

Electronic Supplementary Information

Catalyzed or Non-Catalyzed: Chemoselectivity of Ru-Catalyzed Acceptorless Dehydrogenative Coupling of Alcohol and Amine via Metal-Ligand Bond Cooperation and (De)aromatization

Siwei Shu,^{a,‡} Meijie Huang,^{a,‡} Jingxing Jiang,^b Ling-Bo Qu,^c Yan Liu^{*a} and Zhuofeng Ke^{*b}

^aSchool of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, P. R. China

^bSchool of Materials Science and Engineering, PCFM Lab, Sun Yat-sen University, Guangzhou 510275, P. R. China.

^cCollege of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, P. R. China.

*Correspondence Author: yanliu@gdut.edu.cn; kezhf3@mail.sysu.edu.cn

Contents

1. Free energies of dehydrogenation of amine.	2
2. Free energies of amine and alcohol coupling (Route g) or alcohol and alcohol coupling without 1Cat.....	3
3. The elimination of H ₂ O from 20 to regenerate 1cat.....	3
4. The dehydrogenation or dehydration of hemiaminal by PNN-Ru or PNP-Ru catalysts via (de)aromatization mechanism.	4
5. Cartesian coordinates of all structures.	5

1. Free energies of dehydrogenation of amine.

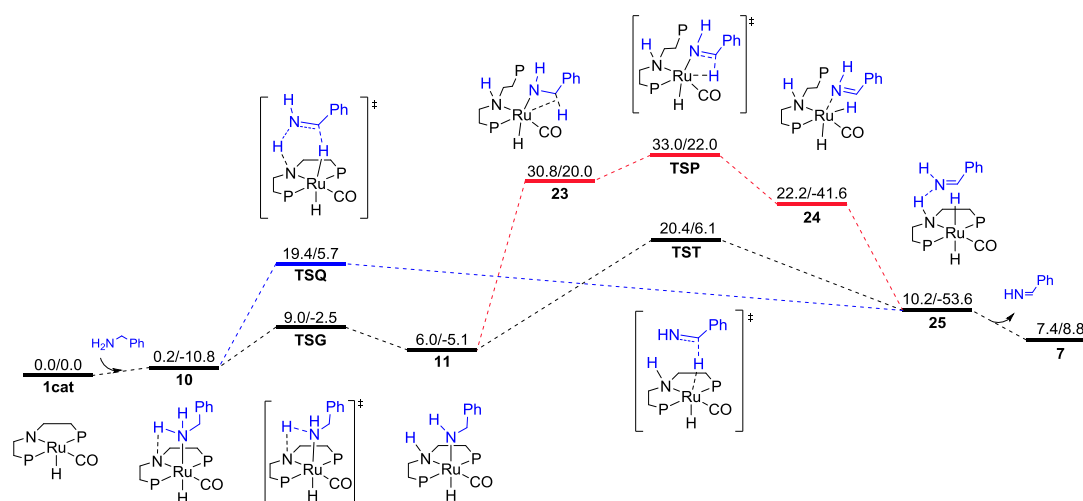


Fig. S1. Free energy profiles for the Macho-Ru catalyzed dehydrogenation of amine. Free energy/enthalpy values are in kcal/mol.

Because alcohol and amine co-exist in the reaction system, **1cat** can dehydrogenate either alcohol to aldehyde or amine to imine (**pimi**), which can further influence the subsequent coupling reaction. To figure out why aldehyde is preferred over **pimi** during the first dehydrogenation process, we have taken both of them into consideration. Similar to the mechanism of dehydrogenation of alcohol (Fig. 1), possible pathways for the dehydrogenation of amine are shown in Fig. S1. As can be seen, the dissociation of the phosphine arm raises the free energy of the system. The energy barrier of **TSP**, the β -H elimination pathway is 33.0 kcal/mol. And the energy of outer sphere β -H elimination **TST** is 20.4 kcal/mol. Unexpectedly, the bifunctional outer sphere **TSQ** of M-L bond cooperation pathway is just 19.4 kcal/mol. We can see the preferred pathway for dehydrogenation of amine (**TSQ**, 19.4 kcal/mol), cannot compete with the preferred pathway for dehydrogenation of alcohol (**TSD**, 5.1 kcal/mol). The chemoselectivity between dehydrogenation of alcohol and amine should be attributed to the less stable C=N bond of the imine as compared with the formed C=O bond in aldehyde, which facilitates the synergetic the hydride transfer to the metal center. This is in accordance with the experiment fact that alcohol dehydrogenations were observed in Macho-Ru system.

2. Free energies of amine and alcohol coupling (Route g) or alcohol and alcohol coupling without 1Cat.

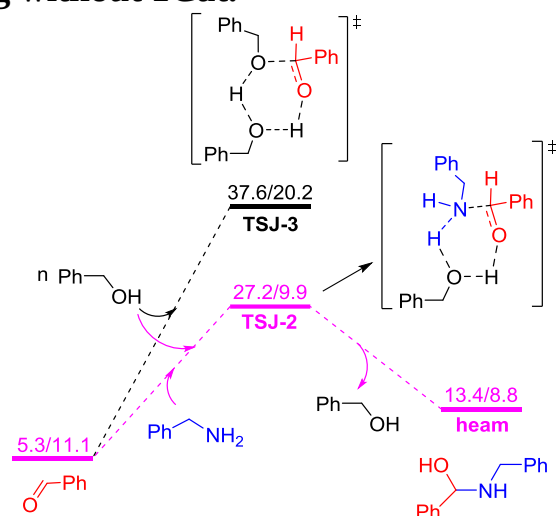


Fig. S2. Free energy profiles for amine and alcohol coupling (**Route g**) or alcohol and alcohol coupling without **1Cat**. Free energy/enthalpy values are in kcal/mol.

3. The elimination of H₂O from 20 to regenerate 1cat.

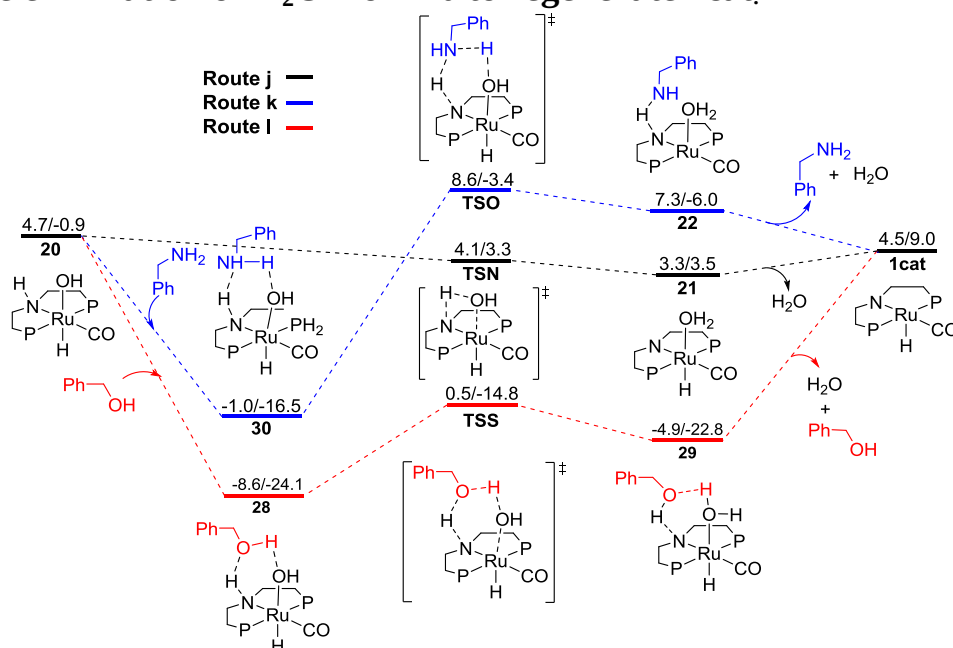


Fig. S3. Free Energy profiles of possible reaction pathways for the elimination of H₂O from **20**.

There are three possible pathways for the elimination of water, showing in the Fig. S3. Under the assistance of amine and alcohol respectively, we obtained the transition states **TSO** and **TSS**, along with the free energy of 8.6 kcal/mol and -3.0 kcal/mol. Meanwhile, by crossing the transition state **TSN** (4.1 kcal/mol), the direct elimination of water will also finally regenerate **1cat**. In comparison, the preferred pathway of dehydration is under the assistance of alcohol (**TSS**), among the three pathways of water elimination.

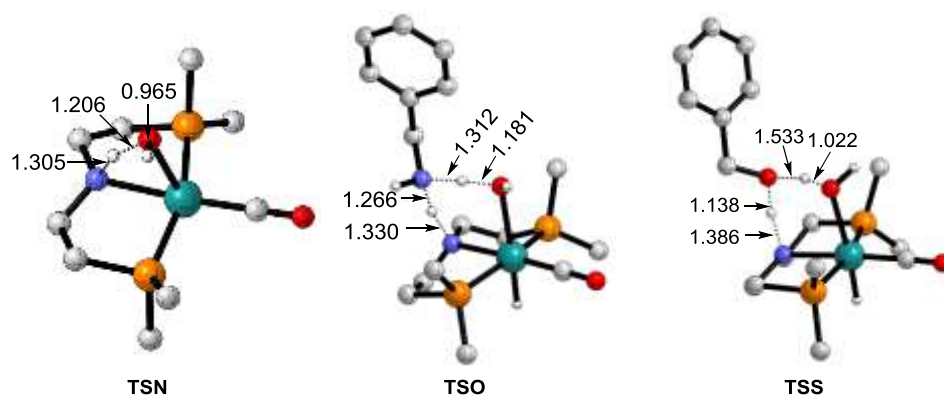
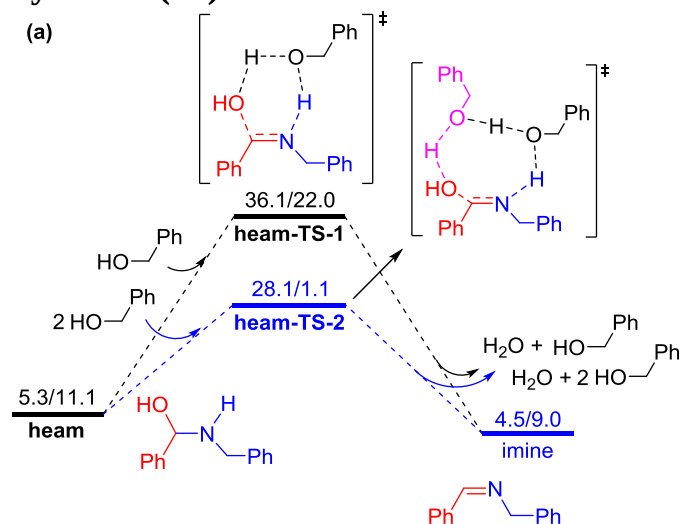


Fig. S4. Optimized transition state structures for elimination of water from complex **20**, along with the key bond lengths (in Å). Trivial hydrogen atoms are omitted for clarity.

4. The dehydrogenation or dehydration of hemiaminal by PNN-Ru or PNP-Ru catalysts via (de)aromatization mechanism.



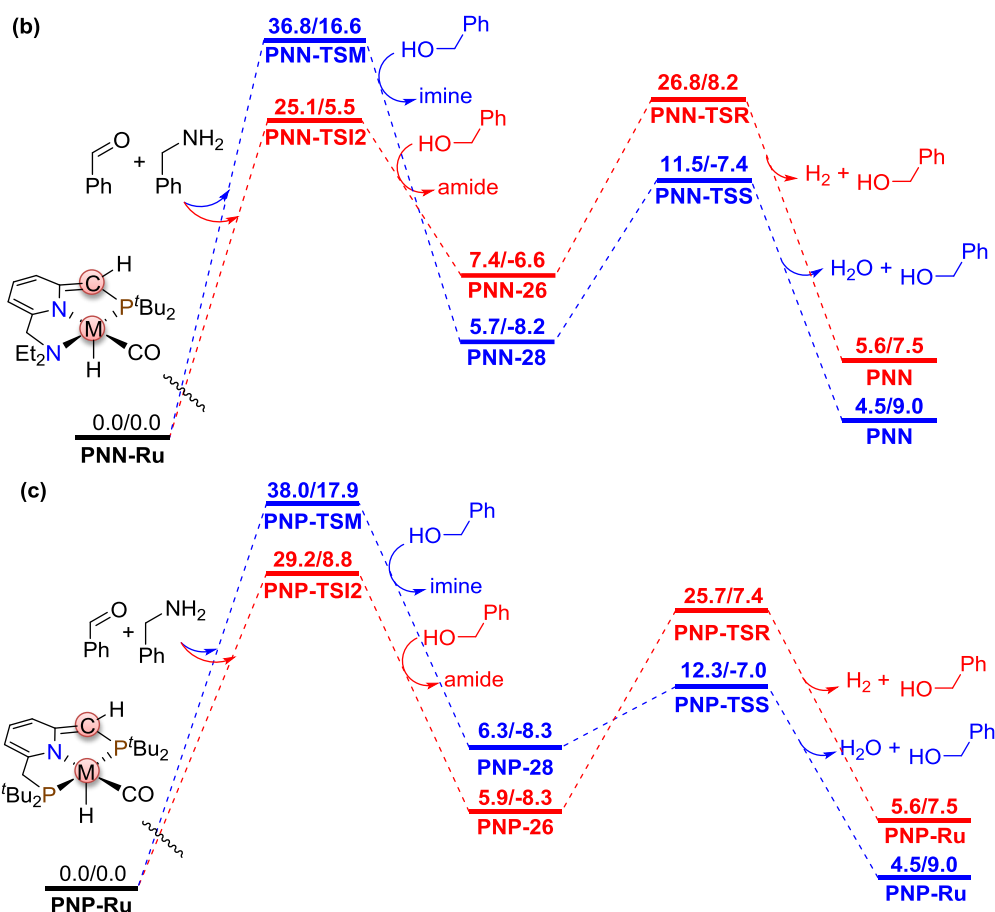


Fig. S5. The dehydrogenation or dehydration of hemiaminal **heam** via (a) non-catalyzed, (b) PNN-Ru catalyzed, and (c) PNP-Ru catalyzed reactions.

5. Cartesian coordinates of all structures.

alcohol

C	0.5083130	1.2978990	-0.0221220
C	-0.4371260	0.2680740	0.0565920
C	0.0030830	-1.0589290	0.0840640
C	1.3681710	-1.3492150	0.0343240
C	2.3068290	-0.3185500	-0.0367960
C	1.8722100	1.0088790	-0.0641060
H	0.1747460	2.3331510	-0.0541220
H	-0.7314130	-1.8549110	0.1336380
H	1.6983140	-2.3843700	0.0507090
H	3.3683010	-0.5463540	-0.0754870
H	2.5943740	1.8182560	-0.1264510
C	-1.9086840	0.6054030	0.1540890
H	-2.1365430	0.9036280	1.1923810
H	-2.1222300	1.4819130	-0.4801760
O	-2.6891210	-0.5176220	-0.2330040
H	-3.6093610	-0.3316990	-0.0127360

amine

C	0.4956440	1.2918830	-0.0209880
C	-0.4300620	0.2535560	0.1362300
C	0.0371260	-1.0669680	0.1718720
C	1.4009030	-1.3392230	0.0578640
C	2.3184290	-0.2962280	-0.0909000
C	1.8612630	1.0222090	-0.1295060
H	0.1441420	2.3206840	-0.0610490
H	-0.6833690	-1.8713420	0.2795920
H	1.7487540	-2.3684560	0.0853890
H	3.3799270	-0.5095150	-0.1806040
H	2.5655740	1.8405160	-0.2522100
C	-1.9081210	0.5583120	0.2959140
H	-2.1524340	0.5823660	1.3673480
H	-2.1000350	1.5780480	-0.0822510
N	-2.7454150	-0.4793450	-0.3151390
H	-3.7277480	-0.2775400	-0.1500200
H	-2.6079950	-0.4805940	-1.3231340

1cat

Ru	0.0028820	0.4163940	0.0648000
H	0.0050980	0.8578410	1.5862460
N	-0.0029210	-1.5978110	-0.3001320
P	2.2983790	0.0526030	0.1068540
P	-2.3008410	0.0629730	0.1049120
C	3.2432320	0.2300450	-1.4711120
H	3.2807620	1.2853430	-1.7548800
H	4.2638570	-0.1560030	-1.3780120
H	2.7171740	-0.3162890	-2.2583160
C	-3.5617330	1.1433470	-0.6966640
H	-4.5565700	0.6864630	-0.6747410
H	-3.5957070	2.1039310	-0.1753220
H	-3.2678860	1.3276640	-1.7330920
C	2.3573750	-1.7628820	0.4699670
H	3.3236040	-2.2099250	0.2069220
H	2.2256890	-1.8464740	1.5546230
C	1.1850810	-2.4534260	-0.2440900
H	1.4949350	-2.7528400	-1.2618820
H	0.9638210	-3.3947920	0.2880770
C	-1.2140980	-2.4067200	-0.4223270
H	-1.4262370	-2.9451120	0.5222760
H	-1.0799450	-3.1908610	-1.1870230
C	-2.4274250	-1.5492200	-0.8016160
H	-2.3809890	-1.2958950	-1.8668190
H	-3.3745860	-2.0668090	-0.6082440
C	3.4427600	0.8078470	1.3371090
H	4.4391000	0.3558300	1.2926450
H	3.5245720	1.8799980	1.1383490
H	3.0224280	0.6772430	2.3370510
C	-3.0596630	-0.2889440	1.7490230
H	-3.0357310	0.6178670	2.3585690
H	-4.0924780	-0.6395080	1.6516540
H	-2.4579300	-1.0511160	2.2502160
C	0.0110690	2.2692840	-0.2634970
O	0.0097490	3.4083920	-0.5194770

