

Supporting Information

Mechanistic Insights on the Full Hydrogenation of 2,6-substituted Pyridine Catalyzed by the Lewis Acid $C_6F_5(CH_2)_2B(C_6F_5)_2$

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Full representation of Ref. 17

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Table S1. Cartesian coordinates of all species.

1				F	0.449997	2.60215	-0.000261
B	-0.000079	1.394679	0.0006				
C	-1.372643	0.668189	-0.057298	3			
C	-2.512129	1.308421	0.433345	C	3.563598	-0.295268	0.776563
C	-1.572245	-0.584502	-0.641561	C	2.325803	-0.544265	1.341645
C	-3.770154	0.733603	0.387599	C	1.575141	-1.675151	1.025013
C	-2.81764	-1.179273	-0.719223	C	2.160314	-2.566118	0.122016
C	-3.918235	-0.515801	-0.195063	C	3.400395	-2.344174	-0.450222
C	1.372583	0.668332	0.05804	C	4.103143	-1.193027	-0.130359
C	1.572516	-0.584342	0.64222	F	1.499691	-3.664562	-0.239063
C	2.511804	1.308612	-0.433149	F	3.908628	-3.21052	-1.3154
C	2.81798	-1.17906	0.719284	F	5.272895	-0.945567	-0.693021
C	3.769869	0.733832	-0.388045	F	4.201924	0.837209	1.053395
C	3.918284	-0.515564	0.194549	F	1.841289	0.384968	2.168316
F	-5.112481	-1.077515	-0.253792	C	0.2186	-1.952463	1.51682
F	5.112562	-1.077257	0.252622	H	-0.534894	-1.438624	-1.158474
F	4.827899	1.360701	-0.885595	H	-0.148475	-2.941345	1.266138
F	2.411675	2.50871	-0.996577	C	-0.595547	-1.117154	2.169379
F	0.552831	-1.244185	1.186508	H	-0.322795	-0.109776	2.451257
F	2.975859	-2.365576	1.291213	H	-1.583696	-1.460905	2.450913
F	-0.552271	-1.244304	-1.185358	B	-0.9726	-0.412738	-0.761784
F	-2.975191	-2.365794	-1.29123	C	-2.511955	-0.321564	-0.522765
F	-4.828468	1.360465	0.884548	C	-3.216844	-1.446189	-0.097976
F	-2.412347	2.508551	0.99676	C	-3.268867	0.820854	-0.774903
H	-0.000155	2.577761	0.000914	C	-4.58477	-1.438989	0.109172
2				C	-4.641126	0.858132	-0.59974
C	-1.240188	1.008825	0.000089	C	-5.297412	-0.277804	-0.150041
C	0.110111	1.312719	-0.000175	C	0.00998	0.783689	-0.588672
C	1.106452	0.334268	-0.000313	C	1.248334	0.76279	-1.229089
C	0.663005	-0.98874	-0.000314	C	-0.201664	1.847626	0.290458
C	-0.681366	-1.318347	-0.000079	C	2.214352	1.73374	-1.030574
C	-1.63901	-0.317223	0.000155	C	0.740992	2.833213	0.515283
C	2.514799	0.755645	-0.000638	C	1.959095	2.770315	-0.147692
H	2.648141	1.831246	-0.002588	F	-6.607038	-0.25396	0.029542
C	3.596634	-0.021802	0.001424	F	2.882181	3.684697	0.081094
H	3.556081	-1.10091	0.003556	F	0.511997	3.811698	1.380534
H	4.576863	0.438099	0.000918	F	-1.319647	1.90968	1.013526
F	1.532298	-1.999002	-0.000656	F	1.569132	-0.244575	-2.039818
F	-1.058212	-2.591224	-0.000098	F	3.401593	1.637004	-1.617917
F	-2.926594	-0.628179	0.000424	F	-2.685324	1.927255	-1.232479
F	-2.149012	1.976199	0.000282	F	-5.333552	1.959765	-0.858645
				F	-5.218485	-2.520838	0.544525

F -2.564898 -2.580569 0.162432

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C	3.798842	-0.648812	0.725517
C	2.493875	-0.666183	1.190777
C	1.585596	-1.637691	0.775146
C	2.055662	-2.603395	-0.115803
C	3.3549	-2.613019	-0.582562
C	4.230442	-1.623667	-0.159315
F	1.215609	-3.528358	-0.571139
F	3.761744	-3.541281	-1.433861
F	5.474033	-1.611345	-0.599819
F	4.63295	0.300046	1.122676
F	2.145303	0.299266	2.036604
C	0.152527	-1.684058	1.141486
H	-0.406577	-1.226759	-0.387672
H	-0.312104	-2.64757	0.975227
C	-0.527768	-0.768858	1.971727
H	0.007622	0.013172	2.484328
H	-1.424646	-1.133434	2.452526
B	-0.858116	-0.31344	0.331383
C	-2.441881	-0.369849	0.06456
C	-3.187616	-1.513315	0.318846
C	-3.158439	0.703112	-0.450286
C	-4.548508	-1.610765	0.096294
C	-4.525818	0.648087	-0.686272
C	-5.2248	-0.514022	-0.413328
C	0.029361	0.971402	-0.012809
C	1.027276	0.968103	-0.974266
C	-0.112317	2.149884	0.708653
C	1.864381	2.051532	-1.197413
C	0.684407	3.260899	0.50456
C	1.685797	3.205636	-0.454917
F	-6.530129	-0.580598	-0.636465
F	2.469275	4.255139	-0.656249
F	0.514828	4.36805	1.217561
F	-1.049061	2.223038	1.659546
F	1.251455	-0.128858	-1.715558
F	2.832152	1.985908	-2.106571
F	-2.552321	1.855842	-0.747491
F	-5.166637	1.70321	-1.175547
F	-5.204309	-2.735613	0.36073
F	-2.571471	-2.605372	0.813926

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C	-5.082138	0.963723	-0.000843
C	-3.714043	1.027375	0.208198
C	-2.946933	-0.110186	0.41254
C	-3.604107	-1.332029	0.383563
C	-4.970072	-1.427496	0.17564
C	-5.710646	-0.271389	-0.015705
F	-2.906558	-2.455596	0.556763
F	-5.572164	-2.610567	0.157941
F	-7.019213	-0.347013	-0.214972
F	-5.79208	2.06999	-0.186445
F	-3.126551	2.226377	0.208511
C	-1.457814	-0.032695	0.607154
H	-1.213047	0.920532	1.079988
H	-1.152692	-0.833724	1.282443
C	-0.711709	-0.157767	-0.750748
H	-1.046154	0.663237	-1.388052
H	-1.001706	-1.097478	-1.221857
B	0.829785	-0.048766	-0.472138
C	1.743543	-1.316223	-0.347895
C	1.225648	-2.581664	-0.059596
C	3.126279	-1.264931	-0.551734
C	2.01193	-3.717407	0.029289
C	3.939068	-2.38167	-0.487469
C	3.375679	-3.613688	-0.192181
C	1.431876	1.382603	-0.202034
C	2.270288	1.627774	0.883305
C	1.117072	2.487238	-0.989761
C	2.75934	2.884763	1.186797
C	1.603305	3.757398	-0.728254
C	2.423151	3.954855	0.370667
F	4.140404	-4.687492	-0.118156
F	2.890655	5.161802	0.639965
F	1.297339	4.778595	-1.517547
F	0.356605	2.347154	-2.077949
F	2.62461	0.624886	1.69094
F	3.543647	3.077338	2.239046
F	3.726044	-0.112358	-0.844717
F	5.244402	-2.28826	-0.701817
F	1.47737	-4.894927	0.322485
F	-0.074913	-2.743287	0.181794

5

C -0.416054 0.34149 -0.037982

C	-0.945132	1.619919	-0.243717	H	0.210457	-3.767632	0.567103
C	-2.321751	1.773892	-0.258381	C	3.152207	-2.372703	1.502807
C	-3.129303	0.65979	-0.07806	H	3.359995	-0.71168	2.85286
C	-2.522868	-0.583199	0.100651	H	2.630722	-3.99319	0.191527
N	-1.197274	-0.730559	0.11762	H	4.217404	-2.474939	1.328021
H	-2.761927	2.751437	-0.419038	C	5.212289	1.758751	-0.085502
H	-0.292258	2.465255	-0.41503	C	3.910036	1.874434	-0.547034
H	-4.208917	0.74352	-0.083828	C	3.21296	0.794459	-1.067779
C	-3.331463	-1.836423	0.293873	C	3.875762	-0.424665	-1.104784
H	-3.140706	-2.250431	1.286197	C	5.17008	-0.573225	-0.637739
H	-4.399934	-1.647181	0.190028	C	5.842081	0.525547	-0.12644
H	-3.028129	-2.58796	-0.436848	F	3.246802	-1.50184	-1.57545
C	1.05247	0.103738	-0.008766	F	5.761775	-1.765335	-0.650502
C	1.553246	-1.159916	-0.33062	F	7.082935	0.395823	0.325761
C	1.949389	1.115357	0.341066	F	5.854488	2.813748	0.403566
C	2.920495	-1.398154	-0.324266	F	3.317283	3.06793	-0.465546
H	0.850916	-1.944529	-0.581077	C	1.759829	0.891332	-1.448016
C	3.317808	0.874384	0.353013	H	1.51302	1.929105	-1.678179
H	1.580522	2.090974	0.634969	H	1.581159	0.289917	-2.341639
C	3.808174	-0.381552	0.014642	C	0.91177	0.361619	-0.263943
H	3.295624	-2.380844	-0.584556	H	1.153534	0.963169	0.615176
H	4.000436	1.66694	0.635392	H	1.238608	-0.656511	-0.06149
H	4.875223	-0.569219	0.02174	B	-0.630321	0.444725	-0.545087
<hr/>				C	-1.442932	-0.822408	-1.005338
6				C	-0.806502	-1.967242	-1.487845
C	-1.057635	-1.883181	2.087967	C	-2.816364	-0.95472	-0.784578
C	-1.958764	-2.946385	2.070049	C	-1.461326	-3.172247	-1.67872
C	-3.312045	-2.672592	2.230196	C	-3.500565	-2.14286	-0.959847
C	-3.71684	-1.362271	2.422493	C	-2.814933	-3.262109	-1.40192
C	-2.750217	-0.351622	2.439167	C	-1.346165	1.844737	-0.426062
N	-1.454711	-0.610473	2.254996	C	-2.247848	2.284695	-1.393214
H	-4.039993	-3.475901	2.212003	C	-1.09694	2.731506	0.618871
H	-1.601919	-3.96314	1.96509	C	-2.876668	3.514492	-1.335957
H	-4.762457	-1.112251	2.55307	C	-1.728071	3.961052	0.722838
C	-3.145405	1.086299	2.637288	C	-2.615199	4.355971	-0.264471
H	-3.934219	1.175159	3.385843	F	-3.449846	-4.413715	-1.547922
H	-2.28053	1.668894	2.952605	F	-3.214011	5.53331	-0.187439
H	-3.526781	1.500099	1.698825	F	-1.497052	4.754698	1.762018
C	0.402146	-2.098598	1.920776	F	-0.274008	2.40608	1.616083
C	1.302918	-1.242553	2.559457	F	-2.534705	1.504557	-2.437885
C	0.895182	-3.105539	1.087006	F	-3.722354	3.895878	-2.285478
C	2.669113	-1.382257	2.354717	F	-3.540293	0.074631	-0.341821
H	0.912687	-0.45472	3.192233	F	-4.792813	-2.234069	-0.666365
C	2.26184	-3.233826	0.869928	F	-0.797549	-4.245067	-2.096925

