.105284
B	1.110909	2.952036	0.369709
H	-0.124071	0.102358	-1.100389
C	1.677629	-3.483602	-0.582335
C	2.796798	-0.931021	-1.555575
C	3.169676	-1.632544	1.285115
C	-3.602222	0.564306	1.673354
C	-3.674572	-1.088262	-0.774062
C	-2.702944	1.849956	-0.826494
O	2.458974	2.665813	0.326965
O	0.812349	4.239185	-0.023794
H	2.482070	-3.674960	-1.306941
C	0.326960	-3.705904	-1.300765
C	1.831579	-4.519620	0.550495
H	2.917897	0.122820	-1.267137
C	1.995200	-0.951509	-2.874013
C	4.198685	-1.532860	-1.811593
H	3.904513	-2.399222	0.993417
C	3.908318	-0.276183	1.396814
C	2.607059	-1.999327	2.678004
H	-4.529157	1.050099	1.339246
C	-2.844651	1.554184	2.587172
C	-4.017231	-0.685667	2.478755
H	-3.727774	-1.888066	-0.020013
C	-5.121928	-0.686804	-1.125866
C	-2.972955	-1.705575	-2.003618
H	-1.871523	2.390691	-0.360637
C	-3.974442	2.714075	-0.657296
C	-2.356334	1.727073	-2.325761
C	3.149660	3.930619	0.136033
C	2.035779	4.816411	-0.551612
H	-0.484292	-3.500801	-0.584331
H	0.204133	-3.000743	-2.129139
C	0.177040	-5.144151	-1.826535

C	1.703247	-5.957833	0.016127
H	2.798646	-4.405250	1.051380
H	1.056916	-4.353540	1.311089
H	1.867462	-1.990563	-3.210955
H	0.996890	-0.535935	-2.708628
C	2.722633	-0.166133	-3.978745
C	4.942762	-0.754499	-2.913213
H	4.808466	-1.543265	-0.903349
H	4.096899	-2.580160	-2.129884
H	3.193951	0.500298	1.684290
H	4.334164	0.033694	0.438231
C	5.038264	-0.348721	2.440479
C	3.732250	-2.088525	3.724387
H	1.896279	-1.222085	2.974250
H	2.059657	-2.944205	2.654899
H	-1.910368	1.088006	2.923114
H	-2.555002	2.454718	2.034059
C	-3.686729	1.942649	3.814059
C	-4.856888	-0.297451	3.710186
H	-4.600665	-1.375397	1.858005
H	-3.127119	-1.231229	2.810712
H	-5.638196	-0.276649	-0.250044
H	-5.106997	0.108077	-1.883051
C	-5.912715	-1.887895	-1.678809
C	-3.760966	-2.909968	-2.545949
H	-2.873913	-0.955359	-2.796367
H	-1.952019	-2.007010	-1.743090
H	-4.837956	2.219007	-1.121539
H	-4.223387	2.855606	0.399045
C	-3.777722	4.101406	-1.300311
C	-2.141642	3.114131	-2.955138
H	-1.458085	1.115232	-2.452733
H	-3.176458	1.224814	-2.858571
C	4.396442	3.680698	-0.710375
C	3.549761	4.434625	1.529552
C	1.989151	4.650541	-2.077246
C	2.068210	6.299074	-0.185057
H	-0.807393	-5.264455	-2.297085
H	0.923542	-5.316147	-2.616415
C	0.369774	-6.178690	-0.710486
H	2.533363	-6.162251	-0.676613
H	1.807820	-6.667690	0.846608
H	2.137571	-0.202483	-4.907007
H	2.779594	0.893231	-3.686726
C	4.139411	-0.705764	-4.220028
H	5.129920	0.270894	-2.561340
H	5.927030	-1.208924	-3.086670
H	5.802134	-1.066083	2.101831
H	5.536578	0.627845	2.505760
C	4.517315	-0.774054	3.819354
H	3.301641	-2.346422	4.700550
H	4.418863	-2.907631	3.459219
H	-3.112416	2.625769	4.452549
H	-4.579367	2.496492	3.485105
C	-4.122312	0.705061	4.610561
H	-5.115850	-1.201742	4.275900
H	-5.807337	0.144608	3.374692
H	-6.026620	-2.640706	-0.884650
H	-6.926711	-1.569355	-1.953281
C	-5.208828	-2.525719	-2.885380
H	-3.256864	-3.316814	-3.432244
H	-3.765535	-3.710959	-1.791393
H	-4.697747	4.690479	-1.189646
H	-2.992459	4.637969	-0.748666
C	-3.377992	4.006076	-2.778665
H	-1.274038	3.591566	-2.477760
H	-1.898159	3.004601	-4.020394

H	5.090621	3.036701	-0.160498
H	4.913165	4.621710	-0.931934
H	4.152117	3.186882	-1.654038
H	2.669516	4.613704	2.154776
H	4.132850	5.360076	1.474090
H	4.159784	3.670611	2.021270
H	1.959546	3.593439	-2.360969
H	2.852134	5.117508	-2.563997
H	1.080473	5.127294	-2.458219
H	1.243312	6.817998	-0.684189
H	3.006525	6.762546	-0.511263
H	1.958240	6.450251	0.891098
H	-0.454657	-6.089790	0.012559
H	0.319846	-7.196083	-1.118965
H	4.662707	-0.095041	-4.967171
H	4.071396	-1.721181	-4.638550
H	5.349295	-0.872926	4.529134
H	3.855454	0.010651	4.211289
H	-4.760479	0.997133	5.454649
H	-3.232954	0.221614	5.040127
H	-5.767439	-3.405322	-3.229797
H	-5.204665	-1.810076	-3.720912
H	-4.214718	3.583766	-3.355850
H	-3.191867	5.008136	-3.186672
C	0.328686	0.836497	1.343947
O	0.860624	0.865629	2.433797
O	0.119034	2.080003	0.696601
C	-0.654396	-1.744084	1.964641
O	-0.825504	-2.398139	2.909601

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Ru	0.499395	0.613032	0.392296
P	-1.422678	2.036807	0.008495
P	2.570930	-0.642023	0.118813
B	-1.908008	-2.503481	-0.061462
H	0.885998	1.177669	-1.210767
C	-1.013146	3.830100	-0.445062
C	-2.513589	1.399275	-1.403246
C	-2.685166	2.294177	1.423639
C	3.082660	-1.843474	1.489123
C	4.091661	0.477895	-0.000080
C	2.453916	-1.763989	-1.409052
O	-3.198526	-2.045692	0.074413
O	-1.828429	-3.823065	-0.431354
H	-1.988239	4.321324	-0.582949
C	-0.215990	3.964645	-1.759286
C	-0.275702	4.560383	0.700069
H	-3.076355	0.592353	-0.916666
C	-1.751525	0.724965	-2.565224
C	-3.529039	2.431315	-1.942454
H	-3.084397	3.308903	1.266572
C	-3.880095	1.311400	1.415563
C	-2.011861	2.246556	2.814973
H	3.985461	-2.350103	1.119165
C	2.008942	-2.923108	1.755204
C	3.456176	-1.156432	2.821647
H	4.183371	0.829512	1.038008
C	5.422674	-0.212626	-0.368706
C	3.889547	1.746614	-0.857085
H	1.441941	-2.178338	-1.291219
C	3.437376	-2.954467	-1.494234
C	2.474091	-0.978806	-2.739927
C	-4.063076	-3.216122	0.055638
C	-3.180297	-4.269163	-0.728880
H	0.723832	3.407962	-1.664143
H	-0.759888	3.502019	-2.588973
C	0.080018	5.434417	-2.104439