2

Ru	-0.6007040	-0.5939510	0.3718220
H	-1.5956180	-1.7867170	0.1564670
N	-0.7454850	0.0422520	-1.6858390
P	0.9741590	-2.0853420	-0.5099260
P	-2.5548400	0.7073400	0.4735940
C	2.7792090	-1.7142330	-0.4940620
H	3.1532270	-1.7788040	0.5299310
H	3.3350200	-2.4087990	-1.1326010
H	2.9372130	-0.6889330	-0.8343820
C	-2.5722690	2.4021930	1.1982160
H	-3.5384690	2.8936350	1.0431960
H	-2.3619010	2.3486580	2.2701760
H	-1.7838480	2.9713790	0.6982440
C	0.5288190	-2.0248210	-2.3093610
H	1.3214770	-2.4389660	-2.9457690
H	-0.3768390	-2.6275610	-2.4399360
C	0.2243090	-0.5439880	-2.6149040
H	1.1680430	0.0187640	-2.5448230
H	-0.1152850	-0.4434100	-3.6567480
C	-2.1232650	0.0416360	-2.1891510
H	-2.5798280	-0.9636170	-2.1938230
H	-2.1524470	0.4035810	-3.2305550
C	-2.9708690	0.9890940	-1.3221900
H	-2.7009710	2.0254030	-1.5459550
H	-4.0441530	0.8638990	-1.4996290
C	0.9268070	-3.8677030	-0.0496750
H	1.5730190	-4.4669660	-0.6990120
H	1.2550350	-3.9802470	0.9874090
H	-0.1029310	-4.2250800	-0.1237510
C	-4.0535740	-0.0816920	1.2000590
H	-3.8917220	-0.2496890	2.2683350
H	-4.9425800	0.5416590	1.0610100
H	-4.2055630	-1.0520380	0.7212890
C	-0.4691110	-1.0874930	2.1872460
O	-0.3852190	-1.4140980	3.3036800
O	-0.2255940	2.6184260	-1.1811910
H	-0.3919110	1.6411160	-1.4170080
C	1.1498380	2.8568870	-1.3036850
H	1.3144570	3.9389980	-1.1939200
H	1.5270940	2.5943750	-2.3086730
C	2.0073850	2.1416830	-0.2668630
C	1.4360540	1.5787670	0.8804190
C	3.3993570	2.0833650	-0.4194390
C	2.2365280	0.9797170	1.8595730
H	0.3585700	1.6568890	1.0210320
C	4.2013700	1.4912960	0.5572490
H	3.8580710	2.5117210	-1.3084650
C	3.6218640	0.9382700	1.7033440
H	1.7697480	0.5441630	2.7374780
H	5.2791930	1.4565560	0.4225760
H	4.2452850	0.4756610	2.4630520

3

Ru	1.1513750	-0.4769580	-0.2133840
----	-----------	------------	------------

H	2.2455330	-1.3641460	0.5945380
N	0.2594850	0.4674050	1.6115450
P	-0.2623330	-2.2211220	0.4158590
P	2.5640330	1.3803870	-0.0916310
C	-2.0150490	-2.3938390	-0.1370610
H	-2.0336940	-2.6151280	-1.2078580
H	-2.5300120	-3.1937900	0.4054440
H	-2.5412050	-1.4492490	0.0125350
C	2.4602540	2.6265420	-1.4362830
H	2.8860010	3.5934960	-1.1499540
H	2.9770840	2.2486010	-2.3226280
H	1.3928460	2.7143520	-1.6577130
C	-0.4222670	-1.8604570	2.2377010
H	-1.2160710	-2.4538590	2.7078410
H	0.5352090	-2.1427980	2.6875850
C	-0.6697170	-0.3589150	2.4301600
H	-1.6927990	-0.1068010	2.1284200
H	-0.5722670	-0.0916560	3.4891150
C	1.1915760	1.3328120	2.3601030
H	1.9274910	0.6961640	2.8637330
H	0.6580780	1.9049600	3.1345830
C	1.8759170	2.2995810	1.3858400
H	1.1288390	2.9920630	0.9828520
H	2.6471220	2.8891370	1.8922570
C	0.3391780	-3.9600450	0.3617850
H	-0.3175150	-4.6340720	0.9210930
H	0.3836040	-4.2878790	-0.6806080
H	1.3499370	-3.9925630	0.7737130
C	4.3613370	1.2120890	0.2699850
H	4.8471260	0.7074050	-0.5695530
H	4.8377990	2.1840240	0.4343870
H	4.4843580	0.5850030	1.1565880
C	1.7990090	-1.1925720	-1.8010430
O	2.2003660	-1.6443270	-2.7977210
O	-0.3023990	1.1028090	-0.8737740
H	-0.2922850	1.0322100	0.9374900
C	-1.3818980	0.8597970	-1.7066450
H	-1.3543130	-0.1471540	-2.1632820
H	-1.3879050	1.5628500	-2.5675940
C	-2.7370820	1.0021460	-1.0138560
C	-3.8789420	0.3668000	-1.5214580
C	-2.8714000	1.7787970	0.1429070
C	-5.1147020	0.4880190	-0.8839960
H	-3.7915650	-0.2424660	-2.4192030
C	-4.1045520	1.9025320	0.7880810
H	-1.9939290	2.2943010	0.5206460
C	-5.2317290	1.2537080	0.2794140
H	-5.9850140	-0.0221260	-1.2889470
H	-4.1872460	2.5106220	1.6857410
H	-6.1909300	1.3440300	0.7816250

4

Ru	1.4021700	-0.1459550	0.6775260
H	1.2525070	1.3379610	1.3117790
N	-0.0353090	0.3364260	-1.0327270

P	-3.2073770	2.3048520	0.8065120
P	2.9388490	0.5946070	-0.7560960
C	-4.3198280	2.3287160	-0.6927500
H	-5.3179270	2.6665600	-0.3973010
H	-3.9440120	2.9916890	-1.4814220
H	-4.4179960	1.3162100	-1.0954410
C	4.3698970	-0.5040160	-1.1056990
H	4.9519010	-0.1535760	-1.9638970
H	5.0124370	-0.5414210	-0.2218790
H	3.9858870	-1.5097310	-1.2928860
C	-1.5481080	2.0926840	-0.0394900
H	-1.3910700	2.9104150	-0.7551240
H	-0.7756560	2.1677100	0.7343760
C	-1.4324440	0.7281760	-0.7177570
H	-1.8300740	-0.0502050	-0.0642910
H	-2.0323740	0.7078980	-1.6398640
C	0.5846430	1.1655010	-2.0898950
H	0.5968290	2.2023960	-1.7414960
H	-0.0178290	1.1345860	-3.0103450
C	2.0131490	0.6894130	-2.3669950
H	1.9982750	-0.3272820	-2.7761370
H	2.5165920	1.3414160	-3.0888870
C	-3.1100120	4.1378090	1.1321740
H	-2.8702470	4.7101140	0.2283730
H	-4.0665350	4.4911110	1.5290150
H	-2.3412840	4.3316300	1.8863760
C	3.6967930	2.2567380	-0.5439880
H	4.2463690	2.2734210	0.4006460
H	4.3744500	2.5010320	-1.3684120
H	2.8989970	3.0004470	-0.4816850
C	2.6463930	-0.4773730	2.0145240
O	3.4565460	-0.6440610	2.8337340
O	0.9650110	-2.1382150	-0.1810280
H	-0.0418840	-0.6438260	-1.3385520
C	0.0234060	-2.2960470	0.7868990
H	-0.0940680	-1.3303860	1.4649420
H	0.2848880	-3.0526700	1.5530300
C	-1.3998060	-2.5269020	0.2854920
C	-2.5007300	-2.3800250	1.1387490
C	-1.6173450	-2.8475380	-1.0576680
C	-3.7994320	-2.5281260	0.6523340
H	-2.3389460	-2.1206400	2.1831340
C	-2.9175090	-2.9996380	-1.5469890
H	-0.7514900	-2.9681760	-1.7010590
C	-4.0117140	-2.8340730	-0.6960410
H	-4.6456340	-2.3944230	1.3204100
H	-3.0759190	-3.2470120	-2.5935490
H	-5.0231570	-2.9436960	-1.0772030
5			
Ru	1.2275010	-0.0058800	0.7596090
H	0.8636510	1.4443220	1.3183350
N	-0.1836590	0.3517600	-1.0023690
P	-3.8000450	1.6836880	0.6416460
P	2.7904100	0.9990760	-0.7712690

C	-4.6165470	2.1100530	-0.9832900
H	-5.6725950	2.3394810	-0.8106460
H	-4.1454440	2.9717630	-1.4715300
H	-4.5708830	1.2516500	-1.6600530
C	4.2884060	0.0749380	-1.3086300
H	4.7438020	0.5023810	-2.2078790
H	5.0206110	0.0824530	-0.4963480
H	3.9901740	-0.9607760	-1.4882780
C	-2.0047490	1.7097650	0.1053570
H	-1.8058250	2.6386670	-0.4449440
H	-1.3916300	1.7160690	1.0116040
C	-1.6410540	0.4788850	-0.7195870
H	-1.9305610	-0.4235970	-0.1809350
H	-2.1883850	0.4864950	-1.6749940
C	0.3102470	1.3919000	-1.9398640
H	0.2242180	2.3605910	-1.4395750
H	-0.3240920	1.4279560	-2.8390070
C	1.7675340	1.1231380	-2.3233440
H	1.8475160	0.1563850	-2.8347330
H	2.1411930	1.8955170	-3.0045850
C	-3.8542060	3.3663040	1.4419950
H	-3.4642560	4.1526000	0.7850490
H	-4.8861340	3.6118920	1.7104570
H	-3.2614650	3.3495320	2.3613890
C	3.4025690	2.7187450	-0.5192790
H	4.0315430	2.7456050	0.3746110
H	3.9774360	3.0790690	-1.3786880
H	2.5478950	3.3777910	-0.3457220
C	2.3220220	-0.1986060	2.2462990
O	2.9933460	-0.2922360	3.1908160
O	1.7329890	-1.9108510	-0.3338700
H	-0.0660920	-0.5489170	-1.4686960
C	0.8483960	-2.2529440	0.5285840
H	-0.0493360	-0.2281040	1.7380290
H	1.1666560	-2.6501450	1.5031640
C	-0.5271890	-2.6368070	0.1028250
C	-1.5591450	-2.7759240	1.0423270
C	-0.8007430	-2.8695150	-1.2528270
C	-2.8485970	-3.0998940	0.6287270
H	-1.3490550	-2.5796720	2.0900040
C	-2.0944150	-3.1924460	-1.6676300
H	0.0170810	-2.8062460	-1.9651640
C	-3.1228340	-3.3006240	-0.7297090
H	-3.6463570	-3.1812650	1.3611030
H	-2.2972250	-3.3682000	-2.7206400
H	-4.1311940	-3.5454480	-1.0504630

6

Ru	0.9588200	0.5824100	-0.3406420
H	2.0492990	1.6324200	0.4166300
N	0.6289000	-0.3816540	1.6916030
P	2.7547730	-0.8785330	-0.3369510
P	-0.6964620	2.0247100	0.4040460
C	2.5621910	-2.6389500	-0.8632050
H	2.4011850	-2.6691740	-1.9444450

H	3.4391850	-3.2451700	-0.6112110
H	1.6739590	-3.0452970	-0.3712890
C	-2.3714550	2.1900820	-0.3502640
H	-3.0429320	2.7875370	0.2759480
H	-2.2707770	2.6725620	-1.3267150
H	-2.7945070	1.1965350	-0.5014430
C	3.0713150	-1.0178020	1.4906730
H	3.7787370	-1.8207770	1.7328110
H	3.5091080	-0.0617500	1.7913530
C	1.7372650	-1.2530150	2.2064790
H	1.4178650	-2.2867930	2.0533900
H	1.8523140	-1.1021350	3.2865730
C	0.1429000	0.6197700	2.6719740
H	0.9616850	1.3187440	2.8656400
H	-0.1208660	0.1301440	3.6222380
C	-1.0772320	1.3528900	2.1066820
H	-1.9084490	0.6474950	1.9864900
H	-1.4083780	2.1434060	2.7889960
C	4.3977020	-0.4149160	-1.0267580
H	5.1751280	-1.1340310	-0.7489250
H	4.3273780	-0.3659310	-2.1169830
H	4.6567260	0.5794230	-0.6561100
C	-0.2570590	3.7891790	0.7204910
H	-0.0238480	4.2696680	-0.2338230
H	-1.0701600	4.3341940	1.2124320
H	0.6446100	3.8159030	1.3357940
C	1.1997800	1.3332760	-2.0207080
O	1.3441950	1.7975210	-3.0814560
O	-0.5949870	-2.7607690	0.6655100
H	-0.1366790	-1.0293770	1.4941090
C	-1.1182640	-2.3862850	-0.3864360
H	-0.6731570	-2.6401910	-1.3628280
H	-0.1494830	-0.5503630	-0.9700930
C	-2.4585500	-1.7484380	-0.4372180
C	-3.0179060	-1.3716910	-1.6648480
C	-3.1881770	-1.5635110	0.7453840
C	-4.2905180	-0.8065280	-1.7099010
H	-2.4388110	-1.5016800	-2.5751150
C	-4.4579480	-0.9902600	0.7015130
H	-2.7459090	-1.8884340	1.6822820
C	-5.0107280	-0.6115990	-0.5260520
H	-4.7193640	-0.5089110	-2.6621180
H	-5.0214450	-0.8456180	1.6188790
H	-6.0010270	-0.1667330	-0.5611330
7			
Ru	0.0124430	-0.4271210	-0.1828970
H	0.0048850	-0.2090470	1.5129040
N	-0.0152020	1.8366300	-0.4016110
P	-2.2629280	-0.1331710	0.0861020
P	2.2858560	-0.0471460	0.0301260
C	-3.4818560	-0.2181480	-1.3026130
H	-3.5505290	-1.2551150	-1.6428220
H	-4.4767040	0.1337790	-1.0076860
H	-3.1084140	0.3774760	-2.1390930

C	3.5521960	-0.4335730	-1.2604000
H	4.5329490	-0.0065710	-1.0235190
H	3.6446020	-1.5203360	-1.3420390
H	3.2006580	-0.0540760	-2.2227660
C	-2.3156330	1.6636510	0.5905640
H	-3.3281430	2.0822150	0.5449480
H	-1.9715750	1.6996800	1.6287890
C	-1.3690530	2.4579010	-0.3129560
H	-1.7761060	2.4818820	-1.3292750
H	-1.2852760	3.4990570	0.0274090
C	1.0166910	2.4276750	0.4843080
H	0.7383770	2.1864950	1.5135580
H	1.0444130	3.5232420	0.3742450
C	2.3849730	1.8283000	0.1376410
H	2.7091670	2.1961920	-0.8441240
H	3.1397960	2.1438440	0.8652600
C	-3.1787290	-0.9767360	1.4439690
H	-4.1857300	-0.5673180	1.5760020
H	-3.2532440	-2.0430470	1.2129200
H	-2.6010470	-0.8674810	2.3640080
C	3.1472570	-0.6116900	1.5614220
H	3.1633060	-1.7050970	1.5749070
H	4.1737130	-0.2335380	1.6186760
H	2.5676860	-0.2745080	2.4228130
C	0.0558160	-2.2809780	-0.1159820
O	0.0830430	-3.4465670	-0.0850750
H	0.3016010	1.9339690	-1.3630390
H	-0.0036930	-0.4458960	-1.8818650

9

Ru	-1.7556100	0.2707530	-0.3562210
H	-2.8984220	0.5922390	0.7048140
N	-0.5305990	-0.5150070	1.2842920
P	-0.8701120	2.2845050	0.4459480
P	-2.6378310	-1.8997750	-0.2681400
C	0.7842050	2.8104820	-0.1725060
H	0.6842950	3.1822450	-1.1965110
H	1.2211620	3.5949620	0.4544130
H	1.4332090	1.9279450	-0.1835210
C	-2.6142780	-3.0822880	-1.6846890
H	-2.9523850	-4.0783930	-1.3807390
H	-3.2663600	-2.7099780	-2.4797880
H	-1.5966640	-3.1508630	-2.0781660
C	-0.5717580	1.8347900	2.2096590
H	0.0302970	2.5899770	2.7324440
H	-1.5555300	1.7700410	2.6863660
C	0.1104140	0.4530270	2.1858170
H	1.1574080	0.6130710	1.8819010
H	0.1517820	0.0658130	3.2141860
C	-1.1618660	-1.6058140	2.0171680
H	-2.0417170	-1.2888680	2.6159240
H	-0.4537980	-2.0545360	2.7352450
C	-1.6043060	-2.7021220	1.0408620
H	-0.7220320	-3.1168270	0.5400540
H	-2.1433920	-3.5172880	1.5367260

C	-1.8508960	3.8401390	0.4778340
H	-1.3369740	4.6208670	1.0474940
H	-2.0140330	4.1900180	-0.5451430
H	-2.8238350	3.6347720	0.9308060
C	-4.3673400	-2.0573550	0.3467140
H	-5.0487580	-1.5746280	-0.3587910
H	-4.6555680	-3.1056690	0.4754370
H	-4.4410120	-1.5342050	1.3027960
C	-2.8779020	0.9708690	-1.7111280
O	-3.6170880	1.4258280	-2.4858940
H	1.1293350	-0.8102010	0.2338400
H	-0.4901840	-0.4678800	-1.6106360
N	2.0308770	-0.6188330	-0.2319620
H	2.0239870	-1.0684220	-1.1440530
C	3.1425380	-1.1302570	0.5642810
H	3.1391260	-2.2280740	0.6913840
H	3.0318920	-0.7191590	1.5778950
C	4.5007960	-0.7173250	0.0224450
C	5.6402820	-1.4727970	0.3287420
C	4.6499710	0.4322880	-0.7625270
C	6.9010430	-1.0853160	-0.1262220
H	5.5367900	-2.3747860	0.9286230
C	5.9094850	0.8199150	-1.2242900
H	3.7651970	1.0102310	-1.0084010
C	7.0401940	0.0648970	-0.9066730
H	7.7731540	-1.6847620	0.1211320
H	6.0076680	1.7138060	-1.8349390
H	8.0198140	0.3660330	-1.2674280
H	-0.1472150	0.2199060	-1.4288340

10

Ru	1.1267080	0.0263620	-0.3926820
H	2.7080640	0.3344180	-0.3144770
N	0.9214470	0.1423290	1.7755050
P	1.8878330	-2.1146890	0.0933010
P	1.0359580	2.3536920	-0.1166770
C	0.7684460	-3.5930290	0.0383180
H	0.4426790	-3.7674000	-0.9911680
H	1.2685620	-4.4922550	0.4131390
H	-0.1159090	-3.4067100	0.6552030
C	-0.3265960	3.5103990	-0.6163640
H	-0.1056040	4.5372700	-0.3057630
H	-0.4540080	3.4863800	-1.7024900
H	-1.2657060	3.2008630	-0.1498300
C	2.2876030	-1.9648730	1.8961080
H	2.3965850	-2.9440060	2.3820650
H	3.2382570	-1.4260480	1.9717330
C	1.1453940	-1.1074600	2.4913600
H	0.2251160	-1.7171890	2.4664000
H	1.3480060	-0.9259010	3.5593970
C	1.6401960	1.2687620	2.3494340
H	2.7375360	1.2348150	2.1903960
H	1.4905120	1.3160750	3.4434130
C	1.0926900	2.5631870	1.7314730
H	0.0575600	2.7042410	2.0628830