F	0.488253	-1.947745	-1.79863
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6a

B	-0.856727	0.009127	0.133911
C	-2.361792	-0.538221	-0.251562
C	-3.520676	-0.429384	0.510353
C	-2.569559	-1.135191	-1.49259
C	-4.77361	-0.85721	0.090927
C	-3.79377	-1.586396	-1.952239
C	-4.91386	-1.443917	-1.151362
C	0.269971	-1.153195	0.445619
C	0.140424	-2.517169	0.217239
C	1.495557	-0.775254	0.984041
C	1.13906	-3.440198	0.49318
C	2.517511	-1.660663	1.284276
C	2.341448	-3.009498	1.026417
F	-6.101659	-1.861896	-1.570542
F	3.310803	-3.874744	1.287265
F	3.677897	-1.219952	1.767016
F	1.743457	0.522696	1.244837
F	-1.016633	-3.029489	-0.223039
F	0.947043	-4.735087	0.262237
F	-1.534289	-1.32171	-2.319319
F	-3.902537	-2.15497	-3.148556
F	-5.835914	-0.700078	0.8776
F	-3.509705	0.135676	1.73658
C	-0.921554	2.189596	1.699021
C	-0.536096	2.823111	2.873622
C	-0.278897	2.075757	4.008817
C	-0.521812	0.716682	3.95885
C	-0.88992	0.111661	2.763496
N	-0.972495	0.832309	1.614391
H	0.039213	2.551739	4.928368
H	-0.488344	3.90353	2.881906
H	-0.437485	0.097129	4.842475
C	-1.245049	-1.351001	2.821129
H	-1.741272	-1.714533	1.927777
H	-0.356188	-1.959524	3.002581
H	-1.924739	-1.48273	3.665613
C	-1.387171	3.052533	0.584432
C	-2.673259	2.884029	0.074365
C	-0.580397	4.086048	0.106146
C	-3.132999	3.721245	-0.935896
H	-3.314493	2.113724	0.48205

C	-1.037359	4.909875	-0.911551
H	0.425496	4.205983	0.494152
C	-2.313418	4.725401	-1.437452
H	-4.133385	3.587416	-1.329116
H	-0.393979	5.689001	-1.301074
H	-2.669014	5.368815	-2.233012
C	-0.234389	0.994578	-1.026791
H	-1.042183	1.495965	-1.565521
H	0.322925	1.79335	-0.5423
C	0.728725	0.392215	-2.090857
H	0.570854	0.919062	-3.035611
H	0.531989	-0.659277	-2.281521
C	2.185021	0.533343	-1.724742
C	2.77008	1.772864	-1.496597
C	3.008129	-0.570566	-1.557728
C	4.078043	1.911939	-1.066111
C	4.314323	-0.468407	-1.106647
C	4.854737	0.782116	-0.863163
F	2.526129	-1.800036	-1.76687
F	5.032074	-1.564574	-0.885761
F	6.105375	0.901312	-0.436024
F	4.592153	3.118552	-0.841851
F	2.049921	2.888547	-1.668785

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C	3.171309	-2.413461	-1.770693
C	4.240613	-3.011181	-1.100766
C	5.147987	-2.201726	-0.43337
C	4.970594	-0.825866	-0.454204
C	3.881592	-0.300849	-1.151074
N	3.006653	-1.088156	-1.793047
H	5.982993	-2.638345	0.101744
H	4.342638	-4.090077	-1.096233
H	5.668744	-0.165994	0.043277
H	0.35629	0.07787	-1.824258
H	1.017509	-0.246517	-1.593437
C	-5.944915	0.795039	-0.128826
C	-4.59798	0.694604	0.174368
C	-3.93753	-0.525287	0.218734
C	-4.682526	-1.658315	-0.072353
C	-6.032933	-1.590062	-0.378823
C	-6.66466	-0.357461	-0.405623
F	-4.096131	-2.856769	-0.061629
F	-6.722806	-2.693146	-0.646947

F	-7.956067	-0.278822	-0.699239	H	2.478121	3.528064	-3.365935
F	-6.549319	1.97738	-0.157868	H	4.034748	4.007347	0.599559
F	-3.916506	1.815449	0.427302	H	3.101447	4.997475	-1.473047
C	-2.466642	-0.589893	0.523365				
H	-2.242619	0.143456	1.30324				
H	-2.228483	-1.577071	0.922029	TS _{7/8}			
C	-1.615492	-0.310179	-0.734328	C	2.538419	-2.386349	-1.991993
H	-1.980832	0.609367	-1.201705	C	3.546889	-3.200866	-1.489415
H	-1.761267	-1.123491	-1.445845	C	4.638938	-2.611121	-0.864022
B	-0.101462	-0.097575	-0.262574	C	4.713578	-1.230024	-0.777413
C	0.711525	-1.310547	0.40585	C	3.671471	-0.46558	-1.301123
C	0.353483	-2.638793	0.184274	N	2.610553	-1.051192	-1.87809
C	1.874573	-1.141759	1.160095	H	5.428255	-3.226723	-0.449014
C	1.076176	-3.719424	0.6649	H	3.462453	-4.277266	-1.57557
C	2.612572	-2.193735	1.671054	H	5.562366	-0.739941	-0.319715
C	2.21568	-3.494086	1.412983	H	0.452499	-0.029473	-1.647379
C	0.164134	1.406736	0.220914	H	1.248887	-0.367408	-1.654496
C	0.264837	1.761476	1.55924	C	-5.87006	1.199228	-0.158806
C	0.160362	2.463253	-0.681047	C	-4.527033	1.068411	0.153193
C	0.435402	3.069321	1.980528	C	-3.899335	-0.167478	0.221176
C	0.330014	3.78292	-0.302834	C	-4.675149	-1.283755	-0.05662
C	0.484347	4.08427	1.03851	C	-6.02101	-1.185119	-0.372012
F	2.951218	-4.510614	1.837081	C	-6.61959	0.063344	-0.421281
F	0.672103	5.341079	1.420367	F	-4.120762	-2.497401	-0.02465
F	0.357535	4.754171	-1.210462	F	-6.739573	-2.273809	-0.626604
F	-0.021545	2.224837	-1.989454	F	-7.9079	0.171604	-0.722814
F	0.173322	0.820595	2.508089	F	-6.443293	2.397134	-0.20759
F	0.54666	3.360997	3.272426	F	-3.821856	2.177066	0.39247
F	2.378753	0.072253	1.388103	C	-2.432076	-0.279562	0.531417
F	3.731245	-1.970158	2.353039	H	-2.165061	0.504889	1.243975
F	0.713734	-4.963196	0.364175	H	-2.247344	-1.240253	1.0158
F	-0.707736	-2.948148	-0.568956	C	-1.570175	-0.152592	-0.739434
C	2.160056	-3.239616	-2.518864	H	-1.828924	0.785458	-1.241483
H	1.204618	-2.71598	-2.568957	H	-1.826995	-0.964667	-1.422378
H	2.501115	-3.409636	-3.543642	B	-0.008033	-0.112079	-0.33465
H	2.009704	-4.213052	-2.047951	C	0.627637	-1.415912	0.39571
C	3.643442	1.164725	-1.220793	C	0.088328	-2.691273	0.248007
C	3.092605	1.727252	-2.374144	C	1.818432	-1.381943	1.121473
C	3.976085	1.999662	-0.149666	C	0.676658	-3.842314	0.753608
C	2.904465	3.101518	-2.466063	C	2.436258	-2.503244	1.645769
H	2.827189	1.077342	-3.1998	C	1.861598	-3.748551	1.458383
C	3.781508	3.37116	-0.240635	C	0.381629	1.342752	0.241262
H	4.359224	1.568662	0.767745	C	0.506776	1.629841	1.592814
C	3.255893	3.927365	-1.403513	C	0.484662	2.434351	-0.611006
				C	0.795736	2.896105	2.074568

C	0.768234	3.716464	-0.173153
C	0.941936	3.943915	1.180584
F	2.460817	-4.838734	1.918837
F	1.240845	5.162147	1.618076
F	0.887441	4.723899	-1.035627
F	0.30077	2.270175	-1.931022
F	0.333981	0.660148	2.502256
F	0.929967	3.116072	3.379735
F	2.476749	-0.230685	1.304053
F	3.603476	-2.402032	2.277143
F	0.129631	-5.033762	0.528602
F	-1.032994	-2.889225	-0.457082
C	1.33163	-2.947247	-2.688796
H	0.444388	-2.343543	-2.489324
H	1.496795	-2.947396	-3.769258
H	1.13436	-3.971623	-2.370346
C	3.686725	1.015076	-1.254601
C	3.219278	1.745607	-2.348089
C	4.184878	1.690683	-0.136792
C	3.26383	3.134214	-2.331827
H	2.828781	1.218836	-3.211171
C	4.21917	3.078048	-0.120401
H	4.506749	1.127268	0.731202
C	3.765976	3.80161	-1.220428
H	2.894161	3.695167	-3.181192
H	4.589052	3.597096	0.755788
H	3.784745	4.884615	-1.202104

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C	2.136588	2.403212	2.023951
C	2.331629	3.560216	1.287129
C	3.148175	3.529378	0.164738
C	3.803528	2.358198	-0.197112
C	3.611512	1.212649	0.556463
N	2.779785	1.286562	1.624044
H	3.28027	4.425251	-0.431664
H	1.816862	4.463903	1.586122
H	4.461341	2.318858	-1.054013
H	0.207134	0.258583	1.93468
H	2.543752	0.411103	2.10023
C	-5.927305	-2.19991	0.057208
C	-4.564959	-2.084115	-0.172477
C	-3.925324	-0.854685	-0.226283
C	-4.715543	0.26978	-0.027049

C	-6.078014	0.187566	0.204
C	-6.686295	-1.057296	0.244989
F	-4.150678	1.481205	-0.056557
F	-6.807331	1.285816	0.384131
F	-7.994109	-1.152437	0.464669
F	-6.510049	-3.395674	0.096032
F	-3.862778	-3.20745	-0.345577
C	-2.441051	-0.726185	-0.433269
H	-2.085687	-1.609332	-0.962884
H	-2.256878	0.132883	-1.08462
C	-1.694904	-0.544437	0.90233
H	-1.72824	-1.493838	1.449564
H	-2.257231	0.170961	1.50852
B	-0.141591	-0.031145	0.808176
C	-0.022044	1.358783	-0.071766
C	-0.780546	2.464892	0.316063
C	0.811997	1.616152	-1.150981
C	-0.732108	3.7068	-0.298188
C	0.900235	2.841089	-1.79777
C	0.121481	3.899298	-1.371944
C	0.833276	-1.250847	0.303317
C	0.787211	-1.804862	-0.972418
C	1.689276	-1.909797	1.170652
C	1.529898	-2.905081	-1.365447
C	2.429918	-3.035633	0.841909
C	2.356713	-3.529974	-0.444988
F	0.22615	5.093383	-1.951736
F	3.109672	-4.566298	-0.810376
F	3.229773	-3.619632	1.736638
F	1.906259	-1.431115	2.428275
F	0.009335	-1.248193	-1.911828
F	1.476259	-3.364365	-2.614956
F	1.684357	0.68977	-1.597571
F	1.797381	3.026867	-2.771206
F	-1.463868	4.723649	0.153482
F	-1.584061	2.386399	1.389603
C	1.245765	2.333212	3.220453
H	0.201454	2.362358	2.899275
H	1.396005	1.410329	3.779437
H	1.440712	3.188784	3.868583
C	4.285329	-0.069379	0.289824
C	4.857267	-0.789156	1.342816
C	4.375973	-0.549112	-1.018861
C	5.515867	-1.983111	1.085196