C	0.032988	6.025914	0.346822
H	-0.870083	4.536731	1.618568
H	0.662386	4.031607	0.918337
H	-1.120383	1.452549	-3.089329
H	-1.074316	-0.037791	-2.169000
C	-2.735926	0.087999	-3.562457
C	-4.505510	1.786838	-2.942502
H	-4.092181	2.893250	-1.122691
H	-2.994407	3.244886	-2.449859
H	-3.511468	0.284055	1.522452
H	-4.423138	1.356839	0.466824
C	-4.874192	1.622758	2.550937
C	-3.004582	2.584525	3.940203
H	-1.620065	1.236497	2.976216
H	-1.158326	2.927107	2.868162
H	1.107930	-2.442493	2.149771
H	1.710001	-3.427637	0.830207
C	2.506364	-3.961218	2.776346
C	3.947052	-2.185379	3.857444
H	4.238281	-0.402869	2.675260
H	2.581859	-0.629709	3.221719
H	5.590268	-1.103503	0.247347
H	5.379597	-0.553140	-1.411535
C	6.612063	0.751946	-0.211114
C	5.080554	2.707947	-0.700903
H	3.777345	1.473511	-1.913885
H	2.957787	2.243660	-0.570296
H	4.463658	-2.584195	-1.611922
H	3.421640	-3.551043	-0.577735
C	3.092054	-3.868683	-2.685215
C	2.125248	-1.890487	-3.928912
H	1.779997	-0.134286	-2.690704
H	3.477453	-0.559898	-2.900839
C	-5.378313	-2.837845	-0.622062
C	-4.312956	-3.602300	1.519834
C	-3.348774	-4.194126	-2.252206
C	-3.325583	-5.714427	-0.255519
H	0.668347	5.479929	-3.030177
H	-0.863925	5.962176	-2.309174
C	0.819180	6.145686	-0.964181
H	-0.911982	6.582184	0.253699
H	0.587375	6.490304	1.172436
H	-2.179098	-0.365591	-4.392726
H	-3.272547	-0.730172	-3.058661
C	-3.757129	1.102816	-4.095294
H	-5.121757	1.042266	-2.417010
H	-5.195782	2.547497	-3.330091
H	-5.331453	2.607491	2.368483
H	-5.692918	0.891360	2.524994
C	-4.202025	1.627467	3.928961
H	-2.487089	2.539510	4.906889
H	-3.360866	3.619672	3.822472
H	1.721233	-4.707640	2.951911
H	3.367866	-4.504537	2.358646
C	2.914774	-3.295196	4.097400
H	4.182232	-1.671839	4.798478
H	4.887210	-2.633905	3.502212
H	6.721170	1.018737	0.850551
H	7.541059	0.244750	-0.502461
C	6.415942	2.029811	-1.039276
H	4.929091	3.589083	-1.337809
H	5.113235	3.074406	0.336156
H	3.813439	-4.694848	-2.734866
H	2.106115	-4.323847	-2.510959
C	3.067499	-3.098971	-4.012326
H	1.088783	-2.242432	-3.820044
H	2.162766	-1.311405	-4.860900

H	-5.894563	-2.079945	-0.023916
H	-6.037804	-3.709345	-0.705185
H	-5.216593	-2.426700	-1.621377
H	-3.378596	-3.859303	2.028041
H	-5.003421	-4.448414	1.603428
H	-4.749756	-2.745777	2.042115
H	-3.236418	-3.167899	-2.616171
H	-4.326469	-4.570771	-2.570883
H	-2.573630	-4.805423	-2.724913
H	-2.653921	-6.358819	-0.832056
H	-4.350532	-6.072797	-0.405542
H	-3.069032	-5.820122	0.800849
H	1.811878	5.689329	-0.835502
H	0.988295	7.200978	-1.214383
H	-4.467726	0.611686	-4.772662
H	-3.233772	1.865920	-4.690564
H	-4.926721	1.904697	4.705808
H	-3.852883	0.612653	4.166269
H	3.313762	-4.041507	4.796661
H	2.022754	-2.862678	4.572941
H	7.250715	2.722833	-0.873556
H	6.430165	1.771771	-2.108800
H	4.084109	-2.749192	-4.247485
H	2.768688	-3.763957	-4.832994
C	-0.621869	-0.832774	1.194999
O	-1.175128	-1.114405	2.232384
O	-0.783192	-1.723822	0.073864
C	0.948325	1.234318	2.061889
O	1.352739	1.753912	3.029708

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Ru	-0.091688	-0.927768	0.298627
P	2.382901	-0.941494	0.007436
P	-2.497877	-0.475700	0.022765
B	0.327287	2.399259	0.312845
H	-0.135016	-0.633138	-1.307832
C	3.263402	-2.618751	0.122101
C	2.998453	-0.206183	-1.630550
C	3.391368	0.053495	1.302529
C	-3.408015	-0.031948	1.618478
C	-3.499015	-1.952479	-0.609946
C	-2.787135	1.027113	-1.085008
O	0.818380	3.420381	1.163282
O	0.055656	2.953647	-0.963626
H	4.334666	-2.372386	0.078285
C	2.960373	-3.582628	-1.046322
C	3.004721	-3.317357	1.475634
H	2.837473	0.867733	-1.469290
C	2.191667	-0.564037	-2.897053
C	4.507826	-0.430131	-1.893499
H	4.324756	-0.521707	1.406677
C	3.774688	1.494362	0.893216
C	2.695191	0.098122	2.680872
H	-4.413458	0.284676	1.309829
C	-2.742727	1.161904	2.340885
C	-3.591893	-1.227070	2.581289
H	-3.279950	-2.701107	0.166416
C	-5.034493	-1.777786	-0.657650
C	-3.027363	-2.565822	-1.950092
H	-2.000702	1.709463	-0.743809
C	-4.145821	1.753778	-0.945374
C	-2.510277	0.745450	-2.578139
C	0.613905	4.689447	0.525970
C	0.573590	4.298212	-1.002481
H	1.889971	-3.809322	-1.076816
H	3.208396	-3.116408	-2.003803
C	3.744871	-4.901097	-0.910886