H	1.6709140	3.4501540	2.0142600
C	3.4091970	-2.7712630	-0.7093440
H	3.7469550	-3.6977210	-0.2338300
H	3.2102140	-2.9593480	-1.7681220
H	4.1905120	-2.0112590	-0.6388650
C	2.5088050	3.2806200	-0.7315910
H	2.5472050	3.2177970	-1.8226020
H	2.4807280	4.3321220	-0.4270760
H	3.4053290	2.8010020	-0.3334930
C	1.2325300	-0.0533940	-2.2721280
O	1.3156030	-0.1119590	-3.4355230
N	-1.1118770	-0.4339150	-0.1094060
H	-1.1087920	-0.0794640	0.8527870
C	-2.1535130	0.1989950	-0.9436840
H	-2.0337060	-0.1763540	-1.9643670
H	-1.9338300	1.2684090	-0.9754790
C	-3.5600330	-0.0445140	-0.4408290
C	-4.0174880	0.6160990	0.7085710
C	-4.4085730	-0.9600900	-1.0734150
C	-5.2918270	0.3657150	1.2151780
H	-3.3662590	1.3309710	1.2078610
C	-5.6873250	-1.2128140	-0.5707080
H	-4.0665260	-1.4744730	-1.9686950
C	-6.1310240	-0.5511680	0.5750880
H	-5.6334120	0.8868760	2.1050800
H	-6.3359150	-1.9237760	-1.0748280
H	-7.1252010	-0.7456560	0.9669620
H	-1.2946020	-1.4330790	-0.0551500

11

Ru	-1.1666170	0.0834010	-0.4156290
H	-2.7808220	0.4129320	-0.2623720
N	-0.8202590	-0.0654260	1.8071730
P	-1.0871280	2.3639440	0.0769340
P	-1.7785590	-2.1447580	-0.1551210
C	0.4202240	3.4395820	0.1532380
H	0.8316350	3.5680490	-0.8513700
H	0.1823620	4.4234940	0.5716530
H	1.1833450	2.9601350	0.7717710
C	-0.9744080	-3.5489990	-1.0436160
H	-1.2575490	-4.5171920	-0.6177770
H	-1.2732850	-3.5188180	-2.0951700
H	0.1114170	-3.4348330	-0.9962130
C	-1.6126590	2.3083230	1.8647110
H	-1.4830300	3.2761960	2.3648560
H	-2.6770840	2.0540340	1.8620380
C	-0.8109010	1.2082320	2.5724750
H	0.2323910	1.5270970	2.6843800
H	-1.2013220	1.0438140	3.5842480
C	-1.5118820	-1.1917160	2.4602100
H	-2.5753040	-0.9413740	2.5510450
H	-1.1225030	-1.3551810	3.4769960
C	-1.3271750	-2.4658650	1.6278000
H	-0.2669280	-2.7455030	1.6278840
H	-1.8972960	-3.3001220	2.0505920

C	-2.3072970	3.4963580	-0.7096540
H	-2.3532700	4.4629660	-0.1976690
H	-2.0247520	3.6572370	-1.7538730
H	-3.2852970	3.0115440	-0.6911830
C	-3.5624920	-2.5928820	-0.2545330
H	-3.9094880	-2.4370170	-1.2794700
H	-3.7407000	-3.6330200	0.0384560
H	-4.1256330	-1.9182180	0.3938720
C	-1.2686580	0.1819960	-2.2667090
O	-1.3109020	0.2426810	-3.4306890
N	0.9726170	-0.4665980	-0.1220320
H	1.1122460	-1.4473240	-0.3709100
C	2.0142730	0.2660980	-0.8234370
H	1.8565070	1.3379850	-0.6504440
H	1.9702980	0.1517790	-1.9230740
C	3.4398110	-0.0626660	-0.3828580
C	4.5276690	0.2551690	-1.2082660
C	3.6986290	-0.6575870	0.8569920
C	5.8374910	-0.0045380	-0.8044590
H	4.3414090	0.7075000	-2.1807970
C	5.0076760	-0.9243100	1.2649650
H	2.8506610	-0.9119970	1.4858590
C	6.0834320	-0.5970600	0.4373920
H	6.6668090	0.2478140	-1.4605480
H	5.1886460	-1.3899130	2.2309600
H	7.1023330	-0.8058110	0.7523630
H	0.1589410	-0.3217760	1.5284210

12

Ru	-2.15138100	0.18591400	-0.21957500
H	-3.63877400	-0.51615600	-0.46950000
N	-1.42868900	-1.81332000	0.55403200
P	-2.93999400	0.39427300	1.94721700
P	-1.54708900	-0.80423200	-2.23932200
C	-1.94873400	1.18647100	3.29570500
H	-0.94315700	0.75745600	3.30660900
H	-1.85374200	2.25515800	3.08429600
H	-2.40833200	1.05140900	4.28049200
C	0.03763200	-0.36300900	-3.07412100
H	-0.07426800	0.59819600	-3.58330200
H	0.78927700	-0.25320700	-2.28811600
H	0.34933200	-1.12094200	-3.79984300
C	-3.00427300	-1.39327200	2.46495100
H	-3.13168100	-1.51275300	3.54771400
H	-3.87520500	-1.82779400	1.96423400
C	-1.71883500	-2.07870300	1.98991500
H	-0.86621500	-1.69503400	2.56108700
H	-1.76372100	-3.15974500	2.17764100
C	-1.85346300	-2.88908300	-0.37630200
H	-2.94583400	-2.90982500	-0.40518700
H	-1.48966000	-3.86431200	-0.02024900
C	-1.26321700	-2.59503900	-1.76062900
H	-0.18023900	-2.74993600	-1.71765100
H	-1.67304700	-3.27315500	-2.51590600
C	-4.63595000	1.01882300	2.29598500

H	-4.93164000	0.84311600	3.33534300
H	-4.67176300	2.09214300	2.08945900
H	-5.33043700	0.51786800	1.61797300
C	-2.75165600	-0.88967200	-3.63027900
H	-2.93888600	0.12144500	-4.00266200
H	-2.38725600	-1.51689200	-4.45039900
H	-3.69322900	-1.28734700	-3.24448500
C	-2.80325800	1.79142200	-0.88058000
O	-3.22102500	2.79925500	-1.29409900
C	2.13244300	-1.51350900	0.31982600
H	-0.40780700	-1.77617800	0.46951500
N	-0.03503500	0.81513100	0.11285400
H	0.10057800	0.94032400	1.11947400
C	0.29716300	2.11123100	-0.48536400
H	-0.28244700	2.95667000	-0.06626500
H	0.03146300	2.07835800	-1.54893300
C	1.77276700	2.46257400	-0.37615300
C	2.64922200	2.28109200	-1.45547400
C	2.29946500	2.96957000	0.82140600
C	4.00296000	2.60950700	-1.35186600
H	2.25911400	1.88615400	-2.39041800
C	3.65273800	3.29333600	0.93663200
H	1.63242000	3.12299600	1.66743300
C	4.51006400	3.12083100	-0.15466600
H	4.66184000	2.46683800	-2.20424600
H	4.03778300	3.69084700	1.87210900
H	5.56096500	3.38436900	-0.07257800
H	1.65704900	-0.51384700	0.19983500
C	3.59684600	-1.56601700	0.46783900
C	4.30545600	-0.35851800	0.53350400
C	4.27991400	-2.79103800	0.54593900
C	5.69265400	-0.37303600	0.67249000
H	3.76815000	0.58110500	0.47859500
C	5.66351700	-2.80233200	0.68229000
H	3.70417800	-3.71016800	0.49513900
C	6.36967700	-1.59254300	0.74457000
H	6.23737300	0.56499700	0.71916900
H	6.19930700	-3.74552700	0.74011700
H	7.45122400	-1.60578400	0.84959200
O	1.41622100	-2.51786000	0.32220900

13

Ru	1.6543790	0.4268580	-0.1654320
H	3.2170530	0.8024010	-0.1091140
N	2.1540840	-1.3706720	1.0198610
P	2.3655450	-0.9220420	-1.9324790
P	1.6198380	1.3255150	1.9909730
C	1.2133880	-1.9494350	-2.9573350
H	0.5637140	-1.2979260	-3.5477870
H	1.7638530	-2.6146460	-3.6310580
H	0.5838060	-2.5512920	-2.2972670
C	0.0265840	1.6520670	2.8655380
H	0.1891400	1.9734320	3.8993460
H	-0.5443550	2.4204950	2.3355980
H	-0.5317740	0.7119550	2.8580340

C	3.3654350	-2.1934570	-1.0244280
H	3.5807150	-3.0721020	-1.6463040
H	4.3129910	-1.7148130	-0.7549200
C	2.5674850	-2.5457940	0.2461490
H	1.6690770	-3.1040330	-0.0571840
H	3.1545610	-3.2389110	0.8677360
C	3.0768860	-1.0370630	2.1075130
H	4.0364190	-0.6335390	1.7411590
H	3.3148890	-1.9357220	2.7019260
C	2.4077640	-0.0064260	3.0309530
H	1.6003350	-0.4882890	3.5913630
H	3.1135490	0.4236710	3.7491120
C	3.5018650	-0.2413610	-3.2123200
H	3.9350470	-1.0346310	-3.8297770
H	2.9538760	0.4548400	-3.8536080
H	4.2971630	0.3123500	-2.7082910
C	2.5996710	2.8503240	2.3206490
H	2.1670560	3.6838360	1.7602450
H	2.6158230	3.0989200	3.3867120
H	3.6191770	2.6919740	1.9611020
C	1.3845130	2.0160930	-1.1158760
O	1.2844970	3.0197270	-1.7064670
N	-0.6542970	-0.1767330	-0.1426900
H	-1.0127890	0.5078130	0.5198490
C	-1.3775830	0.0543770	-1.4400160
H	-1.7599700	-0.9023370	-1.8067180
H	-0.6505860	0.4156540	-2.1694380
C	-2.5053340	1.0549100	-1.3006760
C	-2.2106370	2.4263690	-1.2498190
C	-3.8388140	0.6458930	-1.1701230
C	-3.2260070	3.3648370	-1.0591950
H	-1.1856140	2.7612120	-1.3739320
C	-4.8544390	1.5847820	-0.9847240
H	-4.0828040	-0.4106440	-1.1984650
C	-4.5516580	2.9463630	-0.9241670
H	-2.9814240	4.4229850	-1.0263030
H	-5.8823000	1.2483540	-0.8815740
H	-5.3428850	3.6764080	-0.7778160
H	0.7462370	-1.5366970	1.5252670
O	-0.2988780	-1.5502960	1.7306600
C	-0.9231790	-1.5201630	0.5031140
H	-0.5067000	-2.2530220	-0.2101760
C	-2.4077340	-1.8009300	0.6705330
C	-3.1464260	-1.1059770	1.6356220
C	-3.0625850	-2.7257510	-0.1468710
C	-4.5177070	-1.3133330	1.7619450
H	-2.6373720	-0.3996460	2.2838210
C	-4.4385760	-2.9411230	-0.0217470
H	-2.4929650	-3.2816220	-0.8882540
C	-5.1700460	-2.2287680	0.9292890
H	-5.0819960	-0.7606710	2.5077770
H	-4.9350790	-3.6625830	-0.6646600
H	-6.2399320	-2.3892290	1.0274430

14

Ru	1.3481550	-1.0176350	0.6040980
H	2.2644030	-2.1654560	1.1701760
N	1.5404440	-1.3696050	-1.4986880
P	3.3295310	0.1534820	0.1719600
P	-0.3513600	-2.6114290	0.3515590
C	3.2724150	1.8699310	-0.4936890
H	2.9235780	2.5592640	0.2788760
H	4.2594260	2.1831110	-0.8497160
H	2.5492700	1.8952070	-1.3124010
C	-2.0241020	-2.5892370	1.1197290
H	-2.6241070	-3.4368850	0.7735040
H	-1.9217410	-2.6420340	2.2072100
H	-2.5424750	-1.6661280	0.8591430
C	3.9804590	-0.8548460	-1.2357270
H	4.8095850	-0.3553350	-1.7518110
H	4.3625930	-1.7735060	-0.7770150
C	2.8297630	-1.1981720	-2.1973140
H	2.7452720	-0.4041780	-2.9590610
H	3.0994290	-2.1148700	-2.7436720
C	0.7215510	-2.3973030	-2.1561030
H	1.2306320	-3.3785520	-2.1465410
H	0.5681230	-2.1446030	-3.2189850
C	-0.6444650	-2.5161930	-1.4726670
H	-1.2155820	-1.5940560	-1.6315780
H	-1.2187070	-3.3710900	-1.8478230
C	4.7169750	0.2109630	1.3799370
H	5.6335770	0.5936910	0.9196500
H	4.4379830	0.8591450	2.2152450
H	4.8908650	-0.7951240	1.7690030
C	0.1874540	-4.3527390	0.6342110
H	0.3801960	-4.5004590	1.6999470
H	-0.5687710	-5.0689240	0.2963020
H	1.1217270	-4.5190910	0.0935670
C	1.0256310	-0.4722480	2.3735510
O	0.8091190	-0.1079290	3.4605330
N	-1.6952910	0.8650990	-1.0115350
H	-2.0692890	1.3716060	-1.8123770
C	-2.5152890	1.0950900	0.1730530
H	-2.5803580	2.1573790	0.4620290
H	-2.0087980	0.5976160	1.0139290
C	-3.9170660	0.5309650	0.0378570
C	-4.9162660	0.9541270	0.9255560
C	-4.2400590	-0.4302990	-0.9272520
C	-6.2033090	0.4225290	0.8592690
H	-4.6799320	1.7075840	1.6737540
C	-5.5310560	-0.9599010	-0.9996960
H	-3.4709340	-0.7579360	-1.6179600
C	-6.5161440	-0.5384650	-0.1063890
H	-6.9643820	0.7617180	1.5565940
H	-5.7652750	-1.7030260	-1.7572750
H	-7.5198110	-0.9502480	-0.1626510
H	0.7946310	0.0154500	-1.9159670
O	0.3899190	0.9506860	-2.0465380
C	-0.2782660	1.2299860	-0.8677000

H	0.0901020	0.5924370	-0.0182900
C	-0.0434720	2.6708650	-0.4361860
C	-0.0075030	3.6944820	-1.3901470
C	0.1212380	2.9893410	0.9157860
C	0.1898340	5.0174870	-0.9958070
H	-0.1062750	3.4370180	-2.4403220
C	0.3198170	4.3143990	1.3126030
H	0.1147160	2.1945760	1.6579080
C	0.3536840	5.3315910	0.3570190
H	0.2249500	5.8051670	-1.7436540
H	0.4529410	4.5488590	2.3651760
H	0.5117260	6.3621880	0.6622190

14'

Ru	1.31267400	-1.02348200	0.59484300
H	2.27642600	-2.23324800	0.96374600
N	1.45696400	-1.36221000	-1.60807500
P	3.27398000	0.22110600	0.15295700
P	-0.41720300	-2.59659600	0.36535900
C	3.52654700	2.00917700	0.51235000
H	3.47545600	2.17774100	1.59100900
H	4.50206500	2.33888600	0.14037500
H	2.73554300	2.59134400	0.03715500
C	-2.11794800	-2.40698900	1.03575100
H	-2.75548800	-3.24268800	0.73011400
H	-2.07738300	-2.36613000	2.12759900
H	-2.55126600	-1.47929900	0.66266100
C	3.39498400	0.12682500	-1.69823300
H	2.75591400	0.92995000	-2.08077600
H	4.42218800	0.27616300	-2.04723800
C	2.81523400	-1.20988000	-2.17138300
H	2.77167100	-1.22558600	-3.27093800
H	3.44088500	-2.05298600	-1.85220700
C	0.74178900	-2.54422400	-2.13105600
H	1.33093500	-3.44768700	-1.92434200
H	0.63474200	-2.46524200	-3.22322400
C	-0.64034900	-2.62966200	-1.47603100
H	-1.21361800	-1.72708700	-1.72349700
H	-1.19520200	-3.51350500	-1.80967500
C	4.84491700	-0.53697500	0.75221900
H	5.72045900	-0.00709200	0.36304600
H	4.86179100	-0.51381100	1.84511700
H	4.87376700	-1.58258800	0.43676900
C	-0.00031700	-4.33761600	0.80666700
H	0.14068400	-4.40756400	1.88846200
H	-0.78930000	-5.03030800	0.49626400
H	0.94199500	-4.61023500	0.32595000
C	1.14091500	-0.64315500	2.41867600
O	1.03424700	-0.39991000	3.55227700
N	-1.75167800	0.82144700	-1.04640100
H	-2.09604900	1.25054300	-1.90289300
C	-2.55531400	1.20966300	0.10217500
H	-2.56136200	2.29577600	0.29536400
H	-2.08577500	0.76339400	0.99202400
C	-3.99050000	0.72116400	0.01346900

C	-4.94449200	1.22955900	0.90685900
C	-4.39370700	-0.24382200	-0.91706500
C	-6.26330600	0.77945600	0.87955600
H	-4.64665400	1.98705200	1.62876200
C	-5.71685200	-0.69302300	-0.95043900
H	-3.66007300	-0.63866700	-1.61191200
C	-6.65574100	-0.18632000	-0.05210800
H	-6.98731400	1.18510300	1.58104500
H	-6.01237900	-1.43989500	-1.68269400
H	-7.68432200	-0.53495700	-0.07832000
H	0.89936400	-0.46064000	-1.94147900
O	0.27095000	0.82107300	-2.16505500
C	-0.29365400	1.10604500	-1.00187600
H	0.04527500	0.40838000	-0.11131200
C	0.06380300	2.50334700	-0.46499500
C	0.37290500	3.52021700	-1.37513400
C	0.12476200	2.77844000	0.90549200
C	0.72810700	4.79185600	-0.92207300
H	0.35819800	3.27839300	-2.43310000
C	0.47785500	4.04968600	1.36324500
H	-0.06846400	1.98004900	1.61812300
C	0.78028400	5.06149100	0.44908000
H	0.97530600	5.57188700	-1.63773300
H	0.53025800	4.24528900	2.43107400
H	1.06429700	6.04929100	0.80154700

15

Ru	-2.0577840	0.3622210	0.1404450
H	-3.4760560	1.0215750	0.2925500
N	-2.1571380	-0.8756090	-1.5179530
P	-2.7508050	-1.6183790	1.1590890
P	-1.3886560	1.9086680	-1.4810900
C	-1.3951700	-2.7907900	1.5929320
H	-0.7632640	-2.3642090	2.3748810
H	-1.7846820	-3.7656000	1.9043740
H	-0.7636170	-2.9101540	0.7091000
C	0.0795790	2.9986610	-1.2741070
H	0.3224840	3.5247590	-2.2032870
H	-0.1127540	3.7281160	-0.4836400
H	0.9305450	2.3861900	-0.9679140
C	-3.6207490	-2.4399490	-0.2507050
H	-3.7857300	-3.5101270	-0.0762560
H	-4.5961060	-1.9458050	-0.3199990
C	-2.8181560	-2.1812060	-1.5362710
H	-2.0761800	-2.9924600	-1.6724110
H	-3.5030140	-2.2643060	-2.3974690
C	-1.8842740	-0.4121050	-2.8789740
H	-2.8223890	-0.1431440	-3.4021690
H	-1.4299960	-1.2220470	-3.4765900
C	-0.9244550	0.7831340	-2.8752030
H	0.0851860	0.4250970	-2.6438920
H	-0.9113460	1.3051840	-3.8392400
C	-3.9109640	-1.7494940	2.5821060
H	-4.1991250	-2.7882380	2.7732270
H	-3.4286650	-1.3404890	3.4742050