H	4.807864	-0.408412	2.357285
C	5.016383	-1.756436	-1.263065
H	3.90208	-0.003165	-1.825169
C	5.586622	-2.472331	-0.214781
H	5.955843	-2.541046	1.901704
H	5.053577	-2.148636	-2.272095
H	6.074504	-3.419365	-0.409195

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C	0.379384	-2.471738	2.737706
C	0.470432	-1.698128	3.88114
C	1.590093	-0.902965	4.083986
C	2.615043	-0.874629	3.151491
C	2.509799	-1.644967	2.005228
N	1.413396	-2.427001	1.872636
H	1.660067	-0.290582	4.97479
H	-0.345158	-1.716298	4.590885
H	3.4877	-0.25301	3.28889
H	0.543062	0.121909	1.482554
H	1.304139	-2.929524	0.995009
C	-5.529167	-1.521165	0.298217
C	-4.198331	-1.304232	-0.011286
C	-3.743095	-0.128916	-0.594486
C	-4.700983	0.840442	-0.857269
C	-6.044155	0.652582	-0.564023
C	-6.459748	-0.533401	0.017095
F	-4.342213	2.000316	-1.408578
F	-6.935655	1.601106	-0.835112
F	-7.742923	-0.72296	0.30761
F	-5.919989	-2.663437	0.860742
F	-3.322542	-2.280168	0.278036
C	-2.275819	0.088061	-0.855308
H	-1.885431	-0.812967	-1.332847
H	-2.156941	0.910336	-1.558104
C	-1.522031	0.371313	0.458294
H	-1.770521	-0.441997	1.150608
H	-1.955934	1.274605	0.9041
B	0.116488	0.539605	0.422292
C	0.600476	2.106926	0.390789
C	0.057245	3.067679	-0.449439
C	1.596524	2.584796	1.228515
C	0.45373	4.395482	-0.469593
C	2.036696	3.898555	1.245513
C	1.454614	4.816203	0.389864

C	0.846321	-0.34495	-0.765348
C	1.892065	0.072263	-1.583162
C	0.513478	-1.680689	-0.95159
C	2.549817	-0.755317	-2.484881
C	1.144437	-2.552296	-1.82256
C	2.18294	-2.081728	-2.604631
F	1.854884	6.085788	0.390134
F	2.857081	-2.90358	-3.405372
F	0.808037	-3.846654	-1.856595
F	-0.443428	-2.253711	-0.174794
F	2.395838	1.311006	-1.494381
F	3.58293	-0.297278	-3.191259
F	2.242995	1.752105	2.082659
F	3.011401	4.28464	2.07358
F	-0.109444	5.268447	-1.303357
F	-0.895717	2.722172	-1.329802
C	-0.802189	-3.322414	2.403102
H	-1.240339	-3.721457	3.317022
H	-1.551423	-2.718892	1.883518
H	-0.529949	-4.147475	1.744618
C	3.517465	-1.663593	0.932352
C	3.843828	-2.851455	0.273234
C	4.147417	-0.467731	0.572247
C	4.79625	-2.844086	-0.738195
H	3.381623	-3.789703	0.565095
C	5.094053	-0.468007	-0.441587
H	3.848724	0.460614	1.046508
C	5.419708	-1.653399	-1.095626
H	5.04493	-3.765009	-1.250368
H	5.554048	0.46427	-0.743762
H	6.146098	-1.644897	-1.898766

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C	0.694954	-2.485305	2.279081
C	0.291273	-1.301345	2.817502
C	1.07959	-0.128176	2.615204
C	2.418791	-0.310522	2.171057
C	2.796383	-1.505051	1.625972
N	1.916045	-2.552649	1.669319
H	0.84759	0.764259	3.184754
H	-0.669258	-1.243281	3.309602
H	3.112129	0.516054	2.187656
H	0.399144	0.564685	1.369667
H	2.136851	-3.383769	1.13475

C	-4.956027	-2.689659	0.203469
C	-3.748741	-2.096233	-0.119032
C	-3.662687	-0.826807	-0.676848
C	-4.862715	-0.166948	-0.903296
C	-6.089689	-0.737662	-0.596824
C	-6.136063	-2.00421	-0.039761
F	-4.861002	1.056513	-1.432842
F	-7.220036	-0.078883	-0.831307
F	-7.304034	-2.559731	0.263176
F	-4.991677	-3.904755	0.746504
F	-2.627123	-2.785834	0.133985
C	-2.326348	-0.186887	-0.949601
H	-1.708383	-0.901579	-1.497264
H	-2.474061	0.683654	-1.58722
C	-1.631165	0.217387	0.365029
H	-1.553653	-0.686875	0.9809
H	-2.294746	0.90106	0.905068
B	-0.167505	0.891014	0.235781
C	-0.120364	2.508859	0.314673
C	-1.142904	3.341958	-0.115202
C	0.958772	3.163815	0.893376
C	-1.106435	4.724088	0.015916
C	1.042731	4.533953	1.048225
C	-0.006683	5.323066	0.603289
C	0.890075	0.193089	-0.787495
C	1.926603	0.848382	-1.452774
C	0.93858	-1.192708	-0.924066
C	2.932208	0.193932	-2.154158
C	1.933167	-1.88658	-1.590153
C	2.948477	-1.1866	-2.215232
F	0.047733	6.643802	0.739732
F	3.949091	-1.825627	-2.808244
F	1.957195	-3.224596	-1.557676
F	0.016861	-1.972216	-0.326725
F	2.032968	2.180672	-1.428583
F	3.933224	0.8827	-2.700539
F	2.013568	2.441582	1.327538
F	2.108197	5.101225	1.612553
F	-2.114253	5.476549	-0.418876
F	-2.234461	2.832629	-0.704837
C	-0.128251	-3.731929	2.249388
H	-1.059014	-3.585125	2.792896
H	-0.377784	-3.971074	1.21203
H	0.413114	-4.573497	2.687674

C	4.091542	-1.731027	0.954422
C	4.659332	-3.005462	0.878576
C	4.733843	-0.660022	0.322794
C	5.839063	-3.207687	0.174175
H	4.202268	-3.842835	1.395028
C	5.909927	-0.866316	-0.383018
H	4.286854	0.327349	0.346314
C	6.462654	-2.140763	-0.461924
H	6.271485	-4.199219	0.124323
H	6.381641	-0.033665	-0.889918
H	7.375418	-2.302709	-1.021733

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C	3.315376	1.216021	1.44257
C	3.227409	0.073954	2.129137
C	2.010416	-0.313111	2.930377
C	0.891674	0.673769	2.708801
C	1.043357	1.80852	2.009412
N	2.279131	2.160696	1.451967
H	2.255949	-0.367244	3.999691
H	4.091385	-0.579775	2.158193
H	-0.055768	0.491627	3.201366
H	1.685487	-1.329304	2.660999
H	2.223482	2.7317	0.618843
C	4.655604	-1.029062	-1.225332
C	3.329401	-1.119712	-1.615644
C	2.44114	-1.994462	-1.007598
C	2.946296	-2.793179	0.010071
C	4.262893	-2.718187	0.426745
C	5.120155	-1.824922	-0.194011
F	2.134315	-3.648577	0.638967
F	4.698719	-3.455051	1.442878
F	6.371687	-1.694846	0.232065
F	5.472238	-0.155062	-1.805787
F	2.918112	-0.317141	-2.600446
C	0.983028	-2.038901	-1.380438
H	0.823616	-1.334793	-2.197471
H	0.730189	-3.030725	-1.762318
C	0.064266	-1.728058	-0.169264
H	0.619461	-1.09801	0.539989
H	-0.165643	-2.655906	0.353812
B	-1.236322	-0.920055	-0.508877
C	-2.614624	-1.609557	-0.168731
C	-2.833211	-2.920257	-0.578597

C	-3.618332	-1.034933	0.600545
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C	-4.773941	-1.709386	0.950652
C	-4.957399	-3.010354	0.506057
C	-1.168943	0.540193	-1.073877
C	-2.304621	1.267316	-1.456881
C	0.028274	1.265633	-1.100454
C	-2.273938	2.614285	-1.764176
C	0.09193	2.61303	-1.404661
C	-1.06773	3.296221	-1.722452
F	-6.06221	-3.666348	0.822321
F	-1.026662	4.586414	-1.992931
F	1.255423	3.261335	-1.361618
F	1.191168	0.695729	-0.788078
F	-3.496423	0.679542	-1.533852
F	-3.387349	3.269544	-2.065176
F	-3.477754	0.215524	1.055721
F	-5.701555	-1.129775	1.701937
F	-4.16603	-4.865274	-0.697841
F	-1.915842	-3.537948	-1.33138
C	4.506576	1.637866	0.6368
H	4.880663	2.601771	0.991467
H	5.310135	0.905036	0.706052
H	4.234307	1.753987	-0.418443
C	-0.043135	2.795828	1.785774
C	0.253687	4.139708	1.535055
C	-1.381254	2.391567	1.750502
C	-0.759206	5.046135	1.238501
H	1.281124	4.480215	1.584624
C	-2.392795	3.297788	1.465728
H	-1.62908	1.351164	1.916956
C	-2.084901	4.629798	1.196896
H	-0.509696	6.081328	1.038538
H	-3.420563	2.954071	1.427622
H	-2.871723	5.333509	0.953504

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C	-0.355755	0.370369	-0.101855
C	-0.892137	1.577438	-0.313711
C	-2.377172	1.811909	-0.406982
C	-3.134929	0.558356	-0.051638
C	-2.543283	-0.620642	0.147673
H	-2.642925	2.146241	-1.419643
H	-0.223917	2.413482	-0.480422

H	-4.21445	0.611059	0.025323
C	-3.272159	-1.884538	0.490478
H	-2.923849	-2.284828	1.448219
H	-4.343314	-1.704437	0.563965
H	-3.09313	-2.646658	-0.272788
C	1.104387	0.12429	-0.038673
C	1.647384	-1.040279	-0.58973
C	1.961199	1.043	0.572918
C	3.016824	-1.272127	-0.542565
H	0.990374	-1.750534	-1.078826
C	3.329474	0.811236	0.616095
H	1.54284	1.930973	1.0321
C	3.862459	-0.347057	0.059053
H	3.424639	-2.174622	-0.982406
H	3.981413	1.53097	1.096874
H	4.929709	-0.528861	0.097523
H	-2.672627	2.635613	0.255426
H	-0.750784	-1.515743	0.576403
N	-1.154534	-0.779199	0.013125

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C	-2.683196	4.035438	-0.14662
C	-2.600873	2.699868	-0.519853
C	-1.733905	4.931611	-0.616026
C	-0.704727	4.49943	-1.445705
C	-0.630812	3.163854	-1.80156
N	-1.588157	2.334388	-1.334706
F	2.981242	2.261799	-0.823639
C	2.063265	2.724969	0.040506
C	1.07233	1.891363	0.546597
C	0.154418	2.552741	1.35996
C	0.211645	3.89864	1.675366
C	1.229828	4.67614	1.152614
C	2.161546	4.082451	0.323208
B	0.879523	0.30251	0.144508
F	-0.909565	1.892197	1.851868
F	-0.744756	4.473405	2.409309
F	3.112675	4.826966	-0.241928
C	0.354349	-0.593503	1.413859
C	-0.516786	-1.655487	1.227009
C	-0.997081	-2.457556	2.248526
C	-0.573748	-2.229678	3.544949
C	0.322984	-1.201496	3.785654
C	0.762034	-0.417394	2.729521