C	3.777819	-4.642345	1.598325
H	3.286556	-2.662550	2.306200
H	1.930638	-3.517296	1.582039
H	2.296607	-1.630791	-3.133905
H	1.129104	-0.385093	-2.719188
C	2.672176	0.267621	-4.099844
C	4.990050	0.407893	-3.091528
H	5.111445	-0.192944	-1.010413
H	4.688443	-1.489950	-2.115205
H	2.864633	2.089579	0.775162
H	4.309095	1.513068	-0.060387
C	4.659927	2.166260	1.959673
C	3.570038	0.776130	3.749221
H	1.757439	0.653113	2.565940
H	2.439244	-0.908546	3.020678
H	-1.708179	0.911862	2.598177
H	-2.674717	2.025212	1.669851
C	-3.516231	1.556589	3.610005
C	-4.361112	-0.811884	3.848925
H	-4.131364	-2.043721	2.088517
H	-2.616204	-1.627985	2.874381
H	-5.420489	-1.331551	0.264651
H	-5.297178	-1.091131	-1.473329
C	-5.728873	-3.132117	-0.895058
C	-3.690985	-3.934877	-2.176981
H	-3.305159	-1.902416	-2.776202
H	-1.940799	-2.664417	-1.983860
H	-4.959096	1.104021	-1.295595
H	-4.366071	1.997641	0.098829
C	-4.151049	3.058083	-1.766518
C	-2.486218	2.051398	-3.387141
H	-1.560933	0.214464	-2.695360
H	-3.300810	0.099349	-2.981678
C	1.748392	5.636474	0.923233
C	-0.725557	5.249365	1.034788
C	1.969230	4.238848	-1.644799
C	-0.339826	5.172670	-1.864057
H	3.484605	-5.566532	-1.743877
H	4.822099	-4.694460	-1.000027
C	3.471087	-5.589728	0.431849
H	4.857448	-4.431139	1.619795
H	3.534082	-5.119041	2.556330
H	2.099541	-0.013768	-4.993032
H	2.452642	1.328557	-3.909615
C	4.176496	0.098778	-4.355980
H	4.894301	1.476151	-2.847485
H	6.057646	0.221464	-3.266938
H	5.615745	1.625081	2.037704
H	4.904863	3.185304	1.632274
C	3.971764	2.194139	3.328768
H	3.024691	0.796663	4.701617
H	4.476225	0.174385	3.920657
H	-2.993293	2.379420	4.113561
H	-4.509088	1.941588	3.330839
C	-3.687585	0.366680	4.563723
H	-4.444369	-1.674030	4.523008
H	-5.388637	-0.530157	3.573263
H	-5.542423	-3.784048	-0.028745
H	-6.815689	-2.986058	-0.946179
C	-5.223041	-3.823845	-2.169609
H	-3.346495	-4.357872	-3.129344
H	-3.364175	-4.630114	-1.390381
H	-5.131270	3.544338	-1.674532
H	-3.415522	3.749851	-1.332248
C	-3.807659	2.819478	-3.243445
H	-1.652698	2.666869	-3.028590
H	-2.291655	1.826259	-4.444216

H	1.709007	5.823601	2.001780
H	1.659332	6.601281	0.409480
H	2.727833	5.209370	0.693515
H	-1.557378	4.596696	0.749336
H	-0.926974	6.255813	0.651175
H	-0.694481	5.295529	2.128074
H	2.658500	3.641599	-1.040285
H	2.402347	5.236546	-1.777658
H	1.885104	3.766726	-2.629519
H	-0.313704	4.829103	-2.903925
H	-0.008977	6.218101	-1.848130
H	-1.377086	5.133824	-1.522723
H	2.414538	-5.891295	0.475705
H	4.065300	-6.508344	0.518912
H	4.499649	0.743386	-5.183507
H	4.377477	-0.936704	-4.669310
H	4.629555	2.648605	4.081207
H	3.071950	2.820854	3.262181
H	-4.272625	0.662139	5.444172
H	-2.700717	0.050971	4.931678
H	-5.680641	-4.816456	-2.268815
H	-5.545306	-3.242627	-3.046487
H	-4.617469	2.241097	-3.713967
H	-3.757559	3.776740	-3.778505
C	-0.092486	-1.283558	2.266738
O	-0.129331	-1.600064	3.375388
O	0.161561	1.163482	0.713163
C	-0.300534	-2.743245	-0.056990
O	-0.452132	-3.880200	-0.255413

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Ru	-0.261433	-0.960484	-0.216375
P	-2.767712	-0.485048	-0.289414
P	2.156972	-1.581115	0.164977
B	0.097015	2.021640	0.970763
H	-0.328665	-0.828179	1.421675
C	-3.854659	-1.903661	-0.982608
C	-3.549585	-0.080825	1.387029
C	-3.386139	0.950286	-1.405108
C	3.044747	-2.190138	-1.390076
C	2.262044	-3.107943	1.295805
C	3.320729	-0.236693	0.826696
O	-1.162559	2.287178	1.496050
O	1.085917	2.648771	1.710663
H	-4.819434	-1.406948	-1.164065
C	-4.131127	-3.086562	-0.024524
C	-3.358591	-2.455347	-2.338649
H	-3.135264	0.914206	1.585873
C	-3.083087	-0.976791	2.557792
C	-5.093507	0.031140	1.358723
H	-4.420347	0.657777	-1.644423
C	-3.433873	2.336594	-0.725620
C	-2.605449	1.081833	-2.731853
H	4.059480	-2.441046	-1.054167
C	3.172748	-1.091028	-2.470172
C	2.444066	-3.478069	-1.995791
H	1.732230	-3.860395	0.697058
C	3.677193	-3.671908	1.559475
C	1.485109	-3.004436	2.628265
H	2.997399	0.659476	0.281193
C	4.826403	-0.457919	0.530482
C	3.126715	0.018971	2.336640
C	-1.031621	3.420027	2.394862
C	0.467470	3.291425	2.855823
H	-3.199852	-3.614364	0.202612
H	-4.532210	-2.733145	0.926695
C	-5.133801	-4.082781	-0.637771