H	-4.8019910	-1.1531940	2.3705850
C	-2.6628830	3.0373480	-2.1902580
H	-2.9866230	3.7458340	-1.4232950
H	-2.2792570	3.5857220	-3.0569430
H	-3.5272570	2.4384300	-2.4876150
C	-1.6472230	1.3704800	1.6664850
O	-1.4072890	2.0089170	2.6197770
C	2.4308050	3.6768280	1.4144380
C	1.7419120	2.6455340	2.0509430
C	1.9913830	1.3121140	1.6917360
C	2.9412690	1.0160240	0.7006480
C	3.6288190	2.0485850	0.0706410
C	3.3732330	3.3784150	0.4257920
H	2.2331250	4.7100030	1.6844230
H	0.9900760	2.8641380	2.8032550
H	3.1363570	-0.0169940	0.4441090
H	4.3639210	1.8116570	-0.6922280
H	3.9102800	4.1833540	-0.0685240
C	1.2538860	0.2253270	2.3680850
O	1.2944650	-0.9518040	2.0356960
H	0.6330790	0.5452280	3.2265550
C	3.8463720	-2.6316550	0.3431210
C	3.1795310	-2.2734440	-0.8323330
C	3.8553270	-1.4920430	-1.7808480
C	5.1704740	-1.0850430	-1.5609850
C	5.8294230	-1.4489970	-0.3813950
C	5.1643330	-2.2236510	0.5692900
H	3.3180360	-3.2056830	1.0992310
H	3.3258990	-1.1839920	-2.6778450
H	5.6834090	-0.4824000	-2.3061350
H	6.8518120	-1.1264980	-0.2054310
H	5.6649320	-2.5013550	1.4926720
C	1.7228240	-2.6259590	-1.0494610
H	1.6065260	-3.1401090	-2.0127630
H	1.4094220	-3.3403070	-0.2691630
N	0.9227080	-1.3978490	-1.0962830
H	-0.0640420	-1.5819190	-1.2763800
H	0.9532360	-0.9596560	-0.1776920

16

Ru	-1.9765990	-0.6358450	-0.3911170
H	-3.1719470	-1.7269050	-0.3587470
N	-1.2372340	-1.0307360	1.7021460
P	-3.4208270	0.7768080	0.7750660
P	-0.5585630	-2.4245040	-0.8745850
C	-2.8142210	2.4748570	1.1363670
H	-3.0203960	3.1121120	0.2717570
H	-3.2797300	2.9094850	2.0266580
H	-1.7281320	2.4079870	1.2359210
C	0.8134770	-2.3711200	-2.0992590
H	1.4266590	-3.2775330	-2.0580600
H	0.3968710	-2.2649170	-3.1045540
H	1.4244090	-1.4985980	-1.8663490
C	-3.4583440	-0.0855880	2.4253490
H	-3.9253540	0.5309990	3.2034190

H	-4.0815930	-0.9727970	2.2711270
C	-2.0433390	-0.5118540	2.8447740
H	-1.5148540	0.3429970	3.2828450
H	-2.1051990	-1.2794570	3.6240140
C	-0.6262350	-2.3607830	1.9146190
H	-1.4351240	-3.0961560	1.9968560
H	-0.0626070	-2.3824810	2.8597790
C	0.3103350	-2.6999320	0.7491050
H	1.1567100	-2.0039270	0.7366900
H	0.6928130	-3.7223930	0.8409300
C	-5.2035310	0.9982280	0.3790170
H	-5.7307130	1.5405950	1.1703990
H	-5.2922730	1.5554350	-0.5576070
H	-5.6585110	0.0149070	0.2370250
C	-1.3581370	-4.0462200	-1.2368620
H	-1.8960650	-3.9735370	-2.1858540
H	-0.6246840	-4.8576020	-1.2932110
H	-2.0899420	-4.2588060	-0.4541700
C	-2.4770460	-0.2084490	-2.1268010
O	-2.7883460	0.0628090	-3.2166360
O	-0.3486660	0.8310760	0.1108250
C	0.7738140	1.1099370	-0.6169580
C	1.1154700	2.6003380	-0.5114640
C	1.4828200	3.3549090	-1.6283140
C	1.0909790	3.2251780	0.7433010
C	1.8161120	4.7076630	-1.5013890
H	1.5003770	2.8808130	-2.6075560
C	1.4261240	4.5704270	0.8777520
H	0.7873960	2.6400360	1.6072440
C	1.7907330	5.3184980	-0.2477470
H	2.0933370	5.2820530	-2.3815230
H	1.4004220	5.0418410	1.8571200
H	2.0489440	6.3689600	-0.1454140
H	-0.5046190	-0.3327060	1.4703270
N	1.9019470	0.2597590	-0.1215990
H	2.0063490	0.4711070	0.8710300
C	3.1986130	0.4652380	-0.7813740
H	3.5232220	1.5179600	-0.7830610
H	3.0817230	0.1790500	-1.8363510
C	4.2599400	-0.3902660	-0.1263770
C	4.2027000	-1.7891910	-0.2120900
C	5.2935210	0.1927720	0.6146700
C	5.1583360	-2.5829210	0.4198980
H	3.4021480	-2.2512240	-0.7812650
C	6.2539800	-0.5987350	1.2507580
H	5.3459670	1.2761380	0.6922930
C	6.1891040	-1.9889460	1.1548460
H	5.1033570	-3.6652540	0.3377270
H	7.0512730	-0.1283200	1.8196910
H	6.9355680	-2.6065610	1.6463880
H	0.6772740	0.8608120	-1.6918280

17

Ru	1.3477910	-1.0180010	0.6040430
H	2.2637700	-2.1660270	1.1701560

N	1.5397900	-1.3700460	-1.4987450
P	3.3293430	0.1527780	0.1717860
P	-0.3522710	-2.6112490	0.3516210
C	3.2729510	1.8693470	-0.4936330
H	2.9240690	2.5587210	0.2788770
H	4.2601930	2.1821780	-0.8493050
H	2.5499840	1.8949200	-1.3125130
C	-2.0250490	-2.5881780	1.1196630
H	-1.9228510	-2.6417700	2.2071220
H	-2.5425940	-1.6644550	0.8595960
H	-2.6257300	-3.4350980	0.7728250
C	3.9799400	-0.8556880	-1.2359720
H	4.8091470	-0.3563590	-1.7521140
H	4.3619810	-1.7743550	-0.7772010
C	2.8291880	-1.1989570	-2.1974490
H	2.7447580	-0.4051040	-2.9593310
H	3.0986200	-2.1158080	-2.7436480
C	0.7207770	-2.3977720	-2.1560070
H	1.2296670	-3.3791120	-2.1461460
H	0.5675180	-2.1453080	-3.2189610
C	-0.6452750	-2.5161480	-1.4725940
H	-1.2160210	-1.5937880	-1.6316080
H	-1.2199470	-3.3707980	-1.8476660
C	4.7167960	0.2092910	1.3798060
H	5.6336370	0.5916620	0.9196920
H	4.4381620	0.8572990	2.2153650
H	4.8900780	-0.7970530	1.7684820
C	0.1859280	-4.3526690	0.6346910
H	0.3789210	-4.5000310	1.7004280
H	-0.5706110	-5.0687480	0.2972540
H	1.1200100	-4.5195320	0.0938730
C	1.0256210	-0.4725760	2.3735360
O	0.8094330	-0.1084790	3.4606640
N	-1.6948510	0.8658380	-1.0118730
H	-2.0684590	1.3726060	-1.8127340
C	-2.5149480	1.0960660	0.1725930
H	-2.5801210	2.1584380	0.4612590
H	-2.0084650	0.5988830	1.0136440
C	-3.9167060	0.5317820	0.0375660
C	-4.2399020	-0.4291200	-0.9278370
C	-4.9156780	0.9544650	0.9257460
C	-5.5308750	-0.9587970	-1.0001210
H	-3.4709270	-0.7564660	-1.6188430
C	-6.2027000	0.4227900	0.8596200
H	-4.6791870	1.7076100	1.6742140
C	-6.5157440	-0.5378130	-0.1063570
H	-5.7652580	-1.7016280	-1.7579380
H	-6.9635830	0.7616110	1.5573300
H	-7.5193930	-0.9496530	-0.1625080
H	0.7943330	0.0155310	-1.9161740
O	0.3906460	0.9511740	-2.0464730
C	-0.2777270	1.2305180	-0.8677270
H	0.0902490	0.5927420	-0.0183370
C	-0.0426470	2.6712080	-0.4360520
C	-0.0062280	3.6948980	-1.3899190

C	0.1218210	2.9895040	0.9159870
C	0.1913930	5.0178060	-0.9954050
H	-0.1048910	3.4375740	-2.4401340
C	0.3206930	4.3144750	1.3129720
H	0.1148380	2.1946800	1.6580330
C	0.3550610	5.3317360	0.3574870
H	0.2268620	5.8055510	-1.7431640
H	0.4536440	4.5488060	2.3655950
H	0.5133370	6.3622610	0.6628110

19

Ru	1.9182130	-0.1470160	-0.5126370
H	3.2717960	0.6701210	-0.4578260
N	1.1002170	1.0833960	1.1048720
P	2.7840150	-1.2961830	1.3206310
P	1.0755330	1.6057550	-1.8037970
C	1.7205100	-2.5722760	2.1387950
H	1.6779610	-3.4689420	1.5112850
H	2.1079960	-2.8530210	3.1237210
H	0.7088410	-2.1666640	2.2439550
C	-0.1870140	1.3793390	-3.1328100
H	-0.5741420	2.3409410	-3.4856350
H	0.2658790	0.8409110	-3.9700190
H	-1.0118580	0.7757750	-2.7470570
C	2.8766830	0.0616090	2.5708210
H	3.0711900	-0.3154490	3.5839950
H	3.7165330	0.6933000	2.2617640
C	1.5585050	0.8552250	2.4817220
H	0.7951470	0.2915280	3.0522880
H	1.6887080	1.8044710	3.0216720
C	0.9894710	2.5050230	0.7850850
H	1.9750060	3.0086300	0.7224040
H	0.4204930	3.0420790	1.5609680
C	0.2518020	2.6884630	-0.5460480
H	-0.7812620	2.3433360	-0.4375230
H	0.2290940	3.7357900	-0.8677990
C	4.4500210	-2.0797680	1.3349980
H	4.7383340	-2.3968280	2.3423610
H	4.4481900	-2.9477170	0.6698090
H	5.1779100	-1.3591310	0.9543000
C	2.3042220	2.7088410	-2.6241940
H	2.8536350	2.1380150	-3.3774880
H	1.8229860	3.5717610	-3.0959010
H	3.0175280	3.0507470	-1.8706210
C	2.6312720	-1.1834380	-1.9126670
O	3.1208210	-1.7994430	-2.7741780
O	-0.2006140	-1.4646600	-0.5808950
H	-0.4578930	0.0722080	1.3132480
C	-1.4404460	-0.9212610	-0.0909410
H	-1.5873290	-0.0314650	-0.7206910
C	-2.5704520	-1.9003640	-0.3502960
C	-2.7837640	-2.9840280	0.5107640
C	-3.3738320	-1.7631820	-1.4865850
C	-3.7871980	-3.9139560	0.2388230
H	-2.1671380	-3.0745830	1.4005350

C	-4.3802050	-2.6911460	-1.7604650
H	-3.2077340	-0.9240860	-2.1581910
C	-4.5881130	-3.7689700	-0.8973140
H	-3.9490850	-4.7491640	0.9145010
H	-5.0004480	-2.5730450	-2.6444170
H	-5.3717760	-4.4912540	-1.1073600
H	-0.0094730	-2.2473260	-0.0438990
N	-1.2517400	-0.6055720	1.3098490
C	-2.4086660	0.0069690	1.9870490
H	-3.2690510	-0.6644560	1.9002030
H	-2.1570520	0.0704820	3.0512070
C	-2.7692930	1.3889280	1.4689480
C	-2.2343940	2.5336570	2.0722980
C	-3.5797740	1.5472840	0.3349950
C	-2.4840010	3.8036220	1.5507220
H	-1.6054060	2.4244400	2.9523650
C	-3.8263450	2.8151170	-0.1954110
H	-4.0181870	0.6689800	-0.1316520
C	-3.2755090	3.9475870	0.4091440
H	-2.0567710	4.6791040	2.0317250
H	-4.4525350	2.9194890	-1.0773620
H	-3.4665700	4.9345280	-0.0023890

20

Ru	-0.0006530	-0.4524220	-0.1219480
H	0.0996370	-0.4691970	-1.7462850
N	0.1001490	1.7906990	0.0634700
P	2.2986960	-0.1375000	-0.0691180
P	-2.2952610	-0.0495920	-0.1237850
C	3.0504530	0.0667250	1.6045140
H	3.2397960	-0.9208670	2.0355800
H	3.9860630	0.6344050	1.5828030
H	2.3044310	0.5679110	2.2282950
C	-3.2606710	-0.7980100	1.2470940
H	-4.2365930	-0.3219280	1.3859660
H	-3.3988790	-1.8660650	1.0579890
H	-2.6300710	-0.6665250	2.1309690
C	2.4445700	1.5535590	-0.8339050
H	3.4433010	1.9836260	-0.6900720
H	2.2975630	1.3847300	-1.9053470
C	1.3532240	2.5034950	-0.3052860
H	1.7237310	3.0539770	0.5689240
H	1.1215600	3.2493570	-1.0724120
C	-1.1411950	2.4963300	-0.3187920
H	-1.1967880	2.5180310	-1.4134100
H	-1.1219940	3.5393450	0.0338100
C	-2.3528430	1.7723180	0.2775710
H	-2.2996220	1.8256720	1.3699030
H	-3.2890130	2.2363500	-0.0506110
C	3.5494590	-1.1180820	-0.9972210
H	4.5435570	-0.6621450	-0.9487210
H	3.5957210	-2.1263070	-0.5765260
H	3.2290410	-1.1975580	-2.0389390
C	-3.3640170	-0.2315490	-1.6135180
H	-3.4063440	-1.2879080	-1.8928620

H	-4.3794890	0.1379810	-1.4363750
H	-2.9110240	0.3169540	-2.4434140
C	-0.0741280	-2.3043950	-0.1640720
O	-0.1196320	-3.4699880	-0.1983910
H	0.0858500	1.6019260	1.0889140
O	-0.2503740	0.1531740	2.0190350
H	0.2066380	-0.4615350	2.6033110

21

Ru	0.0009830	0.4567270	-0.0056970
H	0.0163680	0.5681960	-1.5855340
N	-0.0174060	-1.7278900	0.1273660
P	-2.2895370	0.1007010	-0.2040010
P	2.3001600	0.0726780	-0.1620080
C	-3.2667130	-0.0068490	1.3556190
H	-3.4229290	1.0026970	1.7456620
H	-4.2362160	-0.4911900	1.2003230
H	-2.6765520	-0.5584850	2.0910480
C	3.5679870	0.7997870	0.9691970
H	4.5530600	0.3452390	0.8200960
H	3.6375720	1.8759200	0.7876210
H	3.2569270	0.6510320	2.0070330
C	-2.3136470	-1.6188320	-0.8906370
H	-3.3156850	-2.0664420	-0.8533740
H	-2.0120870	-1.5220820	-1.9396940
C	-1.2731100	-2.4577040	-0.1250380
H	-1.7253570	-2.7799670	0.8282400
H	-1.0864860	-3.3792260	-0.6952010
C	1.1597000	-2.4363190	-0.3689760
H	1.1914070	-2.4782680	-1.4748220
H	1.1660320	-3.4848400	-0.0248820
C	2.4364840	-1.7563420	0.1425280
H	2.5080610	-1.8888160	1.2290060
H	3.3416640	-2.1757210	-0.3110510
C	-3.3788070	1.0684680	-1.3279760
H	-4.3733490	0.6181070	-1.4089940
H	-3.4755540	2.0889080	-0.9472690
H	-2.9139320	1.1135390	-2.3157860
C	3.0775220	0.3070590	-1.8170220
H	3.0351800	1.3650940	-2.0880670
H	4.1176390	-0.0348210	-1.8292000
H	2.4956620	-0.2536560	-2.5522210
C	0.0099770	2.3350610	0.0679700
O	0.0099090	3.5005640	0.0944000
H	0.0012520	-1.1640440	1.7033720
O	-0.1337300	-0.3887550	2.3585550
H	0.7108130	-0.2530740	2.8053070

22

Ru	1.6061910	0.0351000	-0.3954240
H	3.0522060	0.1989490	0.2500040
N	0.7374850	0.0541670	1.6445690
P	1.8699020	-2.2253140	0.0873740
P	1.4361630	2.3322990	-0.0227670
C	0.5255740	-3.3781070	-0.4331570

H	0.5853850	-3.5250750	-1.5149130
H	0.5925140	-4.3476480	0.0711750
H	-0.4361820	-2.9074870	-0.2182890
C	0.1012740	3.3531430	-0.8000930
H	0.0310500	4.3488140	-0.3495500
H	0.3036270	3.4599160	-1.8699650
H	-0.8521820	2.8313380	-0.6789980
C	1.7807680	-2.2236540	1.9384340
H	1.6262020	-3.2310540	2.3479660
H	2.7430090	-1.8425370	2.2980120
C	0.6465160	-1.2450780	2.3126210
H	-0.3061260	-1.7268190	2.0364310
H	0.6159490	-1.1281470	3.4075180
C	1.3455190	1.0975710	2.4658480
H	2.4359510	0.9773540	2.6046410
H	0.9035240	1.1081430	3.4783740
C	1.0743110	2.4610520	1.8057700
H	0.0127160	2.7131430	1.9079560
H	1.6556930	3.2697380	2.2619330
C	3.4028400	-3.1611550	-0.3180090
H	3.4047860	-4.1530830	0.1451950
H	3.4856780	-3.2689560	-1.4030640
H	4.2640220	-2.5889410	0.0355930
C	2.9255980	3.3891110	-0.2762680
H	3.1867080	3.3976980	-1.3381030
H	2.7599220	4.4156410	0.0664650
H	3.7590040	2.9462470	0.2742370
C	2.4015600	0.0555480	-2.0986790
O	2.9387310	0.0646260	-3.1350200
H	-1.0071060	0.5170330	1.3145170
O	-0.6688700	-0.2923890	-1.2819640
H	-0.6939700	0.2510530	-2.0783500
N	-1.9308760	0.6549950	0.8312870
H	-2.2798540	1.5934030	1.0108300
H	-1.2331040	0.1876910	-0.5870050
C	-2.9226570	-0.3487330	1.2508340
H	-3.1873390	-0.2649730	2.3158720
H	-2.4498950	-1.3296680	1.1215740
C	-4.1779190	-0.2799670	0.4068150
C	-5.4081040	0.0782730	0.9664810
C	-4.1141470	-0.5607060	-0.9667610
C	-6.5581620	0.1551070	0.1755050
H	-5.4675720	0.2976230	2.0302500
C	-5.2592040	-0.4849770	-1.7575110
H	-3.1579330	-0.8334900	-1.4058050
C	-6.4857910	-0.1263110	-1.1885910
H	-7.5068450	0.4343570	0.6256140
H	-5.1984290	-0.7094470	-2.8190300
H	-7.3777730	-0.0687280	-1.8060770