F	-0.988702	-1.939115	-0.010424	C	-1.745842	-0.885586	-3.053521
F	1.625424	0.563348	3.036558	H	-1.587262	0.943545	-4.04201
F	0.745586	-0.97679	5.02772	C	-0.307715	-1.28678	-3.189001
F	-1.887385	-3.426377	1.992668	H	-0.229392	-2.189403	-3.801254
H	0.058698	5.181037	-1.796981	H	0.271271	-0.495948	-3.664994
H	-1.772933	5.969103	-0.304411	H	0.122627	-1.493698	-2.206492
H	-1.552144	1.350054	-1.640379	H	-2.144665	-2.665833	-2.092468
H	-0.010417	0.276865	-0.696235	N	-2.559761	-1.826752	-2.460937
H	-3.457829	4.339296	0.543338	C	-3.721479	0.623566	-3.431599
C	-3.514981	1.650538	-0.042806	H	-4.136036	0.739707	-4.442727
C	-4.890177	1.883714	0.016138	H	-3.872923	1.603726	-2.951069
C	-2.989911	0.429434	0.385143	C	-4.476629	-0.437893	-2.671654
C	-5.734975	0.889538	0.493485	C	-3.916702	-1.581673	-2.251845
H	-5.296266	2.826046	-0.336013	H	-5.51862	-0.259017	-2.439112
C	-3.835599	-0.536899	0.906924	C	-4.657256	-2.623563	-1.501206
H	-1.920573	0.263007	0.358907	C	-4.016991	-3.389584	-0.522184
C	-5.208074	-0.317497	0.944917	C	-6.020359	-2.832923	-1.727793
H	-6.804506	1.058838	0.516721	C	-4.726267	-4.317369	0.231477
H	-3.426731	-1.47426	1.26386	H	-2.967691	-3.233401	-0.298703
H	-5.865976	-1.094573	1.317234	C	-6.72889	-3.759635	-0.974488
C	0.428351	2.589258	-2.685929	H	-6.520484	-2.278255	-2.512751
H	0.712651	1.592028	-2.341415	C	-6.086178	-4.503046	0.011291
H	0.062955	2.519678	-3.713781	H	-4.210495	-4.882941	0.998455
H	1.309627	3.229837	-2.67465	H	-7.784227	-3.912511	-1.167203
F	-1.02244	-2.983876	4.544005	H	-6.640107	-5.227407	0.596045
F	1.264466	5.987142	1.387269				
C	5.742293	-3.321535	-0.480737				
C	4.703681	-2.598334	0.082815	TS _{12/13}			
C	4.561803	-1.230777	-0.106816	C	-2.80266	3.990914	-0.045155
C	5.509051	-0.611007	-0.910041	C	-2.674606	2.693918	-0.535764
C	6.558463	-1.306443	-1.488678	C	-1.889727	4.953119	-0.448971
C	6.675343	-2.669562	-1.270471	C	-0.857076	4.599342	-1.307663
F	5.419121	0.700212	-1.14452	C	-0.768289	3.28809	-1.761008
F	7.450669	-0.679457	-2.251374	N	-1.683535	2.381147	-1.384533
F	7.67729	-3.34995	-1.817953	F	2.897292	2.288996	-0.849417
F	5.851589	-4.631147	-0.273	C	1.991821	2.729688	0.042437
F	3.814163	-3.256754	0.831969	C	1.042116	1.870079	0.580792
C	3.40321	-0.469476	0.478059	C	0.132804	2.504809	1.424376
H	3.120124	-0.941107	1.421772	C	0.157401	3.853693	1.729463
H	3.732748	0.546005	0.705436	C	1.129621	4.660081	1.165662
C	2.194795	-0.439142	-0.474029	C	2.053319	4.091491	0.311273
H	1.921562	-1.479919	-0.694728	B	0.866335	0.28778	0.158127
H	2.51097	0.001986	-1.425795	F	-0.882981	1.810523	1.968168
C	-2.251989	0.279132	-3.501852	F	-0.789929	4.403475	2.493328
				F	2.950913	4.865216	-0.303844

C	0.364453	-0.634272	1.422439	H	3.141878	-0.905686	1.415573
C	-0.493603	-1.70408	1.233642	H	3.717666	0.590336	0.687131
C	-0.970474	-2.516838	2.247901	C	2.190689	-0.429211	-0.473737
C	-0.552908	-2.291844	3.54608	H	1.941948	-1.477155	-0.692391
C	0.33534	-1.257131	3.791743	H	2.489969	0.02282	-1.426163
C	0.769267	-0.463697	2.740437	C	-2.089892	0.44237	-3.196777
F	-0.95678	-1.996832	-0.010239	C	-1.611277	-0.829723	-2.840121
F	1.621096	0.522869	3.055792	H	-1.446961	0.944615	-3.917315
F	0.753759	-1.035243	5.035676	C	-0.173904	-1.211219	-2.981554
F	-1.852001	-3.493141	1.981386	H	-0.05439	-1.770994	-3.914274
H	-0.105246	5.319447	-1.606744	H	0.458614	-0.326691	-3.018437
H	-1.954253	5.963545	-0.062196	H	0.148888	-1.829697	-2.143736
H	-1.771999	1.233506	-2.130282	H	-2.040216	-2.612991	-2.009934
H	-0.032451	0.280571	-0.670854	N	-2.434095	-1.751591	-2.362795
H	-3.580326	4.211475	0.673845	C	-3.589939	0.63765	-3.402483
C	-3.568144	1.600803	-0.088761	H	-3.845902	0.653281	-4.469296
C	-4.953847	1.761352	-0.083172	H	-3.894819	1.614727	-3.008057
C	-3.001761	0.417926	0.390539	C	-4.384248	-0.4411	-2.714234
C	-5.769027	0.73692	0.387814	C	-3.838974	-1.566272	-2.250014
H	-5.391	2.680018	-0.461103	H	-5.449272	-0.29449	-2.586574
C	-3.818032	-0.578925	0.904707	C	-4.569727	-2.658227	-1.57181
H	-1.923797	0.314981	0.402771	C	-3.952069	-3.418919	-0.574499
C	-5.201549	-0.430616	0.888174	C	-5.907774	-2.915021	-1.882491
H	-6.845913	0.856255	0.374558	C	-4.663358	-4.392808	0.115825
H	-3.377144	-1.483435	1.307353	H	-2.926886	-3.225144	-0.279777
H	-5.833747	-1.229222	1.259872	C	-6.617528	-3.886693	-1.190208
C	0.338034	2.826416	-2.665728	H	-6.388601	-2.361202	-2.680172
H	0.684724	1.839398	-2.350969	C	-5.999649	-4.626617	-0.186076
H	-0.000349	2.77496	-3.70423	H	-4.168235	-4.953453	0.899601
H	1.18157	3.515292	-2.616372	H	-7.653982	-4.075542	-1.443136
F	-0.997131	-3.054878	4.540935	H	-6.555122	-5.385184	0.351812
F	1.116235	5.976781	1.375827				
C	5.780606	-3.247734	-0.517204				
C	4.735983	-2.540739	0.055587	13			
C	4.575008	-1.174112	-0.125768	C	-3.046582	4.140334	0.141297
C	5.509318	-0.537753	-0.931327	C	-2.808672	2.877056	-0.398534
C	6.564808	-1.216937	-1.518782	C	-2.212091	5.185508	-0.231072
C	6.701031	-2.579447	-1.308108	C	-1.17506	4.939894	-1.119603
F	5.400398	0.772428	-1.160003	C	-0.996615	3.644476	-1.607693
F	7.444902	-0.575336	-2.283492	N	-1.80545	2.643893	-1.251964
F	7.708983	-3.243905	-1.864854	F	2.75689	2.333071	-0.945935
F	5.906613	-4.557594	-0.318095	C	1.87044	2.736773	-0.016867
F	3.857586	-3.215056	0.804501	C	0.99438	1.832425	0.568787
C	3.407839	-0.432868	0.467387	C	0.09466	2.422002	1.454508
				C	0.052175	3.775101	1.740124

C	0.944412	4.628437	1.117298	F	5.485941	0.959826	-1.027781
C	1.863078	4.102886	0.231335	F	7.608356	-0.307132	-2.091765
B	0.888386	0.254832	0.116032	F	7.933847	-2.974069	-1.714522
F	-0.843304	1.678567	2.068224	F	6.10939	-4.369961	-0.265385
F	-0.875882	4.277802	2.557127	F	3.980901	-3.108012	0.799597
F	2.679357	4.9206	-0.440242	C	3.459047	-0.339988	0.497961
C	0.353839	-0.715444	1.327533	H	3.201521	-0.810443	1.449462
C	-0.503705	-1.773609	1.085157	H	3.705676	0.70307	0.704578
C	-0.97548	-2.637044	2.060083	C	2.263579	-0.415572	-0.466205
C	-0.565327	-2.470798	3.36884	H	2.070827	-1.479835	-0.666806
C	0.313411	-1.441754	3.667328	H	2.563597	0.035536	-1.418618
C	0.748407	-0.600781	2.655197	C	-1.783431	0.161418	-3.061107
F	-0.967497	-2.01132	-0.174544	C	-1.437067	-1.263776	-2.890573
F	1.586827	0.379763	3.018665	H	-1.096655	0.620608	-3.774804
F	0.720723	-1.272925	4.923004	C	-0.033381	-1.718493	-3.01573
F	-1.846324	-3.611847	1.748023	H	0.308522	-1.555893	-4.041093
H	-0.489874	5.727971	-1.409922	H	0.575851	-1.090831	-2.355594
H	-2.348289	6.173901	0.192028	H	0.095746	-2.76403	-2.738597
H	-1.538537	0.636872	-2.091601	H	-2.112066	-3.062478	-2.368945
H	0.037144	0.245441	-0.758717	N	-2.370672	-2.099277	-2.56351
H	-3.836857	4.279889	0.867635	C	-3.249992	0.430799	-3.396533
C	-3.638109	1.703611	-0.016243	H	-3.432897	0.377572	-4.476276
C	-5.031246	1.777218	0.002667	H	-3.482616	1.449849	-3.07997
C	-3.009603	0.511097	0.354131	C	-4.156641	-0.538041	-2.692151
C	-5.788302	0.671681	0.384556	C	-3.743836	-1.749122	-2.323337
H	-5.522903	2.6992	-0.290235	H	-5.171565	-0.243365	-2.453026
C	-3.765815	-0.572546	0.777033	C	-4.526893	-2.774	-1.609258
H	-1.926836	0.465108	0.350107	C	-3.922504	-3.550768	-0.617439
C	-5.156559	-0.50275	0.779354	C	-5.892124	-2.924949	-1.860317
H	-6.870383	0.73434	0.385949	C	-4.676038	-4.448672	0.127965
H	-3.272793	-1.485231	1.092101	H	-2.875487	-3.414342	-0.369644
H	-5.740617	-1.364629	1.084746	C	-6.642146	-3.823764	-1.113978
C	0.10693	3.305673	-2.574081	H	-6.361018	-2.343029	-2.645399
H	0.491978	2.306028	-2.359059	C	-6.037917	-4.584794	-0.116921
H	-0.272629	3.321895	-3.60067	H	-4.194971	-5.020922	0.911866
H	0.931275	4.017533	-2.506683	H	-7.700591	-3.936116	-1.315151
F	-1.0078	-3.284531	4.323937	H	-6.627733	-5.281822	0.465743
F	0.857669	5.945591	1.306069				
C	5.955071	-3.059711	-0.443591				
C	4.869112	-2.393745	0.100021	14			
C	4.674072	-1.02875	-0.062141	F	-1.781203	2.601463	-0.544696
C	5.620519	-0.350388	-0.817753	C	-0.471894	2.504081	-0.813003
C	6.717936	-0.988354	-1.374735	C	0.229663	1.336159	-0.540887
C	6.886108	-2.349961	-1.184563	C	1.580616	1.394558	-0.872815
				C	2.212686	2.511371	-1.390085