C	-4.356087	-3.454553	-2.950610
H	-3.185418	-1.649008	-3.054010
H	-2.395437	-2.959379	-2.192838
H	-3.387451	-2.017869	2.400766
H	-1.990748	-0.974403	2.600783
C	-3.660948	-0.491181	3.899680
C	-5.639132	0.534196	2.707488
H	-5.424894	0.699660	0.556723
H	-5.542408	-0.947828	1.150433
H	-2.417157	2.649143	-0.479599
H	-3.990024	2.302574	0.215704
C	-4.080014	3.386138	-1.647785
C	-3.233902	2.137210	-3.659807
H	-1.574430	1.372480	-2.508658
H	-2.558269	0.130607	-3.266622
H	2.180942	-0.808119	-2.829690
H	3.596712	-0.170396	-2.061090
C	4.008490	-1.584124	-3.663925
C	3.264531	-3.957477	-3.208832
H	2.409492	-4.283583	-1.253522
H	1.409327	-3.296835	-2.310895
H	4.246075	-3.771346	0.628883
H	4.237788	-2.979521	2.199852
C	3.598557	-5.044093	2.255225
C	1.400270	-4.376949	3.318470
H	1.985232	-2.299250	3.301335
H	0.482695	-2.606882	2.455589
H	5.182331	-1.369365	1.027653
H	5.004900	-0.588996	-0.539044
C	5.670459	0.734378	1.016310
C	3.970515	1.212942	2.815649
H	2.070830	0.193582	2.561146
H	3.437760	-0.869082	2.901583
C	-2.062199	3.298594	3.515591
C	-1.307663	4.687199	1.571936
C	0.637281	2.359135	4.063727
C	1.181276	4.616970	3.120486
H	-5.295820	-4.910585	0.064364
H	-6.107010	-3.584820	-0.763943
C	-4.658421	-4.614394	-1.994826
H	-5.291484	-2.928852	-3.193534
H	-3.955020	-3.831963	-3.899837
H	-3.350326	-1.176436	4.699123
H	-3.229945	0.489418	4.143848
C	-5.190329	-0.368089	3.864652
H	-5.281533	1.559136	2.884493
H	-6.734741	0.587934	2.664098
H	-5.128863	3.112639	-1.842891
H	-4.101881	4.354536	-1.130410
C	-3.323156	3.505534	-2.974997
H	-2.637387	2.205215	-4.578334
H	-4.240994	1.810180	-3.962278
H	4.065880	-0.790829	-4.419589
H	5.041240	-1.780341	-3.336925
C	3.416586	-2.862308	-4.272988
H	2.791528	-4.849535	-3.639385
H	4.262566	-4.268484	-2.865095
H	3.126733	-5.766000	1.572189
H	4.612816	-5.416027	2.450002
C	2.792591	-4.977396	3.559311
H	0.858581	-4.277886	4.268012
H	0.810066	-5.060349	2.690636
H	6.730141	0.536699	0.807037
H	5.394865	1.624488	0.435052
C	5.459892	1.015796	2.507744
H	3.603692	2.121952	2.325027
H	3.826719	1.349644	3.896108

H	-3.072529	3.359859	3.097397
H	-1.949430	4.117516	4.235771
H	-1.972723	2.351799	4.052011
H	-0.624973	4.760889	0.721421
H	-1.221584	5.591144	2.184388
H	-2.327274	4.641591	1.176294
H	0.142972	1.397107	3.894953
H	0.225711	2.806377	4.974960
H	1.701215	2.172076	4.228607
H	2.219521	4.425231	3.410292
H	0.697764	5.162476	3.939537
H	1.191994	5.256248	2.234989
H	-3.748079	-5.214515	-1.851363
H	-5.411353	-5.284143	-2.429617
H	-5.564330	0.021671	4.820114
H	-5.635295	-1.366583	3.738549
H	-3.809948	4.236540	-3.633822
H	-2.307204	3.870101	-2.772611
H	4.044547	-3.222430	-5.098156
H	2.430940	-2.634090	-4.703488
H	2.708292	-5.976766	4.005010
H	3.334350	-4.354585	4.286692
H	5.847774	0.170309	3.096436
H	6.034370	1.899515	2.814415
C	-0.207553	-1.079860	-2.222986
O	-0.258446	-1.321572	-3.347970
O	0.319530	1.242833	-0.134741
C	-0.627573	-2.754790	-0.014384
O	-0.813094	-3.892663	0.141236
C	1.314968	4.086855	-2.159865
C	2.694954	3.437810	-1.715269
B	0.893076	1.927645	-1.424938
H	0.521647	1.171002	-2.312802
O	2.342397	2.080824	-1.423045
O	0.348851	3.279966	-1.483373
C	3.773195	3.436940	-2.808713
H	4.042791	4.457191	-3.109836
H	4.678717	2.950578	-2.428114
H	3.446394	2.887317	-3.694918
C	3.279656	4.081375	-0.446958
H	4.148338	3.497228	-0.123131
H	3.615889	5.110236	-0.623891
H	2.552570	4.071799	0.366362
C	1.127832	5.547081	-1.736830
H	1.874283	6.197175	-2.209141
H	0.135407	5.894311	-2.046033
H	1.204596	5.666420	-0.653177
C	1.059977	3.974115	-3.676969
H	0.034791	4.298888	-3.886249
H	1.742783	4.602458	-4.260092
H	1.159952	2.940003	-4.018734

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Ru	0.224118	-1.176325	-0.243548
P	-2.265438	-1.537945	-0.356400
P	2.614721	-0.802910	0.363359
B	-0.913450	2.341208	0.996177
H	0.017149	-0.957612	1.363923
C	-2.830977	-3.285081	-0.880966
C	-3.180525	-1.209596	1.267568
C	-3.253276	-0.485840	-1.617466
C	3.836883	-0.989670	-1.064272
C	3.211568	-2.146288	1.567682
C	2.992474	0.906230	1.065325
O	-2.097449	1.995455	1.653782
O	-0.491605	3.608492	1.378869
H	-3.907996	-3.156227	-1.065060

C	-2.685126	-4.384116	0.196613
C	-2.189306	-3.762782	-2.203444
H	-3.108507	-0.117963	1.347448
C	-2.504049	-1.761775	2.542565
C	-4.677551	-1.604148	1.233052
H	-4.131744	-1.113512	-1.835055
C	-3.759939	0.869580	-1.077743
C	-2.504854	-0.231161	-2.945237
H	4.824494	-0.810149	-0.618315
C	3.623184	0.073815	-2.164509
C	3.867677	-2.405781	-1.680474
H	3.095794	-3.053064	0.958262
C	4.699812	-2.075187	1.980461
C	2.340636	-2.363834	2.827440
H	2.434986	1.572237	0.395018
C	4.476856	1.347660	1.026741
C	2.425569	1.095772	2.487629
C	-2.654455	3.207171	2.221266
C	-1.373296	4.107051	2.411285
H	-1.630126	-4.530248	0.448442
H	-3.190383	-4.091137	1.118759
C	-3.274438	-5.724414	-0.281495
C	-2.771621	-5.108241	-2.672156
H	-2.332335	-3.023319	-2.994757
H	-1.105806	-3.869999	-2.064934
H	-2.480737	-2.858281	2.535284
H	-1.465137	-1.424740	2.576866
C	-3.246241	-1.286832	3.804167
C	-5.408865	-1.128328	2.501600
H	-5.176719	-1.191045	0.349492
H	-4.778171	-2.694895	1.162306
H	-2.902314	1.513112	-0.866319
H	-4.307913	0.749426	-0.140227
C	-4.677936	1.562416	-2.101517
C	-3.412717	0.459610	-3.979060
H	-1.644315	0.414990	-2.744165
H	-2.118898	-1.158098	-3.375758
H	2.641327	-0.067122	-2.624571
H	3.600466	1.083775	-1.747008
C	4.704295	-0.032213	-3.253369
C	4.934774	-2.507563	-2.786888
H	4.074432	-3.164198	-0.916641
H	2.885114	-2.646004	-2.105714
H	5.350416	-1.925322	1.112173
H	4.854667	-1.215182	2.644196
C	5.126423	-3.359360	2.716656
C	2.755083	-3.654853	3.554825
H	2.458641	-1.517101	3.513044
H	1.280339	-2.403066	2.567925
H	5.084986	0.709380	1.680432
H	4.890253	1.255353	0.018586
C	4.616162	2.810548	1.487467
C	2.572529	2.555799	2.947153
H	1.373699	0.792776	2.518144
H	2.968998	0.453414	3.193261
C	-3.397948	2.862085	3.510907
C	-3.638653	3.783491	1.191675
C	-0.684995	3.889598	3.765417
C	-1.591593	5.603737	2.181736
H	-3.137154	-6.480164	0.502376
H	-4.360306	-5.613249	-0.421341
C	-2.640570	-6.192682	-1.596656
H	-3.833979	-4.972634	-2.924000
H	-2.268925	-5.418400	-3.596957
H	-2.765161	-1.714269	4.693696
H	-3.145155	-0.196096	3.884850
C	-4.735324	-1.658893	3.774120