23

Ru	-1.4066600	-0.2100390	-0.6424980
H	-1.2081390	1.2630010	-1.3587090
N	-0.0326690	0.3864520	1.1066250
P	3.1253900	2.1476950	-0.8843750

P	-2.9876720	0.6212190	0.6817120
C	4.3530470	1.9087910	0.5017520
H	5.3583320	2.1370050	0.1340060
H	4.1422170	2.5493340	1.3665100
H	4.3448580	0.8618220	0.8197230
C	-4.4588360	-0.4122330	1.0804930
H	-5.0910580	0.0580540	1.8405300
H	-5.0427430	-0.5654760	0.1688930
H	-4.1120410	-1.3855780	1.4357130
C	1.5265340	2.0969780	0.0947950
H	1.4833680	2.9417720	0.7947100
H	0.7053430	2.2015910	-0.6234900
C	1.3745980	0.7602840	0.8233860
H	1.7851720	-0.0451950	0.2154300
H	1.9481990	0.7732180	1.7620360
C	-0.6932800	1.2982360	2.0648910
H	-0.6834440	2.3026130	1.6313980
H	-0.1313870	1.3419900	3.0105020
C	-2.1348990	0.8523680	2.3176450
H	-2.1461420	-0.1243400	2.8142680
H	-2.6660350	1.5669260	2.9555880
C	3.2702190	3.9940770	-1.0981570
H	3.1997440	4.5329670	-0.1460030
H	4.2289260	4.2343920	-1.5678970
H	2.4742820	4.3459270	-1.7616550
C	-3.7274250	2.2623760	0.2962410
H	-4.2406580	2.1966330	-0.6666660
H	-4.4335340	2.5832610	1.0692250
H	-2.9211330	2.9921320	0.1950690
C	-2.6109110	-0.6207020	-1.9887550
O	-3.4039310	-0.8441210	-2.8141930
H	-0.0425480	-0.5685140	1.4856470
C	0.0414310	-2.3429500	-0.7343900
H	0.0768690	-1.4413790	-1.4771700
H	-0.1609070	-3.1720830	-1.4300580
C	1.4786200	-2.4302130	-0.2307530
C	2.5525620	-2.1278670	-1.0789830
C	1.7424230	-2.7699720	1.0998490
C	3.8631800	-2.1430910	-0.6021400
H	2.3567460	-1.8402670	-2.1097450
C	3.0544330	-2.7876120	1.5804370
H	0.8980750	-2.9931850	1.7440100
C	4.1182550	-2.4677420	0.7343360
H	4.6826680	-1.8865320	-1.2674210
H	3.2453970	-3.0458460	2.6189180
H	5.1377970	-2.4721920	1.1097780
N	-0.9565580	-2.1676890	0.2890230
H	-1.7046080	-2.8368050	0.1268350

24

Ru	-1.2188730	-0.0233250	0.7639830
H	-0.8648040	-1.5253090	1.2000840
N	0.2014300	-0.3078740	-1.0098910
P	3.8328810	-1.6181950	0.6203150
P	-2.7582830	-0.9967980	-0.8032110

C	4.6598410	-2.0162950	-1.0064630
H	5.7187470	-2.2320260	-0.8334750
H	4.2027040	-2.8796420	-1.5050650
H	4.6029630	-1.1516880	-1.6744700
C	-4.2981800	-0.1705630	-1.3969500
H	-4.7349380	-0.6897290	-2.2563020
H	-5.0320040	-0.1455570	-0.5862610
H	-4.0506390	0.8566780	-1.6765960
C	2.0396290	-1.6618370	0.0801060
H	1.8558050	-2.5839360	-0.4866330
H	1.4249440	-1.6928470	0.9845690
C	1.6596080	-0.4212420	-0.7225590
H	1.9341800	0.4738090	-0.1655210
H	2.2101320	-0.4022510	-1.6759960
C	-0.2687000	-1.3426610	-1.9646220
H	-0.1684880	-2.3164480	-1.4775180
H	0.3706480	-1.3544160	-2.8609610
C	-1.7273940	-1.0951350	-2.3507920
H	-1.8216810	-0.1270820	-2.8569530
H	-2.0877390	-1.8703310	-3.0360570
C	3.9070400	-3.3084820	1.4030810
H	3.5270620	-4.0924810	0.7375830
H	4.9415090	-3.5446290	1.6703260
H	3.3128560	-3.3083200	2.3217050
C	-3.3104820	-2.7375890	-0.5468440
H	-3.9552680	-2.7799350	0.3353090
H	-3.8533500	-3.1310420	-1.4127320
H	-2.4331430	-3.3575010	-0.3460380
C	-2.2734710	0.0654390	2.2851940
O	-2.9151050	0.0945060	3.2565880
H	0.0812720	0.5973010	-1.4666910
C	-0.8977060	2.2914150	0.6362050
H	0.0681150	0.1698840	1.7371000
H	-1.1286240	2.6299260	1.6489310
C	0.4582200	2.6514000	0.1515240
C	1.5306220	2.7468940	1.0527570
C	0.6932010	2.9123920	-1.2079680
C	2.8111420	3.0570960	0.6024510
H	1.3564710	2.5285630	2.1024920
C	1.9801380	3.2120120	-1.6606590
H	-0.1483460	2.8901450	-1.8940390
C	3.0442330	3.2796680	-0.7596970
H	3.6335130	3.1076970	1.3099290
H	2.1483660	3.4054190	-2.7167880
H	4.0455930	3.5108280	-1.1109950
N	-1.8583940	1.9746120	-0.2344620
H	-2.7712700	2.0678110	0.2084440

25

Ru	1.0616430	0.5747980	-0.2994070
H	2.0775180	1.4881420	0.7245950
N	0.5787090	-0.6897680	1.5389150
P	2.9018140	-0.8180520	-0.3569800
P	-0.6193220	1.9189920	0.5562710
C	2.8979200	-2.4619780	-1.2118950

H	2.8634120	-2.2977680	-2.2923040
H	3.7754140	-3.0691000	-0.9631660
H	1.9883730	-2.9997150	-0.9310390
C	-2.2587300	2.2162770	-0.2334360
H	-2.9484410	2.7438680	0.4342130
H	-2.1087590	2.8131580	-1.1378050
H	-2.6884070	1.2582500	-0.5245890
C	3.0343320	-1.2876370	1.4404420
H	3.7330800	-2.1167270	1.6090720
H	3.4161770	-0.3996340	1.9518630
C	1.6419460	-1.6521360	1.9646630
H	1.3550220	-2.6363030	1.5829760
H	1.6532880	-1.7342730	3.0588470
C	0.0946330	0.1852990	2.6355610
H	0.9316160	0.8170590	2.9460740
H	-0.2209010	-0.4215980	3.4987120
C	-1.0761200	1.0395110	2.1435000
H	-1.9330810	0.3961500	1.9135690
H	-1.3917050	1.7477380	2.9175080
C	4.5877640	-0.1896840	-0.7528660
H	5.3648460	-0.9238060	-0.5156870
H	4.6380080	0.0554470	-1.8174110
H	4.7502840	0.7276840	-0.1830960
C	-0.1684020	3.6190540	1.1164100
H	0.1244020	4.2104040	0.2442790
H	-0.9969220	4.1169380	1.6322560
H	0.6997650	3.5437500	1.7740630
C	1.4044950	1.5669960	-1.8280460
O	1.6111610	2.1832530	-2.7977160
H	-0.2068510	-1.2697400	1.2312160
C	-1.5729730	-2.4743860	-0.6774610
H	-1.1779640	-2.6167780	-1.6888620
H	0.0280790	-0.4311350	-1.1884000
C	-2.8024810	-1.6660450	-0.6003440
C	-3.3311780	-1.1034800	-1.7704040
C	-3.4760050	-1.4763940	0.6179140
C	-4.5121910	-0.3622690	-1.7281000
H	-2.8038000	-1.2371350	-2.7108770
C	-4.6495620	-0.7284230	0.6610800
H	-3.0693730	-1.9336350	1.5143350
C	-5.1720720	-0.1717320	-0.5119500
H	-4.9111850	0.0730700	-2.6393060
H	-5.1647000	-0.5835540	1.6063970
H	-6.0894270	0.4087130	-0.4763270
N	-1.0308380	-2.9934120	0.3634150
H	-0.2100940	-3.5362810	0.0884540

26

Ru	1.28654000	-0.44661600	-0.22838300
H	2.11836000	-0.94709100	1.15241100
N	-0.29627000	0.40884300	1.16444300
P	0.12620500	-2.41258800	0.16145700
P	2.30619900	1.59858700	0.23232300
C	-1.26316900	-2.99696000	-0.90793000
H	-0.86187000	-3.27584900	-1.88611800

H	-1.78979000	-3.85351200	-0.47254900
H	-1.96190500	-2.17019100	-1.05287300
C	2.45114200	3.00113700	-0.95963700
H	2.82887400	3.90889700	-0.47641800
H	3.13550300	2.71008900	-1.76167300
H	1.46452900	3.18874100	-1.38903300
C	-0.72144900	-1.99261800	1.76607600
H	-1.51217000	-2.70968900	2.01810100
H	0.04770000	-2.03543200	2.54347900
C	-1.29957400	-0.58035500	1.64926400
H	-2.11764400	-0.58201200	0.92656000
H	-1.72269600	-0.25112000	2.60769700
C	0.36565800	1.20493700	2.22622000
H	0.99268900	0.52946300	2.81381500
H	-0.38706200	1.65254800	2.89404500
C	1.20446700	2.30948700	1.57305200
H	0.53750900	3.02341600	1.07775600
H	1.78875200	2.85267100	2.32315800
C	1.01665300	-3.98019200	0.53796800
H	0.34035400	-4.75151300	0.92097200
H	1.49820000	-4.34590500	-0.37325700
H	1.79513700	-3.76321100	1.27231900
C	3.98555000	1.56884100	0.99407000
H	4.69768900	1.17451300	0.26367800
H	4.30768500	2.56616100	1.31199600
H	3.96495800	0.88628900	1.84582100
C	2.57529100	-1.10963200	-1.39076800
O	3.38179200	-1.52242700	-2.12414000
H	-0.79035400	1.07387400	0.56563400
H	0.31728300	0.05235200	-1.56112400
O	-0.77180700	2.26315200	-1.14765700
H	-0.25944600	1.42711000	-1.34458900
C	-2.02231300	2.16923900	-1.82099700
H	-1.89856900	1.73032200	-2.82042100
H	-2.38689000	3.19480900	-1.95488900
C	-3.03852800	1.36801800	-1.02991300
C	-3.49326500	1.84937400	0.20662100
C	-3.50930800	0.13096500	-1.48294700
C	-4.40197800	1.11539000	0.96885000
H	-3.12558100	2.80650300	0.56866300
C	-4.42216700	-0.60811000	-0.72394000
H	-3.15334400	-0.25803000	-2.43337900
C	-4.87074700	-0.11745400	0.50377900
H	-4.74739200	1.50359100	1.92303700
H	-4.77827500	-1.56668700	-1.09084700
H	-5.57959500	-0.69009500	1.09482900

27

Ru	-1.12726200	0.49394600	-0.32049100
H	-2.16951900	1.04055900	0.76553800
N	-0.02760300	-0.47511600	1.30380200
P	0.07507800	2.38197300	0.38979600
P	-2.39876000	-1.46086700	-0.01151500
C	1.62879600	2.90021800	-0.45997400
H	1.39095600	3.24267900	-1.47113100

H	2.13281800	3.70567300	0.08460200
H	2.29984400	2.04069700	-0.53916800
C	-2.21380600	-2.93430900	-1.10088500
H	-2.85411100	-3.75821500	-0.76847400
H	-2.46587700	-2.67136800	-2.13170100
H	-1.16612000	-3.23982200	-1.03889000
C	0.64397400	1.82600300	2.05933000
H	1.46788200	2.44304900	2.43981600
H	-0.20797200	1.92096300	2.74149400
C	1.03623600	0.34401800	1.88571700
H	1.91405300	0.29318900	1.22992200
H	1.35761100	-0.06638300	2.85604900
C	-0.94882300	-1.00799900	2.31211600
H	-1.58002400	-0.22983700	2.77625900
H	-0.38163000	-1.48509400	3.12937700
C	-1.84848400	-2.07174000	1.66000100
H	-1.27048900	-2.98299500	1.48442100
H	-2.71326300	-2.32012700	2.28390200
C	-0.79979900	3.97957900	0.65134400
H	-0.15834500	4.70802800	1.15726400
H	-1.11302000	4.38545000	-0.31463100
H	-1.69388700	3.79497200	1.25123700
C	-4.22438100	-1.24788400	0.11175800
H	-4.61660500	-0.91723200	-0.85399300
H	-4.71791700	-2.18064800	0.40269400
H	-4.43611400	-0.47090900	0.84994700
C	-2.17704500	1.32495100	-1.66302900
O	-2.85773400	1.86178200	-2.43773000
H	0.60984900	-1.85245800	0.58828300
H	-0.10974200	-0.47859600	-1.56328600
O	0.88158000	-2.76625500	0.22101900
H	0.38309300	0.12641100	-1.38427900
C	1.68529700	-2.60612000	-0.92235700
H	2.10964000	-3.59269300	-1.16012500
H	1.09771500	-2.30700900	-1.80980800
C	2.82029500	-1.61619000	-0.73081800
C	3.15096200	-0.67783700	-1.71385700
C	3.55508200	-1.62995400	0.46242400
C	4.19798400	0.22768300	-1.51514700
H	2.58314300	-0.65196000	-2.64118400
C	4.59785700	-0.72754000	0.66671500
H	3.27330000	-2.33956700	1.23440300
C	4.92276300	0.20688300	-0.32200600
H	4.44122200	0.95140000	-2.28848900
H	5.15587100	-0.74766600	1.59899600
H	5.73341200	0.91232700	-0.16258300

28

Ru	-1.76096900	0.36897600	-0.18791100
H	-2.83796100	0.91294800	0.89358100
N	-0.55595700	-0.39946800	1.55583900
P	-0.47858200	2.27561100	0.23159900
P	-2.67759600	-1.77591700	-0.10857300
C	0.84752800	2.74232300	-0.96060300
H	0.39830800	3.12295700	-1.88220600

H	1.52049700	3.50039300	-0.54704600
H	1.41054900	1.83290500	-1.18433700
C	-2.49417600	-2.83982800	-1.59452800
H	-2.61839900	-3.90340900	-1.36782900
H	-3.22969100	-2.54101800	-2.34671700
H	-1.49246400	-2.63356800	-1.98095700
C	0.49089200	1.81836800	1.76140200
H	1.46150100	1.45316900	1.41337200
H	0.64966600	2.68430500	2.41224300
C	-0.22259100	0.68696500	2.50804000
H	0.42107500	0.30457500	3.31479700
H	-1.15780800	1.03816400	2.95594200
C	-1.16854600	-1.57506100	2.21130400
H	-2.04435300	-1.22871300	2.77158200
H	-0.46835600	-2.02240900	2.93290700
C	-1.58174100	-2.60295200	1.15475100
H	-0.69479500	-2.95453100	0.61493500
H	-2.06587800	-3.47263800	1.61236900
C	-1.28374700	3.88121300	0.63968900
H	-0.55302700	4.63786400	0.94354100
H	-1.83238900	4.23833200	-0.23634900
H	-2.00399900	3.71548300	1.44451800
C	-4.38622900	-2.10373500	0.49637400
H	-5.10109500	-1.65863100	-0.20107300
H	-4.58939700	-3.17546200	0.59010400
H	-4.51669700	-1.61649900	1.46598900
C	-2.83337100	1.06568400	-1.53578600
O	-3.52140900	1.51513300	-2.36261600
H	0.33580400	-0.68132200	1.10846600
O	-0.16932300	-0.60276300	-1.46332200
H	-0.08972200	-0.08412400	-2.27165200
O	1.76351600	-0.49331800	0.00477300
H	0.96921800	-0.53311000	-0.73134500
C	2.72083500	-1.48536400	-0.25988100
H	2.66152500	-2.30075500	0.48387900
H	2.52369000	-1.95840900	-1.23747700
C	4.14355200	-0.95040900	-0.26022800
C	5.22630000	-1.83962500	-0.29031100
C	4.40150200	0.42270400	-0.24443200
C	6.53796600	-1.36748400	-0.31108600
H	5.03821800	-2.91185500	-0.29553800
C	5.71488800	0.89964100	-0.26246600
H	3.56108700	1.10716300	-0.21428000
C	6.78769800	0.00811200	-0.29686400
H	7.36623800	-2.07084000	-0.33399700
H	5.89976500	1.97084300	-0.24869600
H	7.80903900	0.37841800	-0.30985000

29

Ru	-1.34338700	-0.64266700	-0.06251300
H	-2.16778400	-1.19492700	1.22047300
N	-0.05907300	0.58823900	1.41899100
P	-2.63310800	1.31098600	0.03098700
P	0.35444300	-2.20963100	0.29743800
C	-2.68168300	2.43551900	-1.42867900