C	1.469003	3.656207	-1.629405	H	2.885864	-0.705264	2.675591
C	0.115248	3.648164	-1.345473	N	2.825039	0.292966	2.485399
B	-0.32057	0.046646	0.31866	C	2.927581	3.07749	2.23941
F	2.374938	0.333496	-0.631816	H	3.402554	3.427134	3.164265
F	3.525604	2.506374	-1.638218	H	2.717353	3.966491	1.643602
F	-0.609275	4.741574	-1.572412	C	3.885274	2.178326	1.509088
C	0.233215	-1.343455	-0.338462	C	3.855201	0.854166	1.652512
C	0.950457	-2.272416	0.393156	H	4.632345	2.611515	0.856494
C	1.536477	-3.403975	-0.1488	C	4.782921	-0.127641	1.058941
C	1.383504	-3.661919	-1.499211	C	4.348942	-1.412731	0.725306
C	0.652646	-2.778062	-2.2763	C	6.113231	0.2248	0.818812
C	0.105658	-1.648215	-1.686666	C	5.22273	-2.326369	0.151682
F	1.203784	-2.068729	1.717641	H	3.316829	-1.701192	0.877049
F	-0.542951	-0.801881	-2.49934	C	6.982518	-0.686296	0.236069
F	0.506421	-3.013428	-3.577689	H	6.471283	1.206341	1.106011
F	2.29276	-4.211285	0.604137	C	6.540886	-1.962935	-0.09817
H	0.964835	2.3277	1.657271	H	4.862366	-3.31487	-0.106943
H	0.264123	0.156747	1.380031	H	8.011857	-0.403224	0.052995
F	1.946866	-4.737502	-2.044113	H	7.22396	-2.67271	-0.548471
F	2.051968	4.746102	-2.123355				
C	-6.152486	-1.498188	0.845006				
C	-4.836575	-1.451769	0.416798	TS _{14/15}			
C	-4.278987	-0.317963	-0.159368	F	1.751426	2.562982	0.793416
C	-5.107584	0.788582	-0.283475	C	0.423639	2.550708	0.971735
C	-6.429626	0.77268	0.134266	C	-0.328821	1.428784	0.651012
C	-6.953752	-0.376947	0.70114	C	-1.695304	1.563222	0.881654
F	-4.636918	1.915946	-0.819844	C	-2.295036	2.716121	1.354476
F	-7.197551	1.850704	-0.00335	C	-1.498248	3.810087	1.658833
F	-8.219271	-0.404598	1.107697	C	-0.130565	3.724576	1.47092
F	-6.652485	-2.603647	1.392506	B	0.193121	0.089334	-0.119911
F	-4.086169	-2.546783	0.573793	F	-2.519765	0.54413	0.577676
C	-2.82942	-0.284052	-0.563552	F	-3.617407	2.794747	1.504383
H	-2.576278	-1.245989	-1.015707	F	0.639034	4.771421	1.757527
H	-2.69099	0.483304	-1.326181	C	-0.305258	-1.258432	0.646426
C	-1.910989	-0.016656	0.641226	C	-0.949284	-2.296196	-0.001997
H	-2.07244	-0.821989	1.370073	C	-1.46008	-3.414285	0.635077
H	-2.24075	0.908489	1.127418	C	-1.292302	-3.541898	2.002754
C	1.610805	2.361289	2.547305	C	-0.623734	-2.547634	2.69924
C	1.787498	0.928955	2.92494	C	-0.153801	-1.436517	2.015044
H	1.041535	2.867489	3.328534	F	-1.165578	-2.236791	-1.344307
C	0.824235	0.255384	3.832783	F	0.466456	-0.497136	2.741767
H	1.066881	0.549189	4.860627	F	-0.453899	-2.666919	4.012764
H	-0.185081	0.59948	3.606067	F	-2.137631	-4.340845	-0.04672
H	0.864587	-0.828636	3.735115	H	-0.840537	2.250013	-1.59633
				H	-0.47904	0.124232	-1.16458

F	-1.772912	-4.604717	2.64045
F	-2.046615	4.929668	2.120523
C	5.937412	-1.533999	-1.055927
C	4.653015	-1.47396	-0.542693
C	4.15521	-0.343451	0.091485
C	5.01024	0.74579	0.186485
C	6.302079	0.715941	-0.316537
C	6.766685	-0.429721	-0.940493
F	4.594498	1.868715	0.773721
F	7.096199	1.77737	-0.208598
F	8.00001	-0.467776	-1.433715
F	6.379107	-2.634563	-1.659125
F	3.871145	-2.550309	-0.676359
C	2.734527	-0.292812	0.585121
H	2.48651	-1.262157	1.025184
H	2.654581	0.457003	1.37176
C	1.750495	0.018195	-0.558491
H	1.861121	-0.778388	-1.307423
H	2.065415	0.950889	-1.042585
C	-1.242246	2.062236	-2.596961
C	-1.343359	0.56958	-2.759028
H	-0.502403	2.433434	-3.308834
C	-0.285857	-0.182054	-3.494962
H	-0.42711	0.006147	-4.565567
H	0.697417	0.185406	-3.203372
H	-0.343304	-1.251955	-3.299239
H	-2.575036	-0.999821	-2.663883
N	-2.512109	0.009537	-2.56437
C	-2.590319	2.767645	-2.768485
H	-2.837907	2.868885	-3.83249
H	-2.514836	3.778457	-2.367451
C	-3.689584	2.006277	-2.080371
C	-3.655516	0.675291	-2.019647
H	-4.527115	2.530654	-1.638878
C	-4.696985	-0.213286	-1.468061
C	-4.350672	-1.392531	-0.803588
C	-6.046232	0.115183	-1.617048
C	-5.336258	-2.226372	-0.292934
H	-3.30869	-1.644658	-0.652513
C	-7.029138	-0.71436	-1.095405
H	-6.322687	1.010054	-2.162391
C	-6.677058	-1.88794	-0.435874
H	-5.050862	-3.135938	0.221813
H	-8.072957	-0.452411	-1.217382

H	-7.445881	-2.538189	-0.036872
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F	-1.955229	2.772825	-1.240534
C	-0.730944	3.093597	-0.813524
C	0.174708	2.091424	-0.474935
C	1.443906	2.516943	-0.091985
C	1.789543	3.851918	0.003468
C	0.854292	4.817005	-0.339054
C	-0.410893	4.439666	-0.762398
B	-0.248754	0.579482	-0.431814
F	2.375845	1.620466	0.234741
F	2.9959	4.21543	0.420587
F	-1.295842	5.366077	-1.106941
C	0.727597	-0.538138	-0.945866
C	0.609024	-1.873651	-0.549573
C	1.387274	-2.89218	-1.063211
C	2.3275	-2.597967	-2.038513
C	2.508708	-1.288179	-2.446059
C	1.718427	-0.290604	-1.900175
F	-0.262355	-2.221297	0.406977
F	1.92981	0.94157	-2.359458
F	3.42969	-1.002156	-3.355854
F	1.265972	-4.136311	-0.619018
H	1.692129	2.142119	2.606598
H	0.44886	0.438154	1.801635
F	3.049964	-3.566572	-2.570043
F	1.170527	6.098891	-0.263971
C	-5.503359	-2.134355	0.696337
C	-4.229079	-1.878248	0.219112
C	-3.935405	-0.749303	-0.532823
C	-4.974952	0.136016	-0.778324
C	-6.26043	-0.09321	-0.31413
C	-6.523563	-1.235465	0.424854
F	-4.743784	1.247956	-1.478187
F	-7.236338	0.770434	-0.56888
F	-7.748777	-1.468011	0.875669
F	-5.755508	-3.227105	1.40745
F	-3.256475	-2.748816	0.498886
C	-2.537344	-0.47532	-1.013442
H	-2.068579	-1.419292	-1.299033
H	-2.592157	0.156731	-1.901781
C	-1.695889	0.220159	0.08257
H	-1.625589	-0.459603	0.937395

H	-2.227727	1.110092	0.423139
C	1.567219	1.37091	3.370001
C	0.920866	0.118473	2.745741
H	0.897035	1.773196	4.134278
C	-0.16388	-0.486569	3.626265
H	0.25503	-0.74689	4.601193
H	-0.982815	0.22284	3.769486
H	-0.568375	-1.397221	3.175402
H	1.557102	-1.615289	1.812214
N	1.91999	-0.916852	2.445938
C	2.954585	1.067897	3.953981
H	2.841259	0.370665	4.795089
H	3.405407	1.980384	4.346132
C	3.803454	0.437756	2.890245
C	3.238975	-0.533955	2.162693
H	4.830342	0.731392	2.72297
C	3.951049	-1.297905	1.112921
C	3.867159	-2.694127	1.069159
C	4.733952	-0.637524	0.162768
C	4.567001	-3.413372	0.107796
H	3.276176	-3.218764	1.813264
C	5.433008	-1.35889	-0.79946
H	4.775513	0.445534	0.178365
C	5.354069	-2.747319	-0.828017
H	4.498199	-4.494753	0.0887
H	6.030062	-0.834353	-1.53591
H	5.891914	-3.307724	-1.582963

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H	2.720445	0.99247	1.661319
H	2.859534	-1.428746	1.358883
C	3.030916	0.611769	0.683579
C	2.496804	-0.818748	0.527715
H	4.123231	0.611888	0.656164
C	2.947859	-1.459724	-0.785327
H	2.479109	-0.956819	-1.63414
H	4.033377	-1.396747	-0.898734
H	2.649381	-2.508468	-0.813459
H	0.646314	-1.139826	1.475777
N	1.034205	-0.836567	0.592583
C	2.453471	1.505912	-0.413349
H	2.955812	1.308297	-1.368348
H	2.655396	2.556093	-0.181439
C	0.970171	1.292403	-0.532492

C	0.343853	0.241102	0.023696
H	0.382218	2.009912	-1.091623
C	-1.133662	0.092055	0.009923
C	-1.716326	-1.172172	-0.118374
C	-1.967056	1.20713	0.133133
C	-3.098611	-1.313701	-0.142861
H	-1.07147	-2.037118	-0.2174
C	-3.347844	1.064959	0.104465
H	-1.522074	2.185725	0.272262
C	-3.919059	-0.196461	-0.034183
H	-3.53621	-2.299087	-0.253947
H	-3.98092	1.93901	0.202696
H	-4.996674	-0.307759	-0.051635

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H	-2.134521	0.56253	1.660956
C	-2.385332	0.616459	0.592303
C	-3.252362	1.84431	0.355881
H	-3.506049	1.915421	-0.704118
H	-4.175636	1.778093	0.935774
H	-2.733241	2.760852	0.649055
H	-0.630776	1.588307	0.178
N	-1.127667	0.77518	-0.166557
C	-2.308199	-1.604906	-0.712473
H	-2.452007	-1.252685	-1.742284
H	-2.696887	-2.623418	-0.669509
C	-0.839992	-1.557816	-0.411374
C	-0.290199	-0.355854	-0.192716
H	-0.220472	-2.440025	-0.499302
C	1.167103	-0.122994	-0.070051
C	1.749371	1.015314	-0.63646
C	1.988466	-1.034384	0.598905
C	3.118399	1.233828	-0.539335
H	1.129281	1.716149	-1.184895
C	3.356413	-0.81583	0.693053
H	1.541661	-1.905869	1.062887
C	3.926872	0.319672	0.126024
H	3.554793	2.11656	-0.99159
H	3.978501	-1.528607	1.221422
H	4.99368	0.490984	0.2042
C	-3.11939	-0.690914	0.221646
H	-4.077396	-0.454318	-0.250436
H	-3.34416	-1.23154	1.143318