H	-5.415615	-0.028751	2.523991
H	-6.459003	-1.446059	2.461229
H	-5.579770	0.950198	-2.259326
H	-5.019810	2.520083	-1.687850
C	-3.964765	1.784083	-3.439719
H	-2.841443	0.629343	-4.900767
H	-4.245837	-0.209545	-4.245114
H	4.515432	0.720429	-4.029141
H	5.688117	0.205766	-2.820765
C	4.745462	-1.437230	-3.870013
H	4.906251	-3.511595	-3.229426
H	5.931483	-2.394165	-2.334813
H	5.064557	-4.208978	2.020536
H	6.179213	-3.278443	3.016613
C	4.241235	-3.637325	3.939160
H	2.132477	-3.788057	4.448881
H	2.553691	-4.516458	2.901623
H	5.674857	3.100993	1.462444
H	4.090799	3.458004	0.772421
C	4.032450	3.022513	2.889376
H	1.952878	3.192886	2.305124
H	2.183467	2.656459	3.968616
H	-4.257038	2.221711	3.283653
H	-3.776573	3.769034	3.996712
H	-2.758154	2.330536	4.219443
H	-3.131687	4.020405	0.251009
H	-4.128244	4.689326	1.565039
H	-4.413082	3.039704	0.980682
H	-0.498248	2.827226	3.950352
H	-1.287092	4.286682	4.589873
H	0.278197	4.407230	3.765839
H	-0.641563	6.134409	2.303259
H	-2.302949	6.014062	2.908260
H	-1.963480	5.808213	1.175157
H	-1.576236	-6.413056	-1.429168
H	-3.106274	-7.126862	-1.935425
H	-5.245471	-1.270356	4.664969
H	-4.838423	-2.754040	3.807487
H	-4.644785	2.244549	-4.168411
H	-3.129929	2.478261	-3.280683
H	5.548235	-1.507419	-4.615215
H	3.802573	-1.624623	-4.403793
H	4.528188	-4.587119	4.408079
H	4.409707	-2.852634	4.691659
H	4.628878	2.455939	3.621194
H	4.107476	4.079367	3.176520
C	0.468113	-1.353343	-2.238027
O	0.609934	-1.555874	-3.362453
O	-0.288707	1.523365	0.118274
C	0.512093	-2.946117	0.069178
O	0.739811	-4.072283	0.258857
C	-0.014877	3.799449	-2.672754
C	1.383992	3.925323	-1.932679
B	0.221461	1.975929	-1.237652
H	0.342341	0.882162	-1.837218
O	1.499952	2.677908	-1.239412
O	-0.736812	2.880544	-1.851961
C	2.585535	4.076486	-2.876979
H	2.514350	4.994512	-3.473843
H	3.508156	4.133512	-2.287833
H	2.674996	3.226040	-3.557778
C	1.426224	5.067445	-0.901889
H	2.363921	4.996563	-0.338188
H	1.397409	6.053411	-1.381780
H	0.604811	4.985473	-0.188862
C	-0.810369	5.106324	-2.758445
H	-0.265714	5.869541	-3.327533

H	-1.764189	4.925362	-3.266982
H	-1.028362	5.503655	-1.763928
C	0.106641	3.193658	-4.086130
H	-0.899110	2.994795	-4.472135
H	0.612034	3.868517	-4.786535
H	0.649738	2.243875	-4.065408

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C	-0.062704	-0.218615	-2.410066
O	-0.094938	-0.342141	-3.553530
Ru	-0.030489	0.189246	-0.439145
P	-2.505133	0.042206	-0.068431
P	2.397803	0.205961	0.049000
H	-0.027808	0.532008	1.159064
H	0.544010	-1.935408	-0.687764
C	-3.419813	-1.530389	-0.650614
C	-2.960727	0.366335	1.740848
C	-3.535695	1.391777	-0.945395
C	3.025551	1.824465	0.810980
C	3.581545	-0.011782	-1.413381
C	2.753095	-1.115020	1.378198
H	-4.441931	-1.168305	-0.843931
C	-3.517873	-2.665670	0.396451
C	-2.850589	-2.086966	-1.977930
H	-2.569235	1.386110	1.870627
C	-2.233144	-0.501959	2.790545
C	-4.479684	0.406886	2.038057
H	-4.572406	1.036707	-0.847081
C	-3.468237	2.793690	-0.293086
C	-3.236604	1.508896	-2.457142
H	3.996370	1.555207	1.247343
C	2.130705	2.342328	1.960469
C	3.287956	2.966752	-0.198893
H	3.354633	0.881367	-2.015133
C	5.086383	0.034400	-1.054947
C	3.300839	-1.226387	-2.327307
H	1.767335	-1.224980	1.846309
C	3.782898	-0.735654	2.468742
C	3.122048	-2.507060	0.811929
H	-2.516206	-3.005286	0.675869
H	-3.996918	-2.301771	1.309291
C	-4.335741	-3.854184	-0.143983
C	-3.684304	-3.269619	-2.502087
H	-2.802340	-1.310236	-2.746443
H	-1.830619	-2.442912	-1.809255
H	-2.572189	-1.540317	2.728489
H	-1.163132	-0.529023	2.581317
C	-2.498355	0.035731	4.207140
C	-4.745410	0.930510	3.462201
H	-5.017200	1.033705	1.318711
H	-4.902341	-0.600667	1.945611
H	-2.447132	3.184647	-0.347769
H	-3.730721	2.748664	0.767324
C	-4.416496	3.786355	-0.992204
C	-4.180807	2.506647	-3.151665
H	-2.199933	1.840060	-2.600762
H	-3.326765	0.537322	-2.949413
H	1.160417	2.647654	1.555240
H	1.916349	1.549304	2.684667
C	2.778545	3.544474	2.668295
C	3.921002	4.183469	0.503242
H	3.955990	2.640604	-1.001988
H	2.349344	3.273260	-0.672969
H	5.321263	0.896082	-0.421084
H	5.350893	-0.859842	-0.476276
C	5.954977	0.088244	-2.325488
C	4.156153	-1.153993	-3.604234