H	-3.21411100	1.94740700	-2.24974800
H	-3.17207200	3.38582200	-1.19403300
H	-1.64635600	2.62184300	-1.72633100
C	1.34605700	-2.74984600	-1.15095600
H	2.31500400	-3.16502800	-0.85715000
H	0.78369400	-3.49607800	-1.71919000
H	1.47586900	-1.85678000	-1.76689100
C	-1.76410000	2.36227000	1.31278400
H	-1.10857900	3.03691500	0.75448100
H	-2.47870200	2.95827100	1.89021300
C	-0.90551300	1.48844400	2.23294800
H	-0.28104500	2.12649900	2.87754600
H	-1.53126100	0.86538700	2.88044700
C	0.84594800	-0.25565300	2.22697000
H	0.23662400	-0.78235400	2.97052800
H	1.57321000	0.36759200	2.76880200
C	1.57876100	-1.24928700	1.32415000
H	2.21237700	-0.70387100	0.62126800
H	2.22469600	-1.91384300	1.90808200
C	-4.38805700	1.24492100	0.58866900
H	-4.81694500	2.24510200	0.70911100
H	-4.97501700	0.68469100	-0.14448000
H	-4.43091800	0.70568100	1.53808900
C	0.06185500	-3.75066700	1.26434100
H	-0.63232900	-4.39179300	0.71425800
H	0.99130900	-4.29792900	1.45291500
H	-0.40827300	-3.48388300	2.21430800
C	-2.44375600	-1.66625200	-1.14850500
O	-3.14819200	-2.31659600	-1.81289600
H	0.85335978	1.57913927	0.36557604
O	0.10170800	0.22686200	-1.70853000
H	-0.44531000	0.32824000	-2.49687500
O	0.70373400	2.35190200	-0.64960800
H	0.34441087	1.11257199	-1.33878260
C	2.00648100	2.74598000	-1.02711100
H	2.05727700	2.95229800	-2.10948100
H	2.24604700	3.68606500	-0.51175800
C	3.05022700	1.69931500	-0.67821100
C	3.76249600	1.76136400	0.52583900
C	3.27041300	0.61049400	-1.53375500
C	4.68702700	0.76939800	0.86456100
H	3.59509800	2.59891900	1.19965700
C	4.19698800	-0.37931300	-1.20356500
H	2.67800600	0.52762100	-2.43920300
C	4.91102000	-0.30098100	-0.00405500
H	5.23593400	0.83591700	1.80005700
H	4.35701500	-1.21604500	-1.87786100
H	5.63352200	-1.07057800	0.25299900

30

Ru	-1.6587890	-0.1183470	-0.3537590
H	-3.1435210	-0.2946410	0.2932890
N	-0.9031500	0.0741130	1.7603390
P	-1.8499840	2.1923700	-0.1482800
P	-1.1833010	-2.3694560	0.0123860

C	-0.7342110	3.2523940	-1.1618080
H	-1.1237950	3.3158310	-2.1819390
H	-0.6262070	4.2624790	-0.7542440
H	0.2336830	2.7446910	-1.1911140
C	0.1713410	-3.0858600	-1.0008640
H	0.6389270	-3.9576800	-0.5329170
H	-0.2205540	-3.3672710	-1.9825360
H	0.8854040	-2.2668310	-1.1310740
C	-1.2581030	2.4996320	1.5987840
H	-0.1822300	2.6969270	1.5443250
H	-1.7408970	3.3768050	2.0428290
C	-1.4934630	1.2458360	2.4460670
H	-1.0449660	1.3739910	3.4432660
H	-2.5646530	1.0597620	2.5766970
C	-1.0677740	-1.1795810	2.5281630
H	-2.1394370	-1.3336780	2.6947520
H	-0.5817860	-1.0953770	3.5124900
C	-0.4752680	-2.3521980	1.7420400
H	0.6069520	-2.2177490	1.6405580
H	-0.6447020	-3.3019760	2.2607620
C	-3.4750480	3.0562010	-0.2323760
H	-3.3880280	4.1220700	0.0025340
H	-3.8882470	2.9388590	-1.2380160
H	-4.1605080	2.5761770	0.4705050
C	-2.4758440	-3.6809020	0.0700910
H	-2.9302260	-3.7758220	-0.9200010
H	-2.0622880	-4.6483720	0.3728730
H	-3.2568810	-3.3759330	0.7711740
C	-2.4119030	-0.3020550	-2.0403950
O	-2.9069820	-0.4231220	-3.0898900
H	0.1153700	0.2734510	1.6783490
O	0.5021720	0.1005290	-0.9208200
H	0.5230990	0.4135410	-1.8322210
H	1.4720620	0.7531760	0.3382150
N	1.8843970	0.8456570	1.2930750
H	2.2787980	1.7804610	1.3794310
C	2.9607290	-0.1465410	1.4311530
H	3.3449680	-0.1288870	2.4587980
H	2.5040060	-1.1333060	1.2839530
C	4.1112370	0.0126400	0.4516980
C	5.4162330	0.2533600	0.8934340
C	3.8651820	-0.0654180	-0.9286330
C	6.4628430	0.4121840	-0.0197450
H	5.6165960	0.3169160	1.9610680
C	4.9080810	0.0918250	-1.8399690
H	2.8453830	-0.2366790	-1.2677260
C	6.2108170	0.3309200	-1.3892530
H	7.4712420	0.5999740	0.3394180
H	4.7072880	0.0267610	-2.9062680
H	7.0217660	0.4536210	-2.1019550

Heam

O	-1.4041440	2.6189120	0.3868070
H	0.6447520	1.5463600	1.5492520
C	-1.2862350	1.3306350	1.0087990

H	-1.5683930	1.4184230	2.0706770
C	-2.1872480	0.2821880	0.3607680
C	-2.8518770	0.5238470	-0.8436850
C	-2.3349540	-0.9627600	0.9852200
C	-3.6632530	-0.4615880	-1.4135240
H	-2.7180610	1.4802970	-1.3385670
C	-3.1432880	-1.9463740	0.4189880
H	-1.8012680	-1.1559250	1.9118880
C	-3.8126050	-1.6969000	-0.7835770
H	-4.1734360	-0.2632690	-2.3520590
H	-3.2516710	-2.9082130	0.9124410
H	-4.4435420	-2.4628770	-1.2253800
H	-2.3173030	2.9205330	0.4896260
N	0.0877030	0.9033250	0.9922090
C	0.6954660	0.7564910	-0.3367220
H	0.0586470	0.0711790	-0.9096210
H	0.7181680	1.7021220	-0.8974680
C	2.0917920	0.1795820	-0.2355720
C	3.1303820	0.6799620	-1.0285150
C	2.3602400	-0.8864510	0.6342960
C	4.4098860	0.1231860	-0.9649570
H	2.9355080	1.5131260	-1.6997950
C	3.6376300	-1.4416440	0.7029380
H	1.5573580	-1.2633310	1.2602220
C	4.6672490	-0.9398360	-0.0982220
H	5.2053180	0.5246210	-1.5869000
H	3.8314930	-2.2677060	1.3819780
H	5.6625570	-1.3719390	-0.0436240

aldehyde

C	1.7384460	1.0582450	-0.0000210
C	0.3640540	1.2944250	-0.0000060
C	-0.5333460	0.2185370	0.0000210
C	-0.0491050	-1.0988620	0.0000310
C	1.3217790	-1.3333050	0.0000100
C	2.2154860	-0.2549350	-0.0000150
H	2.4353310	1.8910210	-0.0000410
H	-0.0184510	2.3127720	-0.0000130
H	-0.7677400	-1.9124460	0.0000540
H	1.7004770	-2.3511730	0.0000150
H	3.2858960	-0.4404290	-0.0000300
C	-1.9923330	0.4714460	0.0000450
O	-2.8436700	-0.3977030	-0.0000710
H	-2.2760450	1.5485660	0.0001910

pimi

C	-1.7470460	-1.0598500	-0.0000110
C	-0.3704520	-1.2828550	0.0000070
C	0.5318160	-0.2083490	0.0000180
C	0.0222060	1.1003330	0.0000240
C	-1.3511160	1.3257700	0.0000090
C	-2.2403810	0.2458130	-0.0000100
H	-2.4326760	-1.9021270	-0.0000230
H	0.0144920	-2.2997840	0.0000080
H	0.7024690	1.9480500	0.0000480

H	-1.7320150	2.3428990	0.0000160
H	-3.3117870	0.4239110	-0.0000210
C	1.9858130	-0.5020650	0.0000230
H	2.2252890	-1.5724840	0.0001430
N	2.9818250	0.2958640	-0.0000550
H	2.6764110	1.2757050	-0.0001490

amide

C	-3.4607290	-1.5802730	-0.1881090
C	-2.4556420	-0.8331920	-0.8034810
C	-1.9909780	0.3480960	-0.2083620
C	-2.5593080	0.7839970	0.9957250
C	-3.5508670	0.0285520	1.6174590
C	-4.0019010	-1.1558430	1.0273600
H	-3.8247310	-2.4884510	-0.6596720
H	-2.0480480	-1.1484930	-1.7590850
H	-2.2144330	1.7197980	1.4231000
H	-3.9785350	0.3650620	2.5573750
H	-4.7798000	-1.7412640	1.5091820
C	-0.9627680	1.2289400	-0.8547220
O	-1.0445660	2.4518320	-0.7881170
N	0.0526580	0.6222260	-1.5733660
H	0.6595460	1.3279140	-1.9781650
C	0.7416850	-0.6112030	-1.1984780
H	0.0494900	-1.2248290	-0.6163860
H	0.9770320	-1.1833620	-2.1042930
C	2.0131480	-0.3871320	-0.3927410
C	3.0380070	-1.3405270	-0.4430000
C	2.1722770	0.7363410	0.4279490
C	4.1952790	-1.1836480	0.3195200
H	2.9289070	-2.2112750	-1.0859590
C	3.3333010	0.8965870	1.1876140
H	1.3949460	1.4934300	0.4684550
C	4.3464300	-0.0619710	1.1382340
H	4.9817680	-1.9313530	0.2681350
H	3.4449880	1.7745920	1.8174910
H	5.2491880	0.0656550	1.7285190

imine

N	-0.1431270	1.6029790	0.0000140
C	-0.5292980	0.3879710	0.0001420
H	0.1715670	-0.4586240	0.0001340
C	-1.9577250	0.0206860	0.0000530
C	-2.3171780	-1.3348040	0.0000740
C	-2.9688420	0.9966430	-0.0000420
C	-3.6602370	-1.7131820	0.0000090
H	-1.5381020	-2.0937230	0.0001470
C	-4.3075240	0.6186140	-0.0001100
H	-2.6776410	2.0418730	-0.0000550
C	-4.6577840	-0.7370090	-0.0000860
H	-3.9271820	-2.7661210	0.0000300
H	-5.0838690	1.3786380	-0.0001800
H	-5.7043510	-1.0285050	-0.0001380
C	1.2848010	1.9313750	-0.0000680
H	1.4543390	2.5732760	-0.8745250

H	1.4543980	2.5733820	0.8742990
C	2.2800290	0.7889300	-0.0000310
C	2.7282460	0.2317180	1.2047860
C	2.7281000	0.2315160	-1.2048090
C	3.6124630	-0.8481220	1.2077830
H	2.3820050	0.6514180	2.1464410
C	3.6123160	-0.8483240	-1.2077320
H	2.3817450	0.6510590	-2.1464920
C	4.0575550	-1.3903420	0.0000440
H	3.9557930	-1.2641670	2.1508590
H	3.9555320	-1.2645280	-2.1507800
H	4.7481300	-2.2288410	0.0000730

TSA

Ru	1.3502340	0.4444900	-0.1445280
H	2.3912080	0.9698690	0.9307000
N	-0.0492770	-0.6169450	1.2171710
P	2.4358020	-1.6158750	-0.0144710
P	0.0115060	2.2568800	0.5073340
C	1.8999710	-2.9238770	-1.1950980
H	2.3583630	-2.7314220	-2.1692200
H	2.1778930	-3.9261930	-0.8536740
H	0.8171840	-2.8329260	-1.3111260
C	-0.8352590	3.4433650	-0.6253950
H	-1.5118400	4.1059200	-0.0756990
H	-0.0829550	4.0464600	-1.1412730
H	-1.4035920	2.8886890	-1.3756410
C	1.8457030	-2.2081060	1.6414470
H	2.0794580	-3.2681120	1.8050550
H	2.4012480	-1.6134040	2.3750420
C	0.3400460	-1.9246010	1.7808740
H	-0.2227750	-2.7288810	1.2790870
H	0.0713230	-1.9826840	2.8442960
C	-0.8731670	0.1825390	2.1285730
H	-0.3017430	0.4681620	3.0279590
H	-1.7428080	-0.3989200	2.4755250
C	-1.3873450	1.4421420	1.4205290
H	-2.1357470	1.1613880	0.6731120
H	-1.8589560	2.1361400	2.1253500
C	4.2644380	-1.8055030	0.0612420
H	4.5535120	-2.8320790	0.3079430
H	4.6932940	-1.5339820	-0.9072510
H	4.6596900	-1.1204360	0.8152540
C	0.7525590	3.3862460	1.7632700
H	1.5936100	3.9222130	1.3160170
H	0.0186350	4.1046230	2.1432760
H	1.1382340	2.7805650	2.5868120
C	2.4000790	1.2738870	-1.4550560
O	3.0628290	1.7914330	-2.2617840
O	-0.5210670	-0.8513540	-1.1762670
H	-0.5641510	-0.7969760	-0.0187970
C	-1.6474610	-0.3390530	-1.8418100
H	-1.6999620	-0.7889740	-2.8469170
H	-1.5647350	0.7480250	-2.0074320
C	-2.9515350	-0.6175180	-1.1093100

C	-3.0908070	-1.7643060	-0.3172630
C	-4.0337010	0.2659260	-1.2082540
C	-4.2806360	-2.0179480	0.3656000
H	-2.2507570	-2.4465010	-0.2345720
C	-5.2284050	0.0126000	-0.5310700
H	-3.9353890	1.1650940	-1.8133190
C	-5.3546380	-1.1303510	0.2612870
H	-4.3703440	-2.9094670	0.9806530
H	-6.0560450	0.7119030	-0.6140260
H	-6.2799400	-1.3253970	0.7959750

TSB

Ru	1.3289750	-0.2715640	0.6309210
H	1.0619430	1.1060090	1.4008200
N	-0.0269420	0.3779900	-1.0936380
P	-3.3680220	2.1429040	0.7159640
P	2.9450660	0.7746080	-0.6490120
C	-4.1445550	2.8223320	-0.8405580
H	-5.1448570	3.2030550	-0.6121680
H	-3.5519370	3.6337660	-1.2800170
H	-4.2553720	2.0240540	-1.5805710
C	4.5018570	-0.1007690	-1.1013720
H	5.0586330	0.4280140	-1.8818960
H	5.1304570	-0.1914340	-0.2110780
H	4.2482180	-1.1077160	-1.4422280
C	-1.6046360	1.9289320	0.1211950
H	-1.2722140	2.8552080	-0.3654260
H	-0.9790960	1.7726790	1.0058400
C	-1.4468870	0.7200580	-0.7973730
H	-1.8873020	-0.1575080	-0.3245890
H	-1.9817740	0.8859710	-1.7454060
C	0.6121590	1.3619630	-2.0026470
H	0.5671200	2.3399100	-1.5153540
H	0.0460010	1.4387830	-2.9433290
C	2.0699910	0.9903970	-2.2783230
H	2.1233810	0.0261270	-2.7974660
H	2.5512290	1.7434620	-2.9122790
C	-3.1295760	3.7434140	1.6417220
H	-2.6315570	4.5068140	1.0325200
H	-4.1014350	4.1293320	1.9639380
H	-2.5267010	3.5588360	2.5358570
C	3.5314780	2.4731010	-0.2376550
H	4.0758760	2.4390050	0.7099270
H	4.1819210	2.8836830	-1.0169010
H	2.6631580	3.1219560	-0.0985010
C	2.4449020	-0.6893170	2.0504920
O	3.1546200	-0.9056540	2.9475450
O	1.0934510	-2.2460710	-0.4456930
H	-0.0249550	-0.5316090	-1.5618690
C	0.2109880	-2.3720680	0.4932510
H	-0.0332040	-1.0194750	1.3452260
H	0.4917230	-2.9313440	1.4011150
C	-1.2386300	-2.5456330	0.1026650
C	-2.2642510	-2.4821680	1.0540260
C	-1.5590780	-2.7767750	-1.2393220

C	-3.5947400	-2.6160800	0.6635140
H	-2.0160040	-2.2871830	2.0945420
C	-2.8927770	-2.9143770	-1.6313640
H	-0.7491140	-2.8514190	-1.9581400
C	-3.9128680	-2.8270260	-0.6829690
H	-4.3856170	-2.5438830	1.4042180
H	-3.1341900	-3.0921940	-2.6758110
H	-4.9511200	-2.9247840	-0.9868310

TSC

Ru	1.7971540	0.1010930	-0.5128170
H	3.1680130	-0.7335010	-0.6416300
N	1.0646440	-1.3438690	1.0263340
P	0.9540030	-1.4914980	-1.9788830
P	2.8433370	0.9757960	1.3733750
C	-0.7783910	-1.2841050	-2.5665500
H	-0.7922810	-0.5040890	-3.3335220
H	-1.1941540	-2.2092790	-2.9782720
H	-1.3808190	-0.9382200	-1.7258880
C	2.3004980	2.5182140	2.2445140
H	2.7598840	2.6179830	3.2336230
H	2.5768280	3.3821650	1.6330100
H	1.2120890	2.5145380	2.3434930
C	0.9183560	-2.9872970	-0.8850240
H	0.3116980	-3.7975640	-1.3090190
H	1.9537280	-3.3348670	-0.7979820
C	0.3774320	-2.5285550	0.4783750
H	-0.6811420	-2.2755860	0.3561260
H	0.4095000	-3.3647390	1.1926500
C	2.1417360	-1.6636150	1.9731210
H	2.9918930	-2.1511980	1.4744220
H	1.7803540	-2.3595960	2.7497550
C	2.6143620	-0.3674500	2.6558010
H	1.8490890	-0.0242140	3.3601570
H	3.5373600	-0.5222410	3.2244740
C	1.8630000	-2.0315340	-3.4855120
H	1.3962610	-2.9081160	-3.9461750
H	1.8823950	-1.2124450	-4.2098640
H	2.8932170	-2.2661340	-3.2070340
C	4.6696010	1.2218290	1.3020490
H	4.8986800	2.0178690	0.5880910
H	5.0848950	1.4811910	2.2814980
H	5.1250920	0.2983870	0.9375600
C	2.4513200	1.3141790	-1.7772710
O	2.8712890	2.0614040	-2.5685420
O	-0.2842030	1.0052370	-0.2747800
H	-0.5899110	0.7513760	0.8095680
C	-0.5607200	2.3592260	-0.5689950
H	-0.1241070	2.6038090	-1.5454100
H	-0.1000500	3.0393530	0.1693020
C	-2.0603210	2.5624920	-0.5943710
C	-2.7482190	2.9842850	0.5491070
C	-2.7996040	2.1960620	-1.7268910
C	-4.1441340	3.0337810	0.5673820
H	-2.1830490	3.2586630	1.4367910