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H	-2.600492	-0.148897	-1.500742
C	-2.502858	-0.548597	-0.478171
C	-3.251236	-1.868714	-0.379685
H	-3.180353	-2.260341	0.637508
H	-4.304357	-1.734654	-0.635048
H	-2.830674	-2.611804	-1.062619
H	-0.659448	-1.453985	-0.768646
N	-1.094159	-0.770172	-0.160754
C	-2.302293	1.827023	0.320852
H	-2.525887	2.485421	1.165277
H	-2.657574	2.350765	-0.575018
C	-0.818142	1.586911	0.239835
C	-0.297004	0.371765	0.009229
H	-0.142765	2.406268	0.45234
C	1.165479	0.11867	0.003928
C	1.67565	-1.072079	0.530415
C	2.056727	1.055767	-0.52586
C	3.04478	-1.31059	0.541442
H	0.99005	-1.797875	0.952659
C	3.424449	0.816759	-0.511958
H	1.666283	1.965469	-0.966904
C	3.924077	-0.366927	0.022233
H	3.426109	-2.233681	0.962305
H	4.102869	1.551526	-0.92956
H	4.991131	-0.554055	0.028915
C	-3.049538	0.501698	0.485454
H	-2.915434	0.124833	1.504655
H	-4.12089	0.6321	0.313873

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C	-3.180873	-4.080214	-0.305764
C	-3.176221	-2.790949	0.217747
C	-2.103867	-4.919731	-0.074838
C	-1.012222	-4.469387	0.65787
C	-1.015624	-3.184616	1.168319
N	-2.102808	-2.408588	0.947251
F	1.199044	-2.598988	-0.814434
C	0.146269	-2.027483	-1.433458
C	-0.159107	-0.685978	-1.245537
C	-1.308306	-0.279576	-1.919617
C	-2.108409	-1.107931	-2.689216
C	-1.759523	-2.440344	-2.828267
C	-0.615656	-2.897671	-2.203085

B	0.608806	0.343624	-0.208374
F	-1.747336	0.984631	-1.786092
F	-3.227117	-0.65362	-3.250103
F	-0.287799	-4.191543	-2.297995
C	0.770227	1.857734	-0.819994
C	0.897088	2.941496	0.037511
C	1.090279	4.249409	-0.376169
C	1.192948	4.514983	-1.730792
C	1.098921	3.469097	-2.633109
C	0.900796	2.17873	-2.164335
F	0.814513	2.754674	1.375891
F	0.843804	1.214259	-3.097158
F	1.210625	3.713275	-3.938171
F	1.182251	5.24389	0.505901
H	-0.13726	-5.086485	0.806986
H	-2.093121	-5.914236	-0.503656
H	-2.117981	-1.464734	1.368729
H	-0.149985	0.419838	0.756762
H	-4.00422	-4.384787	-0.935923
C	-4.256824	-1.825296	-0.025407
C	-5.570277	-2.27918	-0.189536
C	-3.973883	-0.463415	-0.150184
C	-6.582065	-1.378292	-0.482872
H	-5.802927	-3.329837	-0.061962
C	-4.986006	0.430415	-0.465546
H	-2.96494	-0.085881	-0.031202
C	-6.288368	-0.025139	-0.631388
H	-7.598988	-1.732256	-0.597608
H	-4.744629	1.478294	-0.587725
H	-7.077445	0.675764	-0.875875
C	0.121038	-2.600178	1.934516
H	0.240629	-1.548528	1.672533
H	-0.05645	-2.681108	3.010439
H	1.040815	-3.12562	1.682676
F	1.386365	5.759885	-2.159008
F	-2.539651	-3.284657	-3.503647
C	6.768297	0.066121	0.270027
C	5.51909	0.372439	-0.248799
C	4.500553	-0.566387	-0.33641
C	4.790508	-1.840641	0.135105
C	6.025998	-2.176897	0.660247
C	7.022399	-1.215858	0.726028
F	3.848926	-2.791053	0.09466
F	6.264704	-3.4099	1.102683

F	8.21281	-1.523608	1.230569	N	-2.346162	-2.272841	0.955894
F	7.720652	0.992075	0.334751	F	1.216886	-2.603131	-0.881385
F	5.312265	1.622631	-0.669274	C	0.155937	-2.003785	-1.456098
C	3.128764	-0.220695	-0.852679	C	-0.098724	-0.651903	-1.267675
H	3.190017	0.720104	-1.402855	C	-1.249871	-0.21215	-1.915205
H	2.817346	-0.992957	-1.560436	C	-2.102469	-1.017671	-2.650147
C	2.099833	-0.108566	0.286368	C	-1.813314	-2.365948	-2.775573
H	2.457267	0.650294	0.994449	C	-0.664839	-2.855302	-2.185397
H	2.105714	-1.056752	0.829914	B	0.705724	0.341803	-0.227211
H	0.114402	-0.077533	3.095007	F	-1.6396	1.072696	-1.789435
C	-0.306004	0.595476	3.855722	F	-3.213191	-0.522593	-3.195215
C	0.833283	1.351863	4.519725	F	-0.378536	-4.157335	-2.28347
H	0.442078	2.02616	5.285186	C	0.89983	1.866148	-0.802207
H	1.53344	0.655947	4.986135	C	1.012782	2.934021	0.075955
H	1.380215	1.942419	3.781513	C	1.220522	4.248401	-0.308737
H	-0.762231	2.27161	2.671994	C	1.349971	4.537336	-1.65615
N	-1.202885	1.537913	3.20984	C	1.265798	3.508336	-2.579273
C	-2.287818	-0.964948	4.176846	C	1.05241	2.210544	-2.138533
H	-3.031364	-1.232999	4.934213	F	0.891843	2.727709	1.413414
H	-1.944268	-1.923836	3.765832	F	0.997604	1.263944	-3.087111
C	-2.938553	-0.105616	3.117729	F	1.39748	3.778232	-3.87699
C	-2.415315	1.090055	2.750384	F	1.296653	5.226827	0.593857
H	-3.935074	-0.355283	2.768859	H	-0.47946	-5.031704	0.648503
C	-3.142687	2.054704	1.879965	H	-2.507866	-5.777961	-0.6
C	-2.51461	2.604888	0.760458	H	-2.455738	-1.207526	1.718045
C	-4.437384	2.460425	2.2049	H	-0.046468	0.421272	0.735349
C	-3.168491	3.552861	-0.018445	H	-4.385427	-4.163231	-0.910822
H	-1.52549	2.262597	0.477835	C	-4.509908	-1.644934	0.044538
C	-5.087154	3.41659	1.431987	C	-5.853978	-2.028974	0.066699
H	-4.918177	2.041216	3.081104	C	-4.175618	-0.326382	-0.259289
C	-4.452312	3.970031	0.323526	C	-6.845393	-1.100046	-0.21637
H	-2.67242	3.959933	-0.892042	H	-6.120145	-3.048891	0.321492
H	-6.085306	3.739525	1.70352	C	-5.167103	0.594315	-0.566644
H	-4.956464	4.721731	-0.272228	H	-3.136255	-0.023628	-0.278184
C	-1.125369	-0.226381	4.853422	C	-6.502273	0.209774	-0.543035
H	-1.524016	0.468845	5.598932	H	-7.886318	-1.398902	-0.188665
H	-0.470017	-0.928104	5.37624	H	-4.884807	1.606669	-0.828224
<hr/>				H	-7.277619	0.928102	-0.781374
TS _{18/19}				C	-0.076164	-2.603554	1.793429
C	-3.522504	-3.909539	-0.309924	H	0.116975	-1.576417	1.484095
C	-3.43799	-2.639705	0.25801	H	-0.199409	-2.636532	2.878701
C	-2.470368	-4.794639	-0.147297	H	0.787393	-3.209529	1.524228
C	-1.343171	-4.387524	0.551585	F	1.555338	5.789028	-2.058752
C	-1.2966	-3.108744	1.090675	F	-2.641055	-3.184364	-3.424946

C	6.749429	-0.013494	0.548081	H	-0.560864	-1.066672	5.336897
C	5.5149	0.317931	0.012744				
C	4.575085	-0.641336	-0.338121				
C	4.923463	-1.96596	-0.111231	19			
C	6.148887	-2.329329	0.422459	C	-3.089414	-4.239011	-0.356488
C	7.067206	-1.346008	0.752627	C	-3.017973	-2.995644	0.278348
F	4.054361	-2.937242	-0.404967	C	-2.039713	-5.128252	-0.192325
F	6.45032	-3.610393	0.62339	C	-0.953622	-4.751485	0.585321
F	8.245641	-1.679909	1.269609	C	-0.952001	-3.489003	1.173879
F	7.627692	0.932839	0.869791	N	-1.97237	-2.634227	1.02762
F	5.234513	1.612827	-0.158354	F	1.50094	-2.659806	-0.69238
C	3.216495	-0.263282	-0.862958	C	0.434786	-2.171618	-1.353058
H	3.299313	0.693283	-1.383777	C	0.047014	-0.84531	-1.213716
H	2.899488	-1.010608	-1.593158	C	-1.101072	-0.525052	-1.929891
C	2.178831	-0.160979	0.268853	C	-1.841781	-1.419489	-2.681437
H	2.550179	0.566392	1.00334	C	-1.40988	-2.730879	-2.777398
H	2.146965	-1.126688	0.783346	C	-0.252022	-3.101807	-2.122217
H	0.222869	-0.308179	3.089469	B	0.698541	0.223802	-0.150883
C	-0.263	0.387577	3.779111	F	-1.608446	0.727017	-1.858584
C	0.802048	1.213989	4.481857	F	-2.973513	-1.044095	-3.27696
H	0.340255	1.928995	5.167356	F	0.169457	-4.36614	-2.200001
H	1.464143	0.562674	5.053949	C	0.777885	1.764591	-0.715001
H	1.405193	1.760745	3.754073	C	0.731417	2.828781	0.171981
H	-0.699266	2.133467	2.63524	C	0.845644	4.16117	-0.185093
N	-1.109212	1.276052	2.9885	C	1.039366	4.475451	-1.519249
C	-2.317098	-1.113213	4.051266	C	1.107168	3.453937	-2.453223
H	-3.133343	-1.244209	4.76575	C	0.982989	2.135305	-2.037447
H	-2.009388	-2.124793	3.771243	F	0.501798	2.592518	1.493185
C	-2.841774	-0.353607	2.828404	F	1.074793	1.1993	-2.991015
C	-2.306738	0.919485	2.557239	F	1.297	3.752555	-3.736947
H	-3.914735	-0.413727	2.65232	F	0.749328	5.130897	0.723875
C	-3.029968	1.950543	1.769944	H	-0.099654	-5.405193	0.708007
C	-2.398968	2.576452	0.694544	H	-2.050654	-6.088752	-0.693325
C	-4.311401	2.345299	2.15467	H	-5.010275	0.846466	2.420149
C	-3.048554	3.595441	0.007724	H	-0.103084	0.218488	0.778652
H	-1.423136	2.234682	0.369633	H	-3.925741	-4.473804	-1.00228
C	-4.943916	3.385232	1.484924	C	-4.105584	-1.998779	0.093725
H	-4.797965	1.855019	2.990136	C	-5.440734	-2.402958	0.027469
C	-4.312984	4.012052	0.413447	C	-3.796762	-0.645044	-0.070046
H	-2.561007	4.060601	-0.840975	C	-6.448616	-1.476809	-0.213378
H	-5.929597	3.70626	1.798995	H	-5.690955	-3.447227	0.177639
H	-4.810643	4.820313	-0.109428	C	-4.801291	0.272649	-0.358852
C	-1.168483	-0.372721	4.751744	H	-2.758122	-0.334338	-0.01399
H	-1.580401	0.36413	5.448822	C	-6.129246	-0.139668	-0.42348
				H	-7.481036	-1.80321	-0.253202