H	3.532405	-2.156870	-1.799701	C	3.205910	1.767401	-0.067050
H	2.242538	-1.276363	-2.594822	C	3.244941	-0.901785	-1.310443
H	4.786172	-0.658560	2.025402	C	2.873391	-0.530461	1.743203
H	3.559361	0.236559	2.915505	H	-4.218548	-1.738945	-0.467513
C	3.799309	-1.791989	3.591061	C	-2.460537	-2.984900	-0.542201
C	3.101430	-3.564093	1.929038	C	-3.352910	-1.541575	-2.415173
H	2.438850	-2.816321	0.019628	H	-2.879437	0.707733	2.124521
H	4.129004	-2.470747	0.375306	C	-2.146432	-1.207017	2.671517
H	-4.356007	-4.644971	0.616716	C	-4.506536	-0.694958	1.944327
H	-5.380551	-3.541963	-0.299987	H	-4.446155	0.784796	-1.027487
C	-3.762079	-4.391160	-1.459780	C	-3.839575	2.364319	0.292640
H	-4.699354	-2.926461	-2.756557	C	-2.823890	1.867085	-1.962980
H	-3.234713	-3.639041	-3.432537	H	4.287088	1.573705	-0.071134
H	-1.987077	-0.601576	4.939826	C	2.913588	2.688638	1.135041
H	-2.058005	1.040116	4.306107	C	2.840053	2.471231	-1.393121
C	-3.999124	0.108653	4.521837	H	2.755690	-0.520195	-2.217828
H	-4.423651	1.981177	3.524425	C	4.763611	-0.697350	-1.506071
H	-5.825280	0.923696	3.659736	C	2.924101	-2.411486	-1.246090
H	-5.456732	3.460455	-0.841991	H	2.446280	0.254151	2.384005
H	-4.326698	4.770249	-0.514367	C	4.390709	-0.595062	2.018820
C	-4.129746	3.890773	-2.494981	C	2.201916	-1.847072	2.189625
H	-3.918707	2.574580	-4.215121	H	-1.431788	-2.915485	-0.916871
H	-5.209908	2.120119	-3.107673	H	-2.383038	-3.116206	0.541648
H	2.118465	3.896285	3.471272	C	-3.151054	-4.214991	-1.155816
H	3.715446	3.227387	3.150346	C	-4.046187	-2.774674	-3.024034
C	3.070492	4.681460	1.679766	H	-3.935664	-0.650812	-2.672374
H	4.070667	4.987784	-0.228208	H	-2.365959	-1.422190	-2.876811
H	4.920566	3.905541	0.869800	H	-2.253096	-2.262474	2.388275
H	5.768345	1.039154	-2.846673	H	-1.095325	-0.939763	2.538629
H	7.016028	0.090563	-2.044653	C	-2.562859	-1.048360	4.144057
C	5.654146	-1.078880	-3.276136	C	-4.937701	-0.534299	3.414112
H	3.946501	-2.027552	-4.233723	H	-5.158795	-0.093892	1.298845
H	3.864254	-0.269179	-4.189445	H	-4.658222	-1.742349	1.649292
H	4.548542	-1.510633	4.342685	H	-2.912736	2.808419	0.678433
H	2.824399	-1.779859	4.098916	H	-4.374657	1.963783	1.158699
C	4.074589	-3.203671	3.058253	C	-4.702878	3.466164	-0.351111
H	2.077651	-3.640372	2.318075	C	-3.695975	2.954570	-2.611030
H	3.352405	-4.544724	1.505918	H	-1.864834	2.308056	-1.658753
H	-2.752639	-4.781539	-1.278350	H	-2.582001	1.096637	-2.700188
H	-4.375156	-5.221373	-1.834290	H	1.830551	2.827394	1.233624
H	-4.164804	0.537201	5.518788	H	3.249394	2.222211	2.067668
H	-4.413419	-0.910126	4.546180	C	3.605197	4.055874	0.984461
H	-4.846077	4.569486	-2.975076	C	3.542970	3.831495	-1.535228
H	-3.131808	4.328030	-2.644824	H	3.093125	1.835234	-2.250045
H	3.575839	5.512150	2.188517	H	1.751667	2.618270	-1.429301
H	2.119658	5.078984	1.296193	H	5.012295	0.365794	-1.592898
H	6.243854	-0.980070	-4.196166	H	5.313442	-1.079274	-0.636970
H	5.967330	-2.021107	-2.802705	C	5.254902	-1.425984	-2.772009
H	5.106506	-3.252526	2.678460	C	3.406548	-3.138191	-2.512845
H	4.006796	-3.935203	3.873442	H	3.426026	-2.853180	-0.374581
C	-0.083611	1.996341	-0.723513	H	1.849046	-2.566523	-1.107667
O	-0.095723	3.141015	-0.931463	H	4.835935	-1.404612	1.425651
C	-0.021877	-2.716254	-0.023972	H	4.893876	0.330273	1.714306
O	-0.241646	-3.786639	-0.589872	C	4.670836	-0.866093	3.508819
O	-0.289384	-2.279071	1.124610	C	2.478710	-2.125069	3.677871

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C	0.047276	-0.439354	-2.105789
O	0.149860	-0.760812	-3.223848
Ru	-0.035359	0.095574	-0.270976
P	-2.412530	-0.168087	-0.030476
P	2.339223	0.089589	0.036833
H	-0.041256	0.575669	1.362557
H	0.040369	-1.406331	0.160373
C	-3.202646	-1.673656	-0.882880
C	-3.019503	-0.319727	1.759988
C	-3.496650	1.246197	-0.715900