C	-4.1938090	2.2441140	-1.7156050
H	-2.2718160	1.8551420	-2.6140100
C	-4.8704740	2.6603330	-0.5651190
H	-4.6638270	3.3583570	1.4646550
H	-4.7540600	1.9553930	-2.6007940
H	-5.9561060	2.6926400	-0.5523480
N	-0.6922260	0.2534300	2.0527170
H	-0.2403560	0.8799410	2.7169680
H	0.1358410	-0.6339550	1.6773640
C	-2.0247550	-0.1044870	2.5649730
H	-1.9674330	-0.4742740	3.5996840
H	-2.6769660	0.7824790	2.5799190
C	-2.6690740	-1.1644740	1.7003670
C	-3.1764400	-0.8286180	0.4379110
C	-2.7229570	-2.4997070	2.1152090
C	-3.7077020	-1.8119350	-0.3966530
H	-3.1412210	0.2020700	0.1060470
C	-3.2559530	-3.4869310	1.2828930
H	-2.3295220	-2.7703680	3.0922050
C	-3.7443740	-3.1456480	0.0204570
H	-4.0922450	-1.5333620	-1.3739410
H	-3.2856790	-4.5200340	1.6182910
H	-4.1568440	-3.9111580	-0.6309890

TSD

Ru	-0.92730300	0.55754700	-0.34392900
H	-2.01497400	1.60567500	0.39057000
N	-0.45056500	-0.29663800	1.69478000
P	0.61349500	2.16284900	0.30439800
P	-2.64571000	-1.00673900	-0.19178400
C	2.41857000	2.04631500	-0.06811200
H	2.56924400	2.17854100	-1.14262700
H	2.99610800	2.80336700	0.47372800
H	2.78058700	1.05033100	0.19272800
C	-2.64146900	-2.61742600	-1.09295800
H	-3.49343800	-3.24424100	-0.80830400
H	-2.67462100	-2.43155000	-2.16985700
H	-1.71000600	-3.13038300	-0.84225500
C	0.54958000	1.95974400	2.15511800
H	1.37849500	2.47216000	2.65837400
H	-0.39039700	2.41173300	2.48655300
C	0.56870400	0.46210900	2.47326100
H	1.54533200	0.04875300	2.20357300
H	0.42984500	0.29107000	3.54945700
C	-1.71051800	-0.58350700	2.42562600
H	-2.23765000	0.36073900	2.58284300
H	-1.48942000	-1.02602200	3.40930600
C	-2.55381400	-1.55979400	1.59739100
H	-2.06473400	-2.53924100	1.59216700
H	-3.55264700	-1.67832800	2.02935300
C	0.28083400	3.95675200	0.05385600
H	0.98022600	4.58173700	0.61871200
H	0.37114700	4.19068000	-1.01057900
H	-0.74542100	4.16514500	0.36365200
C	-4.38371600	-0.43141100	-0.40906200

H	-4.52935300	-0.13142600	-1.45063000
H	-5.10751700	-1.21223800	-0.15284200
H	-4.53775600	0.44788100	0.21992000
C	-1.30266200	1.20364100	-2.04574700
O	-1.53174400	1.60313400	-3.11728200
O	0.36586000	-2.72938000	0.45837900
H	-0.03817900	-1.20805600	1.45314900
C	0.92725100	-2.25897500	-0.54857500
H	0.20542400	-0.59019100	-0.94765900
H	0.54909900	-2.48583200	-1.55906600
C	2.32152900	-1.72445600	-0.50227300
C	2.93674800	-1.22813200	-1.65816900
C	3.03919400	-1.76441000	0.69946400
C	4.24761500	-0.76096600	-1.60999900
H	2.36870200	-1.18577500	-2.58396500
C	4.35024300	-1.28881200	0.75102000
H	2.55559700	-2.18686600	1.57485000
C	4.95595500	-0.78390600	-0.40296800
H	4.71786100	-0.37047000	-2.50792800
H	4.90304600	-1.32052500	1.68588200
H	5.97675700	-0.41452200	-0.36492700

TSE

Ru	-0.0053750	0.4269960	-0.1564190
H	0.0198500	0.4850750	1.4570150
N	0.0020810	-1.7804580	-0.3981460
P	2.2834570	0.0870040	0.1279730
P	-2.3032140	0.0406590	0.0745840
C	3.4766390	0.1908150	-1.2777990
H	3.5525280	1.2300830	-1.6091630
H	4.4700790	-0.1724740	-0.9931100
H	3.0943540	-0.4021910	-2.1117000
C	-3.5746930	0.7031170	-1.0861370
H	-4.5592530	0.2597220	-0.9041190
H	-3.6418910	1.7879730	-0.9657780
H	-3.2594330	0.4913870	-2.1109000
C	2.3017210	-1.7121280	0.5936140
H	3.3118810	-2.1391530	0.5453740
H	1.9451410	-1.7676100	1.6281420
C	1.3092000	-2.4277350	-0.3449080
H	1.7467760	-2.4486500	-1.3575160
H	1.2051210	-3.4780350	-0.0378600
C	-1.0945520	-2.4500000	0.2793910
H	-1.0007200	-2.3943030	1.3816830
H	-1.1260940	-3.5216540	0.0183890
C	-2.4249940	-1.8054670	-0.1400750
H	-2.5928330	-1.9864380	-1.2078140
H	-3.2737360	-2.2174380	0.4166350
C	3.1967820	0.9410640	1.4791110
H	4.1990980	0.5221750	1.6144270
H	3.2813370	2.0049870	1.2407540
H	2.6240110	0.8423970	2.4036410
C	-3.0628210	0.3584900	1.7227620
H	-3.0275710	1.4301330	1.9358330
H	-4.1003150	0.0104990	1.7620780

H	-2.4692230	-0.1565920	2.4811440
C	-0.0285650	2.3048110	-0.1862890
O	-0.0367930	3.4686220	-0.2014490
H	-0.1260640	-0.9114080	-1.5503340
H	-0.0527480	-0.0748130	-2.0321350

TSF

Ru	-1.3406560	0.0120240	0.4643720
H	-2.9159980	-0.0092980	0.0365730
N	-0.8281040	-0.0176700	-1.7126310
P	-1.5746570	-2.2723660	0.1220420
P	-1.5346260	2.2828130	-0.0072630
C	-0.1853820	-3.4612420	0.4043130
H	0.0419680	-3.4976400	1.4731740
H	-0.4279050	-4.4685200	0.0486680
H	0.7043480	-3.0973830	-0.1157530
C	-0.3383000	3.5679980	0.5763200
H	-0.5094390	4.5377200	0.0965620
H	-0.4366440	3.6806000	1.6597010
H	0.6800210	3.2310110	0.3648270
C	-1.8334810	-2.3325420	-1.7135000
H	-1.7300090	-3.3486140	-2.1171740
H	-2.8563470	-1.9850030	-1.8934540
C	-0.8212400	-1.3470780	-2.3304950
H	0.1834480	-1.7884870	-2.2149020
H	-0.9935430	-1.2793710	-3.4164900
C	-1.6406110	0.9535390	-2.4430080
H	-2.7226060	0.7376900	-2.3890990
H	-1.3745410	0.9614330	-3.5154970
C	-1.3811200	2.3538750	-1.8663470
H	-0.3527350	2.6594150	-2.0942640
H	-2.0532160	3.1086920	-2.2892230
C	-3.0086160	-3.1838980	0.8334020
H	-3.0954080	-4.1925190	0.4164590
H	-2.8919330	-3.2523380	1.9185960
H	-3.9166970	-2.6146260	0.6227670
C	-3.1520210	3.0937330	0.3481420
H	-3.3256180	3.0886020	1.4277340
H	-3.1835330	4.1235140	-0.0228520
H	-3.9398530	2.5026010	-0.1236470
C	-1.8184800	0.0690640	2.2799400
O	-2.1404780	0.0996620	3.3993760
H	0.7356610	0.3934540	-1.5243650
H	0.4309040	-0.0058850	0.9309970
N	1.6754610	0.5356210	-0.9717460
H	2.0337450	1.4842600	-1.0509900
C	2.7140160	-0.4699300	-1.2291760
H	2.9735280	-0.5151600	-2.2953320
H	2.2733480	-1.4416200	-0.9709320
C	3.9562730	-0.2317730	-0.3977930
C	5.2154330	-0.1262960	-0.9972140
C	3.8539760	-0.1077770	0.9961810
C	6.3574470	0.0939860	-0.2226540
H	5.3038660	-0.2167260	-2.0774010
C	4.9922290	0.1145400	1.7698740

H	2.8791490	-0.1861750	1.4707210
C	6.2477900	0.2155040	1.1626660
H	7.3288090	0.1741970	-0.7025550
H	4.9007180	0.2071670	2.8484120
H	7.1335370	0.3889080	1.7671040
H	0.9959500	0.3012040	0.1492960

TSG

Ru	1.2550290	-0.1030110	-0.3759760
H	2.7871310	-0.4004460	0.0955530
N	0.3940320	0.1703380	1.6561960
P	1.1036150	-2.3585600	0.2237630
P	1.8124080	2.1395980	-0.0862890
C	-0.3125120	-3.5205170	-0.0670920
H	-0.4864570	-3.6294460	-1.1409250
H	-0.1060530	-4.5047150	0.3667540
H	-1.2219100	-3.1193170	0.3868020
C	1.2610260	3.4974830	-1.2096240
H	1.4611080	4.4857210	-0.7827620
H	1.7869040	3.4049880	-2.1639920
H	0.1896480	3.3968610	-1.4017730
C	1.1072130	-2.1924010	2.0775700
H	0.8384560	-3.1327560	2.5761130
H	2.1293870	-1.9237850	2.3633590
C	0.1438600	-1.0512420	2.4437150
H	-0.8895280	-1.3822530	2.2588350
H	0.2095120	-0.8410450	3.5198700
C	0.9246980	1.3017380	2.4209630
H	1.9323270	1.0763090	2.8041070
H	0.2920280	1.5164180	3.2981800
C	0.9755770	2.5506900	1.5291830
H	-0.0463580	2.8576690	1.2774870
H	1.4632590	3.3897590	2.0373600
C	2.5391050	-3.4520050	-0.1484150
H	2.4849370	-4.3940520	0.4067440
H	2.5572620	-3.6686290	-1.2203180
H	3.4551720	-2.9159380	0.1069760
C	3.5817350	2.5629350	0.2004790
H	4.1523120	2.3425630	-0.7054840
H	3.7101370	3.6168150	0.4686460
H	3.9628970	1.9249470	1.0008850
C	1.7517190	-0.2978010	-2.1657000
O	2.0490320	-0.4221560	-3.2863290
N	-0.9453350	0.4882580	-0.4184600
H	-1.0928540	1.4486990	-0.7262210
C	-2.0019440	-0.3311420	-0.9942920
H	-1.8143890	-1.3707900	-0.7038300
H	-1.9677230	-0.3315540	-2.0957870
C	-3.4171360	0.0330960	-0.5568120
C	-4.5118440	-0.2918160	-1.3695340
C	-3.6628530	0.6594150	0.6711830
C	-5.8169220	-0.0077410	-0.9660410
H	-4.3361570	-0.7703860	-2.3309810
C	-4.9670440	0.9490370	1.0783110
H	-2.8192810	0.9249230	1.3014220

C	-6.0498600	0.6154790	0.2624840
H	-6.6516120	-0.2655560	-1.6127210
H	-5.1379830	1.4373460	2.0344390
H	-7.0645500	0.8427230	0.5775050
H	-0.5412610	0.4176840	0.8728220

TSH

Ru	1.60202900	0.33601100	-0.21676500
H	3.18385000	0.70052500	0.05570300
N	1.82935200	-1.23167100	1.54922400
P	2.52172800	-1.44387600	-1.40700100
P	1.18282400	1.74582600	1.61683400
C	1.48195700	-2.72540400	-2.23251200
H	0.91542000	-2.25961300	-3.04427100
H	2.08938200	-3.54147200	-2.63902400
H	0.76642800	-3.13416700	-1.51568200
C	-0.48185200	2.45191100	1.98043800
H	-0.48586200	2.99530800	2.93172700
H	-0.76754900	3.13084700	1.17225700
H	-1.22498600	1.65244200	2.02781100
C	3.41147200	-2.36954000	-0.06006300
H	3.75414500	-3.35454900	-0.40195600
H	4.29377000	-1.76709800	0.18085800
C	2.49741400	-2.49741700	1.16915500
H	1.71841400	-3.23877100	0.95033700
H	3.07514100	-2.89975200	2.01358100
C	2.41530500	-0.54156200	2.71044100
H	3.43263300	-0.20102800	2.47453500
H	2.48610600	-1.22233200	3.57464200
C	1.53327500	0.65488500	3.09531400
H	0.56278400	0.28919800	3.44957200
H	1.98538600	1.23612100	3.90659800
C	3.82598700	-1.12954500	-2.66522500
H	4.33545300	-2.05148300	-2.96520400
H	3.37320300	-0.66912000	-3.54877600
H	4.55314500	-0.42625500	-2.25127000
C	2.28211100	3.20481000	1.83685500
H	2.11520000	3.90170600	1.00976600
H	2.09714800	3.72049400	2.78518600
H	3.32300500	2.87410300	1.79474400
C	1.63446900	1.59119500	-1.57091200
O	1.74015900	2.37706800	-2.43215100
N	-0.70595000	-0.31089300	-0.36068400
H	-1.12995900	0.12675400	0.45373200
C	-1.52607700	0.07847100	-1.50907400
H	-2.33721200	-0.65576900	-1.67320800
H	-0.91189200	0.07881800	-2.41687800
C	-2.16018100	1.44052200	-1.29876800
C	-1.61107200	2.60692600	-1.84499500
C	-3.26784700	1.55806100	-0.44391600
C	-2.14488800	3.86140700	-1.53598700
H	-0.75767700	2.53464900	-2.51072000
C	-3.80219400	2.80797500	-0.13138400
H	-3.70387200	0.65846200	-0.01501900
C	-3.23873700	3.96732300	-0.67381300

H	-1.70442500	4.75542800	-1.97006400
H	-4.65969000	2.87903800	0.53302600
H	-3.65267600	4.94233300	-0.43116300
H	0.57317000	-1.55071900	1.84774900
O	-0.76495500	-1.86265200	1.97627300
C	-1.18719500	-2.21161400	0.82699000
H	-0.53105200	-2.75853000	0.14367400
C	-2.62669800	-2.28810100	0.54036900
C	-3.56199500	-1.78983200	1.46339300
C	-3.08026600	-2.83255900	-0.67138200
C	-4.92345000	-1.83933600	1.17717800
H	-3.19735900	-1.37250500	2.39639800
C	-4.44548500	-2.88134900	-0.95554500
H	-2.35835000	-3.21698500	-1.38727500
C	-5.36939500	-2.38514300	-0.03307000
H	-5.64199500	-1.45530100	1.89603500
H	-4.78796000	-3.30317200	-1.89616700
H	-6.43219300	-2.42120100	-0.25479200

TSI1

Ru	1.34352800	-1.00275200	0.60659600
H	2.29686100	-2.19723100	1.01343200
N	1.48951200	-1.27638300	-1.57417000
P	3.31934200	0.18079800	0.14712900
P	-0.37266900	-2.58158600	0.34422500
C	3.25029300	1.88445800	-0.54339600
H	2.91818400	2.58855700	0.22278100
H	4.22982200	2.18769500	-0.92759200
H	2.50633700	1.88920700	-1.34445800
C	-2.04568100	-2.51518200	1.10580700
H	-2.67425800	-3.33370000	0.74091800
H	-1.95056300	-2.59223300	2.19246800
H	-2.52659600	-1.56886400	0.85899500
C	3.95237500	-0.83538700	-1.26608000
H	4.80118900	-0.35481500	-1.76798300
H	4.30125300	-1.77192000	-0.81786500
C	2.80520600	-1.12215200	-2.25004500
H	2.73252800	-0.30062300	-2.97745600
H	3.04680700	-2.02806900	-2.82008200
C	0.69404900	-2.36529200	-2.17882800
H	1.24128000	-3.31780800	-2.10979800
H	0.53560500	-2.16520100	-3.25011500
C	-0.66435600	-2.48125300	-1.48196700
H	-1.23527300	-1.55802300	-1.63928600
H	-1.24039600	-3.33551800	-1.85547300
C	4.72383700	0.24030500	1.33436900
H	5.63230900	0.62571000	0.86068800
H	4.45539400	0.88820000	2.17330700
H	4.90632500	-0.76528200	1.72097300
C	0.12302900	-4.33499700	0.63103800
H	0.31784000	-4.48310700	1.69640100
H	-0.65434400	-5.03211100	0.30135700
H	1.04967200	-4.53117700	0.08716000
C	1.13454700	-0.60590800	2.42677800
O	1.00361100	-0.34783000	3.55516200

N	-1.70707400	0.82007500	-1.01835600
H	-2.05478100	1.27451800	-1.86073600
C	-2.53674400	1.14409300	0.13476900
H	-2.59285100	2.22449400	0.34873300
H	-2.04664900	0.70269300	1.01607800
C	-3.94544900	0.58891500	0.02845800
C	-4.93349200	1.05251100	0.90890500
C	-4.28845900	-0.39811900	-0.90289700
C	-6.22755100	0.53600000	0.86872400
H	-4.68223900	1.82648200	1.63095300
C	-5.58659600	-0.91354900	-0.94929600
H	-3.52830800	-0.75748700	-1.58771900
C	-6.55983200	-0.45157900	-0.06325000
H	-6.97908000	0.90702500	1.56026600
H	-5.83576300	-1.67716200	-1.68142700
H	-7.56900500	-0.85210700	-0.09924300
H	0.88568600	-0.20400500	-1.87588400
O	0.36713000	0.88555100	-2.06172600
C	-0.27205000	1.16416400	-0.90525500
H	0.07711000	0.50834300	-0.02671700
C	-0.02057700	2.59293700	-0.41833300
C	0.03169300	3.63649200	-1.34927900
C	0.16014400	2.87973900	0.93775000
C	0.26027200	4.94633300	-0.92883900
H	-0.07570900	3.39720100	-2.40289500
C	0.39251900	4.19078800	1.36251600
H	0.14234600	2.06783600	1.66149200
C	0.44235000	5.22793400	0.42906500
H	0.30771900	5.74910100	-1.66003900
H	0.53921300	4.39940200	2.41896200
H	0.62687800	6.24778700	0.75514600

TSI2

Ru	1.3362690	-1.0056010	0.5675280
H	2.3844870	-2.2653950	0.8298640
N	1.4026060	-1.4199720	-1.6310320
P	3.2494220	0.2407710	0.0471970
P	-0.3621310	-2.5866390	0.4975600
C	3.5116650	2.0424310	0.3387800
H	3.4906670	2.2401170	1.4135220
H	4.4769190	2.3638560	-0.0663450
H	2.7101860	2.6147350	-0.1286150
C	-2.0473290	-2.3376210	1.1940580
H	-2.7341220	-3.1357810	0.8941570
H	-1.9782140	-2.3181670	2.2854630
H	-2.4391210	-1.3802320	0.8540460
C	3.3225990	0.0931020	-1.8068780
H	2.6752560	0.8827400	-2.2034590
H	4.3387290	0.2357270	-2.1900780
C	2.7512140	-1.2659870	-2.2218520
H	2.6972510	-1.3364310	-3.3189540
H	3.3798180	-2.0869970	-1.8601960
C	0.7207280	-2.6678550	-2.0372500
H	1.3582800	-3.5146290	-1.7584870
H	0.5908010	-2.6943560	-3.1297400