H	-4.547391	1.307405	-0.557086	C	-4.38781	4.559031	0.708368
H	-6.909726	0.577165	-0.649546	H	-4.857692	3.488881	2.50784
C	0.207821	-3.014944	2.004966	C	-3.571115	4.62739	-0.419726
H	0.451222	-1.984426	1.73783	H	-1.959757	3.693756	-1.5166
H	-0.050361	-3.047436	3.068707	H	-5.161047	5.301503	0.861739
H	1.091279	-3.631148	1.841485	H	-3.719445	5.419267	-1.143881
F	1.15312	5.745353	-1.901312	C	-2.461436	-0.545335	4.297312
F	-2.116503	-3.630413	-3.460671	H	-2.423871	0.160966	5.135363
C	6.723636	0.498296	0.788826	H	-2.231898	-1.536976	4.692743
C	5.474926	0.684534	0.216717				
C	4.64295	-0.376136	-0.113541				
C	5.114072	-1.650093	0.173988	20			
C	6.356919	-1.868947	0.745323	F	-0.345995	-2.450722	0.771777
C	7.166388	-0.787129	1.052803	C	-0.735189	-1.828261	-0.359999
F	4.351912	-2.712167	-0.09688	C	-0.550586	-0.456843	-0.489751
F	6.778878	-3.104587	1.003992	C	-0.99961	0.062732	-1.697409
F	8.36024	-0.983131	1.604089	C	-1.620126	-0.699062	-2.680897
F	7.496781	1.53917	1.088615	C	-1.808816	-2.053061	-2.480138
F	5.072525	1.938249	-0.012423	C	-1.356774	-2.62729	-1.304097
C	3.268341	-0.156654	-0.685	B	0.155419	0.367372	0.74851
H	3.270763	0.784448	-1.23938	F	-0.89432	1.369907	-1.967313
H	3.049996	-0.956779	-1.394986	F	-2.086003	-0.130144	-3.792597
C	2.191065	-0.124603	0.413391	F	-1.582487	-3.927743	-1.068022
H	2.4728	0.651748	1.138119	C	-0.160633	1.977624	0.687183
H	2.227596	-1.077794	0.948885	C	-1.166822	2.56319	1.434471
H	-1.364342	-0.971383	2.506574	C	-1.456372	3.919093	1.454452
C	-1.398168	-0.189045	3.272297	C	-0.685034	4.773566	0.689701
C	-0.012918	0.053989	3.848234	C	0.345262	4.249626	-0.076681
H	-0.022822	0.889581	4.55262	C	0.580197	2.884728	-0.062876
H	0.320066	-0.840629	4.37676	F	-1.982685	1.7962	2.219353
H	0.705254	0.265929	3.051221	F	1.570873	2.445486	-0.847599
H	-1.045492	1.482001	2.02463	F	1.085646	5.067027	-0.820803
N	-1.808662	1.023433	2.531007	F	-2.460358	4.395917	2.192601
C	-3.838705	-0.53283	3.639175	H	-3.737761	-3.454643	0.040572
H	-4.61542	-0.837253	4.341523	H	-0.370313	-0.032689	1.772692
H	-3.845468	-1.242974	2.806579	F	-0.931135	6.08063	0.684
C	-4.157788	0.862297	3.102568	F	-2.47769	-2.782839	-3.371992
C	-3.002289	1.481922	2.375963	C	6.192717	0.176611	-0.425426
H	-4.414554	1.547491	3.921704	C	4.830975	0.342295	-0.626873
C	-3.201184	2.59953	1.442537	C	3.90959	-0.642764	-0.299619
C	-2.393515	2.664426	0.304792	C	4.416576	-1.810597	0.254353
C	-4.217177	3.540536	1.634936	C	5.770551	-2.005144	0.469676
C	-2.57911	3.674811	-0.626882	C	6.663683	-1.002892	0.126946
H	-1.669192	1.885593	0.097448	F	3.578169	-2.793953	0.598874
				F	6.218852	-3.139972	1.001935

F	7.967006	-1.172442	0.327264
F	7.050182	1.138124	-0.757592
F	4.413309	1.492968	-1.156572
C	2.428614	-0.438999	-0.471895
H	2.262146	0.293205	-1.262505
H	1.991328	-1.385503	-0.800936
C	1.760995	0.016733	0.83849
H	2.306675	0.888106	1.21804
H	1.912496	-0.779323	1.575183
H	-1.213031	-1.924604	2.891793
C	-2.261785	-1.699925	3.103556
C	-2.348848	-0.690566	4.239042
H	-3.386751	-0.402294	4.421946
H	-1.948497	-1.142504	5.147616
H	-1.76521	0.202693	4.01203
H	-2.39778	-0.105688	1.742542
N	-2.770993	-1.04924	1.870853
C	-3.118194	-3.79416	2.076723
H	-3.604633	-4.755344	2.244824
H	-2.112759	-3.995249	1.697606
C	-3.899235	-3.012218	1.024677
C	-3.514297	-1.561381	0.945377
H	-4.978978	-3.048868	1.211941
C	-3.971669	-0.731407	-0.183981
C	-3.777939	0.657412	-0.190987
C	-4.578171	-1.332163	-1.295803
C	-4.13094	1.412406	-1.29771
H	-3.355931	1.170829	0.662682
C	-4.941298	-0.571728	-2.397423
H	-4.746567	-2.400347	-1.330235
C	-4.703838	0.798197	-2.406893
H	-3.947298	2.47914	-1.294644
H	-5.382757	-1.055718	-3.259013
H	-4.960595	1.385969	-3.279557
C	-3.030293	-2.98329	3.361994
H	-4.034185	-2.742363	3.731234
H	-2.516188	-3.537754	4.148726

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F	0.45057	-2.487443	0.280492
C	-0.417671	-2.110935	-0.680762
C	-0.72276	-0.764797	-0.853606
C	-1.682268	-0.533433	-1.833541
C	-2.308995	-1.538922	-2.556138

C	-1.985584	-2.861447	-2.319349
C	-1.022283	-3.15087	-1.369767
B	-0.110878	0.338735	0.204239
F	-2.133009	0.706022	-2.091235
F	-3.269574	-1.243947	-3.434972
F	-0.729634	-4.421306	-1.081785
C	-0.552488	1.882535	-0.129044
C	-1.191813	2.706921	0.779397
C	-1.497517	4.041438	0.553181
C	-1.14582	4.613066	-0.65438
C	-0.513259	3.833338	-1.61161
C	-0.239943	2.505941	-1.332169
F	-1.608916	2.224784	1.98743
F	0.324895	1.791445	-2.315552
F	-0.192209	4.37021	-2.785988
F	-2.128752	4.766012	1.480176
H	-1.540236	-2.904671	1.473415
H	-0.611901	0.043547	1.272859
F	-1.422933	5.890408	-0.901305
F	-2.625751	-3.838726	-2.959322
C	6.065508	0.659453	0.019488
C	4.750759	0.919253	-0.334615
C	3.819411	-0.091883	-0.524006
C	4.264863	-1.393047	-0.331873
C	5.571392	-1.685117	0.022275
C	6.477064	-0.650866	0.197536
F	3.412035	-2.410066	-0.484235
F	5.963754	-2.944911	0.197807
F	7.734223	-0.915629	0.540025
F	6.932349	1.654574	0.191023
F	4.385968	2.195084	-0.489774
C	2.3802	0.199322	-0.852956
H	2.328948	1.147552	-1.386228
H	2.013382	-0.574253	-1.533122
C	1.510815	0.235808	0.417202
H	1.839981	1.08241	1.03345
H	1.737526	-0.666175	0.994888
H	-0.665716	0.554467	3.454108
C	-1.475508	0.031727	3.975992
C	-2.059376	0.926153	5.056334
H	-2.914788	0.448426	5.539572
H	-1.29863	1.119536	5.813443
H	-2.369922	1.88779	4.641149
H	-3.036175	0.648039	2.694476

N	-2.502226	-0.18327	2.933324	H	-0.450939	-1.869091	2.17027
C	-0.594511	-2.201858	3.302856	H	-0.900185	0.231098	1.197106
H	-0.201505	-3.160052	3.643709	F	-1.336778	5.279905	-2.57127
H	0.180871	-1.720885	2.701413	F	-3.077293	-4.416634	-2.166182
C	-1.816574	-2.445017	2.421246	C	5.737629	0.667026	-0.074545
C	-2.601235	-1.198824	2.139159	C	4.40255	0.809843	-0.414102
H	-2.516646	-3.134074	2.914163	C	3.567819	-0.27945	-0.621867
C	-3.52082	-1.131133	0.996203	C	4.130686	-1.538236	-0.461349
C	-3.837934	0.101938	0.411579	C	5.463273	-1.713737	-0.122656
C	-4.051693	-2.309217	0.459776	C	6.269935	-0.604394	0.069955
C	-4.705714	0.154291	-0.66729	F	3.378039	-2.626629	-0.631831
H	-3.342322	1.011338	0.737395	F	5.971794	-2.93421	0.019963
C	-4.92644	-2.248685	-0.615553	F	7.54851	-0.757815	0.396585
H	-3.791564	-3.271549	0.883914	F	6.509359	1.733575	0.113268
C	-5.258209	-1.018634	-1.174446	F	3.913621	2.047264	-0.539704
H	-4.914424	1.104918	-1.140254	C	2.111421	-0.096969	-0.953197
H	-5.331518	-3.16304	-1.031025	H	2.011675	0.771033	-1.607202
H	-5.918831	-0.976882	-2.031358	H	1.763856	-0.968719	-1.511988
C	-0.971373	-1.310162	4.481305	C	1.262696	0.088989	0.31923
H	-1.746212	-1.784747	5.094681	H	1.598769	1.004939	0.822714
H	-0.108855	-1.129094	5.125265	H	1.49182	-0.744208	0.987287

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F	0.503552	-2.646895	0.233944	H	-0.136258	1.98501	3.212528
C	-0.602129	-2.391154	-0.490513	C	-0.797133	1.528252	3.96007
C	-1.038377	-1.083606	-0.68641	C	-1.371842	2.607967	4.859998
C	-2.203894	-0.988138	-1.446493	H	-2.06326	2.176117	5.587451
C	-2.888587	-2.079553	-1.953436	H	-0.56625	3.10717	5.399687
C	-2.415077	-3.356921	-1.713646	H	-1.899388	3.364055	4.27308
C	-1.256262	-3.513792	-0.976732	H	-2.667958	1.503312	2.97686
B	-0.330387	0.199577	0.026491	N	-1.899349	0.89222	3.223861
F	-2.758199	0.203253	-1.715691	C	0.431439	-0.616878	3.717994
F	-4.022352	-1.912512	-2.632602	H	0.992996	-1.405569	4.221387
F	-0.788781	-4.734974	-0.725569	H	1.099377	-0.161205	2.983794
C	-0.678885	1.62519	-0.680557	C	-0.765613	-1.238448	3.001864
C	-1.104832	2.75478	-0.006633	C	-1.768115	-0.219211	2.509892
C	-1.334776	3.982853	-0.6082	H	-1.321131	-1.871287	3.706526
C	-1.125072	4.115153	-1.967978	C	-2.971783	-0.672078	1.758853
C	-0.701879	3.014262	-2.696455	C	-3.7697	0.260548	1.091744
C	-0.49415	1.81014	-2.046642	C	-3.296402	-2.027571	1.689477
F	-1.356362	2.702329	1.324855	C	-4.891372	-0.153935	0.388782
F	-0.124167	0.772334	-2.811048	H	-3.475018	1.305313	1.058441
F	-0.511524	3.126629	-4.007591	C	-4.421195	-2.438814	0.984486
F	-1.759872	5.022915	0.10909	H	-2.677788	-2.769096	2.178845
				C	-5.221414	-1.504506	0.336595
				H	-5.484773	0.572855	-0.151018