C	3.205910	1.767401	-0.067050
C	3.244941	-0.901785	-1.310443
C	2.873391	-0.530461	1.743203
H	-4.218548	-1.738945	-0.467513
C	-2.460537	-2.984900	-0.542201
C	-3.352910	-1.541575	-2.415173
H	-2.879437	0.707733	2.124521
C	-2.146432	-1.207017	2.671517
C	-4.506536	-0.694958	1.944327
H	-4.446155	0.784796	-1.027487
C	-3.839575	2.364319	0.292640
C	-2.823890	1.867085	-1.962980
H	4.287088	1.573705	-0.071134
C	2.913588	2.688638	1.135041
C	2.840053	2.471231	-1.393121
H	2.755690	-0.520195	-2.217828
C	4.763611	-0.697350	-1.506071
C	2.924101	-2.411486	-1.246090
H	2.446280	0.254151	2.384005
C	4.390709	-0.595062	2.018820
C	2.201916	-1.847072	2.189625
H	-1.431788	-2.915485	-0.916871
H	-2.383038	-3.116206	0.541648
C	-3.151054	-4.214991	-1.155816
C	-4.046187	-2.774674	-3.024034
H	-3.935664	-0.650812	-2.672374
H	-2.365959	-1.422190	-2.876811
H	-2.253096	-2.262474	2.388275
H	-1.095325	-0.939763	2.538629
C	-2.562859	-1.048360	4.144057
C	-4.937701	-0.534299	3.414112
H	-5.158795	-0.093892	1.298845
H	-4.658222	-1.742349	1.649292
H	-2.912736	2.808419	0.678433
H	-4.374657	1.963783	1.158699
C	-4.702878	3.466164	-0.351111
C	-3.695975	2.954570	-2.611030
H	-1.864834	2.308056	-1.658753
H	-2.582001	1.096637	-2.700188
H	1.830551	2.827394	1.233624
H	3.249394	2.222211	2.067668
C	3.605197	4.055874	0.984461
C	3.542970	3.831495	-1.535228
H	3.093125	1.835234	-2.250045
H	1.751667	2.618270	-1.429301
H	5.012295	0.365794	-1.592898
H	5.313442	-1.079274	-0.636970
C	5.254902	-1.425984	-2.772009
C	3.406548	-3.138191	-2.512845
H	3.426026	-2.853180	-0.374581
H	1.849046	-2.566523	-1.107667
H	4.835935	-1.404612	1.425651
H	4.893876	0.330273	1.714306
C	4.670836	-0.866093	3.508819
C	2.478710	-2.125069	3.677871
H	1.125243	-1.792022	2.008619
H	2.584072	-2.686348	1.594534
H	-2.576380	-5.118135	-0.912234
H	-4.143490	-4.343705	-0.697535
C	-3.310832	-4.074604	-2.674804
H	-5.079385	-2.831329	-2.649085
H	-4.115330	-2.653738	-4.112855
H	-1.944585	-1.698299	4.777037
H	-2.359787	-0.015847	4.465509
C	-4.051550	-1.363776	4.355202
H	-4.874074	0.527571	3.694850
H	-5.990701	-0.824153	3.527194

H	-5.681249	3.040396	-0.619956
H	-4.900105	4.254347	0.387240
C	-4.050294	4.058694	-1.606651
H	-3.174287	3.378202	-3.478904
H	-4.622050	2.500094	-2.994526
H	3.339861	4.697504	1.834743
H	4.695426	3.914220	1.030295
C	3.245359	4.745609	-0.338894
H	3.233441	4.312454	-2.472022
H	4.629387	3.673255	-1.608874
H	4.790204	-0.961398	-3.654279
H	6.338543	-1.286417	-2.880565
C	4.908400	-2.921036	-2.746732
H	3.184559	-4.210353	-2.432582
H	2.840447	-2.764055	-3.377852
H	5.753895	-0.925230	3.679024
H	4.306422	-0.015248	4.103588
C	3.982689	-2.152516	3.987128
H	1.997090	-1.343643	4.284386
H	2.013765	-3.075968	3.969205
H	-2.316952	-4.066156	-3.145540
H	-3.846711	-4.939741	-3.086440
H	-4.337938	-1.187131	5.400142
H	-4.224458	-2.432901	4.160522
H	-4.714954	4.801050	-2.066934
H	-3.133014	4.594718	-1.320909
H	3.791845	5.692601	-0.434881
H	2.175679	5.001563	-0.337105
H	5.224445	-3.399942	-3.682430
H	5.474230	-3.409490	-1.938995
H	4.440555	-3.015216	3.480088
H	4.150826	-2.297316	5.062177
C	-0.458213	3.785484	0.419555
O	-0.611319	4.436501	1.340062

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C	-0.068159	1.609899	2.422018
H	-0.090061	1.805637	3.513612
O	0.002586	0.375587	2.100566
O	-0.109772	2.567569	1.629031
Ru	-0.016559	0.191338	-0.092605
P	2.437850	-0.134706	-0.026446
P	-2.460855	0.027997	0.005979
H	-0.050850	-1.375464	-0.032091
C	3.016758	-1.089396	1.513853
C	3.480066	1.456144	-0.034690
C	3.171642	-1.097586	-1.477243
C	-3.114380	-1.138632	-1.343290
C	-3.049141	-0.523675	1.711377
C	-3.464787	1.597576	-0.316878
H	3.104373	-0.294105	2.268552
C	1.970162	-2.093660	2.050059
C	4.390813	-1.791348	1.400115
H	3.100136	1.964045	-0.933991
C	3.175652	2.379328	1.164741
C	5.012137	1.319233	-0.190983
H	4.210210	-1.311409	-1.191347
C	3.216838	-0.293205	-2.797492
C	2.465824	-2.453398	-1.703317
H	-2.699131	-0.667466	-2.245539
C	-2.526731	-2.566707	-1.296448
C	-4.644623	-1.218453	-1.542939
H	-2.596896	0.248607	2.348266
C	-4.569861	-0.520020	1.977299
C	-2.436954	-1.864038	2.172454
H	-4.520481	1.292875	-0.310857

C	-3.282274	2.668526	0.781121
C	-3.156462	2.193474	-1.708798
H	1.829231	-2.906067	1.323600
H	1.011056	-1.590930	2.170649
C	2.411191	-2.694033	3.396741
C	4.833648	-2.374371	2.754762
H	4.321508	-2.612866	0.674222
H	5.162528	-1.112242	1.028224
H	2.099832	2.511964	1.291499
H	3.555254	1.915373	2.087263
C	3.840611	3.757345	0.991060
C	5.667930	2.696687	-0.402039
H	5.431797	0.875330	0.720557
H	5.281362	0.655312	-1.019137
H	2.201226	-0.032025	-3.110115
H	3.756828	0.650081	-2.662390
C	3.889887	-1.103706	-3.920486
C	3.136269	-3.257354	-2.831003
H	2.463464	-3.046675	-0.782212
H	1.414340	-2.275962	-1.958263
H	-1.443319	-2.527854	-1.150868
H	-2.942720	-3.110580	-0.438626
C	-2.862277	-3.341448	-2.582839
H	-5.094167	-0.221751	-1.597019
H	-5.105367	-1.726565	-0.686187
C	-4.990997	-1.993122	-2.828312
H	-5.030568	0.423317	1.664580
H	-5.050624	-1.314703	1.392507
C	-4.858671	-0.757273	3.471764
C	-2.715712	-2.100437	3.666615
H	-2.876106	-2.689165	1.596753
H	-1.361107	-1.871191	1.982461
H	-2.225639	2.943675	0.860728
H	-3.567448	2.266454	1.760637
C	-4.128128	3.920495	0.489892
C	-3.994942	3.452939	-1.988428
H	-2.090509	2.449373	-1.761607
H	-3.337776	1.456468	-2.499941
H	2.433818	-1.894632	4.152451
H	1.661280	-3.419998	3.737044
C	3.794022	-3.353581	3.315009
H	5.806650	-2.870142	2.640864
H	4.983297	-1.552149	3.470161
H	3.376017	4.270810	0.136838
H	3.631508	4.376415	1.872586
C	5.353655	3.649953	0.759183
H	6.753136	2.575180	-0.515779
H	5.301349	3.131117	-1.344027
H	3.884734	-0.517475	-4.848254
H	4.946415	-1.274299	-3.663676
C	3.196266	-2.455367	-4.137906
H	4.157463	-3.531220	-2.525605
H	2.593520	-4.199074	-2.984222
H	-2.369175	-2.852538	-3.435583
H	-2.447618	-4.355978	-2.521025
C	-4.376458	-3.399312	-2.831400
H	-6.081469	-2.051783	-2.940503
H	-4.617399	-1.430813	-3.696762
H	-4.464360	0.090576	4.051104
H	-5.943271	-0.773419	3.641014
C	-4.219296	-2.058949	3.976592
H	-2.291264	-3.064759	3.974821
H	-2.195223	-1.328058	4.250827
H	-5.197142	3.661765	0.537550
H	-3.952348	4.668411	1.273468
C	-3.813923	4.510249	-0.891502
H	-3.721176	3.863859	-2.968749

H	-5.057619	3.174346	-2.052548
H	3.738801	-4.234930	2.658561
H	4.106347	-3.718421	4.302105
H	5.783704	4.641288	0.566672
H	5.835713	3.272186	1.673412
H	2.173954	-2.281566	-4.503653
H	3.715776	-3.030198	-4.915378
H	-4.590244	-3.906486	-3.780961
H	-4.849553	-4.001582	-2.041304
H	-4.392050	-2.173084	5.054500
H	-4.711799	-2.913962	3.489269
H	-2.775679	4.872177	-0.902825
H	-4.452656	5.380204	-1.091430
C	0.398236	3.182359	-1.016352
O	0.516241	4.309607	-0.911054
C	-0.120838	0.078933	-1.926322
O	-0.249314	0.022751	-3.087188

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O	-3.241329	-0.127072	-0.312217
C	-3.042333	1.209354	-0.121861
O	-3.430325	2.026873	-0.904818
H	-2.507185	1.437383	0.816223
C	-2.724822	-1.024033	0.656928
H	-3.490244	-1.781937	0.820886
H	-2.502099	-0.489063	1.589036
O	-1.586590	-1.693130	0.174677
H	4.014495	2.276889	0.427641
C	3.363976	1.427168	0.243661
C	3.891111	0.269352	-0.337296
C	2.007871	1.517438	0.594476
C	3.088279	-0.852433	-0.595749
H	4.945024	0.234796	-0.596655
C	1.229928	0.404995	0.334877
H	1.587099	2.410728	1.043646
C	1.754224	-0.751235	-0.246099
H	3.485855	-1.755033	-1.047191
O	-0.123129	0.216369	0.576154
O	0.751280	-1.692627	-0.387505
B	-0.380320	-1.076142	0.120494

65

Cu	-0.182353	-0.141100	-1.047707
B	-2.042779	-0.653723	-0.762446
O	-3.088382	0.249935	-0.726491
O	-2.484265	-1.956094	-0.650831
C	1.031272	0.318367	0.408066
N	1.973731	-0.479066	0.987324
N	1.186282	1.520156	1.032087
C	2.698700	0.211124	1.953321
C	2.202548	1.472581	1.981065
C	-4.329114	-0.495210	-0.933201
C	-3.932284	-1.947106	-0.464775
C	-0.547532	-0.389809	-2.906640
O	-1.390790	-0.725873	-3.696100
O	0.650572	-0.000684	-2.871047
H	3.487505	-0.258552	2.519380
H	2.470132	2.332315	2.574720
C	0.423563	2.712030	0.735515
C	0.873087	3.564869	-0.292763
C	-0.716244	2.992643	1.515655
C	0.131438	4.728735	-0.531272
C	-1.413498	4.173347	1.236004
C	-0.997663	5.031958	0.222762

H	0.447053	5.408381	-1.317254
H	-2.296917	4.421131	1.816637
H	-1.556906	5.941369	0.019644
C	2.230229	-1.855116	0.622915
C	3.144771	-2.119542	-0.418253
C	1.585440	-2.876013	1.348500
C	3.395146	-3.462095	-0.726131
C	1.875829	-4.199682	0.996310
C	2.768142	-4.491523	-0.030233
H	4.092220	-3.703463	-1.522521
H	1.394089	-5.011285	1.533436
H	2.976624	-5.526082	-0.289630
C	3.893034	-1.014824	-1.159757
H	3.396926	-0.064763	-0.940147
C	3.858293	-1.190289	-2.688568
H	4.364606	-0.344042	-3.167289
H	4.375473	-2.102044	-3.009508
H	2.830009	-1.218760	-3.058215
C	5.345245	-0.912343	-0.648046
H	5.382924	-0.724774	0.431289
H	5.898507	-1.838557	-0.844100
H	5.871392	-0.093313	-1.152396
C	0.627452	-2.589739	2.500253
H	0.434884	-1.512701	2.521729
C	-0.731076	-3.287025	2.307658
H	-0.632944	-4.378825	2.328800
H	-1.413251	-3.004668	3.118496
H	-1.190356	-3.001330	1.356847
C	1.263841	-2.971518	3.852247
H	2.205863	-2.436802	4.021018
H	0.583948	-2.728569	4.677328
H	1.478715	-4.045533	3.900422
C	-1.178486	2.080898	2.648095
H	-0.637928	1.133514	2.558405
C	-2.678618	1.748899	2.555810
H	-2.925634	1.330215	1.576001
H	-2.944618	1.016903	3.328151
H	-3.304239	2.634335	2.719645
C	-0.828206	2.688664	4.021551
H	0.248435	2.867917	4.122419
H	-1.339958	3.646800	4.171442
H	-1.135578	2.013640	4.829028
C	2.139301	3.296643	-1.102326
H	2.495518	2.291619	-0.857704
C	1.885291	3.321516	-2.621011
H	1.529190	4.301216	-2.959700
H	2.817827	3.107951	-3.156233
H	1.153049	2.563661	-2.913042
C	3.252762	4.288978	-0.708487
H	2.966302	5.321084	-0.942443
H	3.474865	4.240697	0.363888
H	4.175196	4.064867	-1.256849
C	-4.517509	-3.081178	-1.305919
H	-4.153803	-4.042371	-0.927696
H	-5.612754	-3.088188	-1.251447
H	-4.218013	-2.996221	-2.352404
C	-4.200419	-2.208245	1.023219
H	-3.748892	-3.164155	1.305722
H	-3.759264	-1.427610	1.650688
H	-5.273653	-2.262127	1.237191
C	-4.646807	-0.396414	-2.431437
H	-5.579921	-0.913460	-2.681971
H	-4.759337	0.659884	-2.696602
H	-3.832511	-0.804065	-3.036405
C	-5.437931	0.170779	-0.120158
H	-6.383442	-0.373097	-0.232650
H	-5.194490	0.224452	0.943508

H -5.591875 1.191850 -0.483835