H	-4.662227	-3.493733	0.928917
H	-6.085191	-1.828856	-0.230601
C	-0.024273	0.451138	4.706814
H	-0.667892	0.018064	5.480725
H	0.833084	0.910062	5.203707

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F	0.405534	-0.963527	-2.259482
C	-0.691832	-1.60022	-1.844554
C	-1.609201	-0.951532	-1.015992
C	-2.754307	-1.687647	-0.706405
C	-2.949105	-2.990051	-1.129927
C	-1.993569	-3.597928	-1.925391
C	-0.856567	-2.896614	-2.295324
B	-1.301422	0.436392	-0.35482
F	-3.706985	-1.174143	0.070565
F	-4.01845	-3.674166	-0.7397
F	0.056433	-3.471491	-3.068203
C	-2.489267	1.362039	0.114839
C	-2.486218	2.039583	1.330491
C	-3.51858	2.872855	1.727817
C	-4.593438	3.07172	0.876193
C	-4.635	2.424356	-0.349182
C	-3.596408	1.581337	-0.700557
F	-1.486123	1.866936	2.203618
F	-3.682234	0.968544	-1.883116
F	-5.665553	2.615084	-1.162546
F	-3.489681	3.476292	2.909385
H	1.877954	-1.605181	-0.657634
H	2.188293	-0.833527	1.685745
F	-5.581411	3.875124	1.234329
F	-2.160456	-4.848507	-2.321829
C	3.690783	3.887714	-0.366113
C	2.371179	3.531512	-0.59879
C	2.02628	2.322428	-1.184014
C	3.067543	1.467048	-1.521193
C	4.393904	1.790591	-1.293449
C	4.705592	3.011033	-0.714045
F	2.792615	0.283194	-2.072517
F	5.363126	0.941745	-1.616934
F	5.971405	3.337451	-0.492106
F	3.987861	5.055101	0.192471
F	1.413422	4.386629	-0.232847
C	0.592067	1.903388	-1.371589

H	-0.041188	2.79161	-1.397694
H	0.497575	1.38835	-2.328664
C	0.173154	0.97083	-0.206758
H	0.267003	1.544855	0.71842
H	0.886932	0.147208	-0.158145
H	4.364638	-1.428203	2.620257
C	4.167436	-2.490602	2.384488
C	4.854529	-3.362485	3.42415
H	4.66105	-4.415566	3.208129
H	5.933138	-3.192918	3.419256
H	4.482339	-3.145297	4.428948
H	2.372337	-2.645264	3.34854
N	2.727721	-2.764087	2.404163
C	3.929651	-1.950707	-0.066807
H	4.272802	-2.187853	-1.076313
H	4.12228	-0.880882	0.085219
C	2.428736	-2.209475	0.063203
C	1.971173	-1.901977	1.492743
H	2.215855	-3.261371	-0.1546
C	0.491038	-2.115117	1.722581
C	-0.30201	-1.095691	2.252539
C	-0.097861	-3.354133	1.464034
C	-1.655891	-1.300963	2.510847
H	0.147653	-0.134958	2.48126
C	-1.448299	-3.56409	1.725744
H	0.517751	-4.163897	1.088945
C	-2.230971	-2.540182	2.251964
H	-2.251955	-0.496987	2.926927
H	-1.892924	-4.532871	1.524387
H	-3.283524	-2.705442	2.448978
C	4.699738	-2.758942	0.977232
H	4.586858	-3.82917	0.769925
H	5.766976	-2.52283	0.940651

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H	-0.144965	2.38873	0.507779
H	-0.40016	0.873287	-1.403164
H	-2.660791	-0.108958	-1.514511
C	-2.515507	-0.536667	-0.504875
C	-3.260668	-1.859816	-0.418695
H	-3.129585	-2.294056	0.575109
H	-4.327302	-1.716592	-0.603675
H	-2.882179	-2.573191	-1.155846
H	-0.744907	-1.490695	-0.861673

N	-1.09479	-0.767081	-0.239759
C	-2.232235	1.774517	0.450757
H	-2.574399	2.476215	1.215402
H	-2.393448	2.257351	-0.520769
C	-0.742414	1.480462	0.623789
C	-0.275469	0.433948	-0.396408
H	-0.550742	1.081359	1.625618
C	1.188564	0.108086	-0.20527
C	2.161514	0.778339	-0.94496
C	1.590525	-0.831296	0.745093
C	3.51248	0.52069	-0.740051
H	1.855759	1.505213	-1.691267
C	2.940651	-1.09283	0.948531
H	0.830032	-1.356186	1.31152
C	3.905395	-0.417338	0.207966
H	4.257805	1.047252	-1.324559
H	3.241697	-1.826437	1.687486
H	4.957281	-0.623268	0.366776
C	-3.041381	0.478734	0.508035
H	-2.95925	0.035014	1.506759
H	-4.100036	0.67355	0.313852

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H	0.377782	0.521956	1.521347
H	1.089389	0.057909	1.636224
C	-5.704742	-1.792348	0.668177
C	-4.415978	-1.505356	0.252593
C	-4.037687	-0.238415	-0.170649
C	-5.011781	0.748842	-0.15172
C	-6.311391	0.491619	0.256873
C	-6.657224	-0.785144	0.668185
F	-4.706527	1.988995	-0.536233
F	-7.225129	1.456749	0.258863
F	-7.897681	-1.043634	1.064401
F	-6.035146	-3.016764	1.066194
F	-3.510296	-2.487843	0.265682
C	-2.617564	0.04473	-0.576382
H	-2.24565	-0.807991	-1.149904
H	-2.604798	0.918244	-1.22899
C	-1.715771	0.274075	0.655253
H	-1.784608	-0.612902	1.290983
H	-2.107529	1.116383	1.229826
B	-0.188377	0.493579	0.209701
C	0.288248	1.958524	-0.268511

C	-0.560491	3.043547	-0.457178
C	1.633125	2.226837	-0.505126
C	-0.115534	4.297619	-0.857785
C	2.118861	3.455639	-0.906534
C	1.232679	4.507173	-1.079956
C	0.423167	-0.776775	-0.571513
C	0.903663	-0.735189	-1.87568
C	0.414698	-2.03886	0.013062
C	1.367413	-1.854887	-2.546914
C	0.86061	-3.18377	-0.624774
C	1.342376	-3.086467	-1.917741
F	1.675805	5.698668	-1.456048
F	1.813032	-4.160712	-2.539132
F	0.84717	-4.360894	-0.006805
F	-0.014475	-2.19272	1.276761
F	0.943277	0.419807	-2.552338
F	1.864516	-1.756713	-3.777764
F	2.541257	1.250726	-0.335525
F	3.421983	3.64201	-1.117061
F	-0.974697	5.296974	-1.024571
F	-1.879651	2.933381	-0.27135
H	4.721584	1.380113	3.622272
C	4.141673	1.583016	2.71203
C	4.75173	2.771083	1.983848
H	4.202839	2.9729	1.062126
H	4.72135	3.65991	2.61629
H	5.796635	2.579599	1.725784
H	5.0193	0.297621	1.258966
N	4.208977	0.404741	1.849007
C	2.051935	0.564849	3.693195
H	0.991201	0.743957	3.893864
H	2.512741	0.316432	4.655447
C	2.210383	-0.566564	2.705047
C	3.320591	-0.61049	1.896562
H	1.625938	-1.470984	2.811623
C	3.606772	-1.760182	0.999069
C	4.050971	-1.545573	-0.309302
C	3.46361	-3.067708	1.466957
C	4.359526	-2.624713	-1.128816
H	4.116468	-0.534457	-0.696137
C	3.776556	-4.143407	0.644684
H	3.125237	-3.238527	2.481975
C	4.23063	-3.925593	-0.651465
H	4.682162	-2.44953	-2.14886

H	3.661765	-5.153636	1.01747
H	4.466602	-4.765273	-1.293323
C	2.690161	1.831913	3.116928
H	2.129691	2.156554	2.231898
H	2.662712	2.650206	3.839409

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H	0.225881	0.524652	1.858491
H	1.841192	-0.604992	1.841069
C	-5.900617	-1.766541	0.481715
C	-4.572107	-1.494942	0.20015
C	-4.126584	-0.222168	-0.130617
C	-5.080149	0.785642	-0.154938
C	-6.417208	0.545345	0.121846
C	-6.828204	-0.738005	0.441653
F	-4.717272	2.034412	-0.452478
F	-7.307352	1.534232	0.084408
F	-8.107718	-0.982609	0.709322
F	-6.294138	-3.000934	0.788027
F	-3.698381	-2.505909	0.252607
C	-2.667796	0.052359	-0.374682
H	-2.240245	-0.809415	-0.893731
H	-2.578403	0.915709	-1.035758
C	-1.904867	0.296804	0.940031
H	-2.051442	-0.580609	1.580834
H	-2.365062	1.140248	1.462909
B	-0.301809	0.520978	0.752641
C	0.151142	1.940054	0.050871
C	-0.675254	3.006936	-0.280342
C	1.488656	2.178937	-0.22419
C	-0.220568	4.186197	-0.863177
C	1.992944	3.319165	-0.8161
C	1.124473	4.348139	-1.137458
C	0.283694	-0.78746	-0.068032
C	0.705827	-0.824448	-1.390917
C	0.314502	-2.02318	0.573034
C	1.139436	-1.97873	-2.030156
C	0.741284	-3.1991	-0.020865
C	1.145957	-3.177733	-1.34394
F	1.578309	5.46648	-1.697697
F	1.585775	-4.291802	-1.931634
F	0.826671	-4.335743	0.675741
F	-0.021542	-2.110937	1.873756
F	0.735727	0.292416	-2.136488

F	1.585658	-1.940239	-3.2885
F	2.415275	1.224729	0.075086
F	3.306158	3.438491	-1.069885
F	-1.072059	5.164412	-1.1622
F	-1.995632	2.956606	-0.06355
H	5.268727	1.298456	3.319515
C	4.47698	1.485117	2.585779
C	4.719057	2.818024	1.894061
H	3.968682	2.987991	1.122148
H	4.651867	3.620056	2.630179
H	5.711389	2.863205	1.438144
H	5.32103	0.539847	0.868818
N	4.602384	0.403988	1.575301
C	2.811321	-0.040827	3.667756
H	1.849039	-0.099076	4.176822
H	3.57622	-0.419435	4.353267
C	2.742156	-0.888191	2.405167
C	3.842536	-0.63625	1.444456
H	2.645734	-1.959789	2.592213
C	4.045847	-1.506017	0.276004
C	4.265968	-0.933897	-0.983637
C	4.010355	-2.896819	0.418146
C	4.459292	-1.752826	-2.086569
H	4.204429	0.14193	-1.108312
C	4.232295	-3.706488	-0.686263
H	3.829018	-3.347718	1.386643
C	4.450443	-3.136136	-1.936636
H	4.583763	-1.311715	-3.067238
H	4.202251	-4.782972	-0.576555
H	4.583361	-3.773161	-2.802165
C	3.118491	1.399148	3.26724
H	2.342128	1.758004	2.582422
H	3.131679	2.060874	4.134987