C	-0.6378170	-2.7577370	-1.3349980
H	-1.2568890	-1.9029880	-1.6319110
H	-1.1635890	-3.6830520	-1.5954900
C	4.8638830	-0.4602710	0.6043230
H	5.7131070	0.0794310	0.1712130
H	4.9168270	-0.4069080	1.6952070
H	4.9025070	-1.5141380	0.3207630
C	0.0160950	-4.3103150	1.0369940
H	0.1930050	-4.3115740	2.1159150
H	-0.7998280	-5.0017290	0.8001260
H	0.9374000	-4.6357310	0.5490610
C	1.2299140	-0.5776080	2.3745350
O	1.1452060	-0.2829620	3.5007940
N	-1.7642810	0.8296160	-1.0069860
H	-2.1947140	0.7842120	-1.9223130
C	-2.6175430	1.2737160	0.0772870
H	-2.6521010	2.3705780	0.1680990
H	-2.1741290	0.9098390	1.0150640
C	-4.0342340	0.7434420	-0.0355600
C	-5.0596010	1.3997410	0.6601660
C	-4.3581020	-0.3984810	-0.7793460
C	-6.3694060	0.9248300	0.6233580
H	-4.8253050	2.2927030	1.2350000
C	-5.6717720	-0.8726600	-0.8238000
H	-3.5794000	-0.9259290	-1.3206130
C	-6.6816820	-0.2154890	-0.1218630
H	-7.1484990	1.4485310	1.1702130
H	-5.9027120	-1.7586850	-1.4088660
H	-7.7027930	-0.5840690	-0.1564650
H	0.8386630	-0.6187750	-1.9840990
O	0.1379980	0.9123020	-2.2350810
C	-0.4079990	1.2176640	-1.1372970
H	0.2076740	0.2404450	0.0652390
C	0.0377280	2.5026570	-0.4472580
C	0.4275020	3.5518620	-1.2910570
C	0.0778530	2.6952930	0.9381500
C	0.8467070	4.7726190	-0.7579860
H	0.4158530	3.3862750	-2.3631600
C	0.4917720	3.9156750	1.4706810
H	-0.1576850	1.8661470	1.5955740
C	0.8784260	4.9591870	0.6252940
H	1.1552410	5.5740040	-1.4238640
H	0.5314430	4.0440880	2.5487990
H	1.2122720	5.9052120	1.0422690

TSJ

Ru	1.9322340	-0.0043010	0.3196280
H	2.9650700	-1.2199930	0.2237740
N	0.3629130	-1.2789000	-0.6599990
P	2.5195520	0.3725540	-1.8955920
P	1.1905500	-1.2056220	2.1873640
C	1.7292160	1.7993450	-2.7578930
H	2.2245740	2.7203430	-2.4387220
H	1.7847710	1.7112820	-3.8478050
H	0.6912130	1.8573680	-2.4251180

C	0.3088800	-0.5373090	3.6726430
H	-0.0186860	-1.3431950	4.3382880
H	0.9814180	0.1288990	4.2202440
H	-0.5616470	0.0434500	3.3576690
C	1.8039760	-1.1233270	-2.7253500
H	1.7806410	-1.0203480	-3.8187170
H	2.4601180	-1.9614510	-2.4661130
C	0.4020470	-1.3425360	-2.1255880
H	-0.2589910	-0.5582820	-2.5374570
H	-0.0094370	-2.2945240	-2.4919380
C	0.2447200	-2.5949790	-0.0287430
H	1.1516280	-3.2132830	-0.1571080
H	-0.5936460	-3.1630830	-0.4655420
C	-0.0310280	-2.4144520	1.4706780
H	-1.0264800	-1.9786750	1.6040820
H	-0.0117590	-3.3672130	2.0117220
C	4.2641630	0.4399280	-2.4798550
H	4.3236560	0.4491800	-3.5729710
H	4.7427660	1.3402490	-2.0848860
H	4.7976160	-0.4305030	-2.0901340
C	2.4593100	-2.2786160	2.9911340
H	3.2299540	-1.6487710	3.4438230
H	2.0178840	-2.9245140	3.7573840
H	2.9322360	-2.8884810	2.2183510
C	3.2516570	1.0335400	1.1574050
O	4.0942520	1.6545950	1.6706980
O	0.3309760	1.8236550	0.1477980
C	-0.8225970	1.7579410	0.6585030
C	-1.7823800	2.9027490	0.4668790
C	-2.9385210	3.0092840	1.2487550
C	-1.5236240	3.8665960	-0.5141500
C	-3.8358100	4.0581460	1.0433130
H	-3.1301580	2.2706090	2.0239310
C	-2.4192720	4.9150870	-0.7207160
H	-0.6068440	3.7801340	-1.0888820
C	-3.5788820	5.0115200	0.0546600
H	-4.7296880	4.1362190	1.6560060
H	-2.2124430	5.6626870	-1.4817230
H	-4.2747500	5.8303390	-0.1050370
H	-0.9088350	-0.3512070	-0.4157460
N	-1.7391220	0.3737650	-0.3287090
H	-1.9077030	0.8033830	-1.2344210
C	-2.9535260	-0.2364410	0.2175690
H	-3.8073890	0.4269420	0.0334070
H	-2.8376700	-0.2897410	1.3080380
C	-3.2234050	-1.6334100	-0.3173340
C	-3.5404880	-2.6811480	0.5540130
C	-3.1329130	-1.9066160	-1.6885210
C	-3.7588810	-3.9736080	0.0717190
H	-3.6059310	-2.4867260	1.6220120
C	-3.3471380	-3.1954280	-2.1750290
H	-2.8713700	-1.1104410	-2.3799270
C	-3.6599710	-4.2353090	-1.2952120
H	-3.9965080	-4.7754670	0.7650180
H	-3.2653670	-3.3899020	-3.2406770

H	-3.8209020	-5.2407790	-1.6728650
H	-0.9734710	1.2271590	1.6174950

TSJ-2

C	1.89396200	0.48656100	-1.17512900
O	1.35678000	1.71493100	-1.16244700
H	1.96657600	0.06737700	-2.19326300
C	-0.22578600	-1.01679300	-1.29863300
H	-0.75754600	-0.13528100	-1.65873500
N	0.87812400	-0.51183000	-0.43038900
H	1.39040400	-1.28972200	-0.01349400
H	0.48416300	0.13685100	0.35975600
O	0.38719900	1.53227600	1.00978600
H	0.87722700	1.84308700	-0.09306500
C	-0.73514600	2.22921600	1.47555200
H	-0.51605900	3.31120600	1.52457000
H	-0.96213000	1.91969300	2.50844800
H	0.23291600	-1.52236500	-2.15520900
C	-1.13488400	-1.94887200	-0.53619000
C	-2.36221400	-1.49972600	-0.03630400
C	-0.73384300	-3.26877500	-0.28638100
C	-3.17273700	-2.35809500	0.70809400
H	-2.68354400	-0.48363200	-0.22913800
C	-1.54211800	-4.12531900	0.46068800
H	0.21227900	-3.63058500	-0.68560600
C	-2.76461600	-3.66886300	0.96100700
H	-4.12262900	-1.99562500	1.08986400
H	-1.22318600	-5.14677200	0.64677200
H	-3.39647800	-4.33503700	1.54136000
C	3.22443000	0.29609500	-0.45628300
C	3.49582800	0.97971700	0.73617300
C	4.17551100	-0.58888300	-0.97556600
C	4.70724800	0.77206700	1.39501300
H	2.74371400	1.64562800	1.14657500
C	5.39035000	-0.79203300	-0.31729500
H	3.97159200	-1.11143200	-1.90843900
C	5.65703900	-0.11015700	0.87099800
H	4.91305500	1.30180000	2.32098700
H	6.12685100	-1.47328800	-0.73414900
H	6.60160500	-0.26263700	1.38561900
C	-1.98858400	2.04251400	0.63125100
C	-1.92430100	2.12843400	-0.76869500
C	-3.22870100	1.78934500	1.22895600
C	-3.07249800	1.95725000	-1.54433300
H	-0.96660800	2.30541900	-1.24975800
C	-4.38076000	1.62027400	0.45523100
H	-3.29160600	1.71097500	2.31196800
C	-4.30558100	1.70035400	-0.93658000
H	-3.00538400	2.02370500	-2.62716800
H	-5.33269000	1.41741000	0.93883100
H	-5.19682100	1.56251700	-1.54216100

TSJ-3

C	-1.95957900	-0.69500500	-1.18651600
O	-1.42662700	-1.85183000	-0.90830600

H	-1.92658300	-0.39743400	-2.24629200
C	0.20014500	0.80050400	-1.40759600
H	0.66576200	-0.13841600	-1.72865500
H	-0.56828100	-0.10203100	0.42231500
O	-0.51477100	-1.06928800	1.14216600
H	-0.94105200	-1.69405000	0.28931000
C	0.69719000	-1.47497900	1.77658000
H	0.49400600	-2.43283800	2.27399400
H	0.91459800	-0.74421000	2.56333300
H	-0.18239000	1.31408100	-2.29971700
O	-0.92580300	0.53400000	-0.55622000
C	-3.24892900	-0.30497400	-0.50802600
C	-3.83245400	0.94376400	-0.75409000
C	-3.87873400	-1.20397100	0.35540000
C	-5.03078600	1.29305100	-0.13586800
H	-3.33217000	1.64366400	-1.41801700
C	-5.07898100	-0.85463100	0.97710100
H	-3.42046400	-2.17283100	0.52223400
C	-5.65592600	0.39284900	0.73350400
H	-5.47776100	2.26463200	-0.32700000
H	-5.56510900	-1.55708700	1.64827900
H	-6.59114200	0.66403300	1.21540600
C	1.19770700	1.66784600	-0.67817700
C	2.56703800	1.39696900	-0.75379100
C	0.75516500	2.75825000	0.08330000
C	3.48537200	2.21186000	-0.08905900
H	2.91517800	0.53117900	-1.30875000
C	1.67168700	3.56829200	0.75230100
H	-0.31077300	2.95052400	0.16012700
C	3.04086500	3.29906300	0.66429500
H	4.54554100	1.98276600	-0.14712400
H	1.31927800	4.40880300	1.34370400
H	3.75470300	3.92958400	1.18700500
C	1.90330500	-1.62194700	0.86799600
C	3.16621600	-1.24307800	1.33762300
C	1.79616800	-2.18469000	-0.41150200
C	4.30556000	-1.42469200	0.55292000
H	3.25842800	-0.78972700	2.32152100
C	2.93482500	-2.35603300	-1.20167200
H	0.82288500	-2.46220700	-0.80370700
C	4.19284800	-1.98105000	-0.72266000
H	5.27680800	-1.12001800	0.93234000
H	2.83759300	-2.78692900	-2.19435500
H	5.07633400	-2.11893100	-1.33945800

TSK

Ru	2.1590970	-0.5430640	0.3630530
H	3.3044810	-1.6351270	0.3722570
N	0.9208040	-1.3869050	-1.2607700
P	3.1762670	0.5373990	-1.4423590
P	0.8980880	-2.0805850	1.6100460
C	3.1681380	2.3767100	-1.5004150
H	3.8802750	2.7680580	-0.7687370
H	3.4220770	2.7588830	-2.4945370
H	2.1635280	2.7005940	-1.2163190

C	-0.0509480	-1.7004900	3.1479690
H	-0.6629280	-2.5535360	3.4590860
H	0.6478840	-1.4473880	3.9501310
H	-0.7001600	-0.8386550	2.9750590
C	2.0922340	0.0440400	-2.8737400
H	1.2823780	0.7801170	-2.9006780
H	2.6324670	0.0853740	-3.8257200
C	1.5027550	-1.3466580	-2.6025680
H	0.7360150	-1.5670510	-3.3657090
H	2.2866390	-2.1157060	-2.7176250
C	0.2227050	-2.6443370	-1.0000210
H	0.9099290	-3.5043290	-1.0897130
H	-0.5747490	-2.8063000	-1.7465380
C	-0.4019710	-2.6191440	0.4003560
H	-1.1898410	-1.8585820	0.4192960
H	-0.8375680	-3.5862780	0.6752560
C	4.8799920	0.0707310	-1.9624630
H	5.1692490	0.5621060	-2.8970640
H	5.5849060	0.3440210	-1.1728480
H	4.9177140	-1.0139970	-2.0903080
C	1.7588330	-3.6462530	2.0662800
H	2.5525440	-3.4243900	2.7842530
H	1.0674710	-4.3782150	2.4963460
H	2.2222670	-4.0592680	1.1673690
C	3.0740230	0.3173040	1.7564530
O	3.6514110	0.8406880	2.6228760
O	0.2113340	0.8210700	-0.4417450
C	-0.9248800	1.0735600	0.3264520
C	-1.1442860	2.5765890	0.4458200
C	-1.6583190	3.1371720	1.6188910
C	-0.8925340	3.4104690	-0.6514230
C	-1.9222690	4.5074250	1.6977690
H	-1.8428800	2.4986490	2.4801920
C	-1.1544280	4.7774320	-0.5766550
H	-0.4751630	2.9712930	-1.5524590
C	-1.6723190	5.3304160	0.5991020
H	-2.3161820	4.9308750	2.6176470
H	-0.9502210	5.4157730	-1.4322270
H	-1.8727730	6.3964430	0.6587630
H	0.2513250	-0.2141500	-0.9157510
N	-2.0644050	0.3704230	-0.2846000
H	-2.2354550	0.7697150	-1.2060320
C	-3.2958810	0.3607950	0.4965450
H	-3.7022040	1.3683320	0.6896940
H	-3.0465910	-0.0534480	1.4858820
C	-4.3682690	-0.5006640	-0.1432090
C	-4.0383210	-1.5861450	-0.9650430
C	-5.7199330	-0.2353460	0.1106670
C	-5.0387110	-2.3905950	-1.5138570
H	-2.9929070	-1.7849290	-1.1771650
C	-6.7209750	-1.0419130	-0.4316950
H	-5.9893890	0.6122960	0.7368320
C	-6.3830570	-2.1242730	-1.2472870
H	-4.7663390	-3.2268960	-2.1522260
H	-7.7643810	-0.8204120	-0.2246240

H	-7.1610070	-2.7501340	-1.6753670
H	-0.8322340	0.6592170	1.3449040

TSL

C	-0.7136980	0.7004510	-0.1942850
H	-0.0927770	0.2104090	-0.9713240
O	-0.5258610	2.0217000	0.0095780
C	-2.1396950	0.1909920	-0.2651030
C	-2.4242640	-1.1017840	-0.7196480
C	-3.1808460	1.0179210	0.1668160
C	-3.7389640	-1.5698590	-0.7307480
H	-1.6153380	-1.7374910	-1.0752560
C	-4.4958390	0.5517030	0.1538870
H	-2.9264400	2.0239790	0.4854960
C	-4.7767360	-0.7431180	-0.2911690
H	-3.9559140	-2.5729050	-1.0877030
H	-5.3037950	1.1991490	0.4837160
H	-5.8013020	-1.1043390	-0.3047390
N	-0.0547980	0.2448960	1.1963270
H	0.0589130	1.4335080	1.1204020
H	-0.7991180	-0.0037570	1.8489980
C	1.0347560	-0.7490270	1.2619850
H	1.2867360	-0.8882910	2.3207090
H	0.6455310	-1.7117340	0.9044520
C	2.2917640	-0.3865260	0.4912980
C	3.2983510	-1.3609940	0.4172990
C	2.5046570	0.8582040	-0.1131860
C	4.4985890	-1.0996000	-0.2391450
H	3.1396760	-2.3328580	0.8805550
C	3.7092620	1.1144320	-0.7763510
H	1.7323260	1.6223240	-0.0997820
C	4.7085170	0.1449300	-0.8396990
H	5.2671240	-1.8659510	-0.2850770
H	3.8580300	2.0817020	-1.2476210
H	5.6416960	0.3520330	-1.3554560

TSM

Ru	-1.95941800	-0.15914600	0.16057600
H	-2.92673400	-1.22605100	-0.51158900
N	-0.20305900	-0.96329700	-0.98229600
P	-2.23521700	1.08410600	-1.80222300
P	-1.30737900	-1.92995700	1.55026400
C	-1.43729000	2.74665400	-1.88727700
H	-2.04814700	3.46271100	-1.32956300
H	-1.32866200	3.09727800	-2.91878300
H	-0.46072700	2.69012700	-1.40131200
C	-0.29400700	-1.63137300	3.05986400
H	0.03298100	-2.57033000	3.51836200
H	-0.86690900	-1.05095000	3.78777300
H	0.57384300	-1.05312500	2.73581800
C	-1.26819600	0.06211000	-3.01253100
H	-1.07220300	0.60732800	-3.94468400
H	-1.88229600	-0.81455200	-3.24679600
C	0.02790400	-0.36566000	-2.30755400
H	0.66043100	0.51968200	-2.15598500

H	0.59956400	-1.05064200	-2.94847500
C	-0.19658600	-2.43606200	-0.97574100
H	-1.08150200	-2.83059600	-1.49503100
H	0.69571100	-2.81457500	-1.49556400
C	-0.16778500	-2.94417100	0.47461300
H	0.83994100	-2.82306700	0.87680500
H	-0.42848500	-4.00600200	0.52961500
C	-3.86408600	1.35281400	-2.61682200
H	-3.74790300	1.79751800	-3.61021500
H	-4.47580900	2.01321100	-1.99610200
H	-4.37669900	0.39162500	-2.70233200
C	-2.60001800	-3.10904500	2.13046500
H	-3.28197500	-2.58991800	2.80971200
H	-2.16177200	-3.97019600	2.64525500
H	-3.17447600	-3.44958300	1.26575100
C	-3.43099600	0.45296300	1.14445600
O	-4.36230200	0.81380800	1.74597800
O	-0.31973100	1.48434700	0.92607600
H	0.66461500	-0.49964200	-0.22079400
C	1.07530900	1.26468500	1.31800700
H	1.09262700	1.13783800	2.42911500
C	1.81919200	2.57095600	1.00925600
C	2.25500400	2.83349300	-0.29488000
C	2.03210400	3.53033500	2.00228200
C	2.87640600	4.04156100	-0.60430400
H	2.10869100	2.06022200	-1.04344800
C	2.65598100	4.74399100	1.69876600
H	1.71329800	3.32179400	3.02248700
C	3.07587600	5.00276700	0.39308300
H	3.21386600	4.23545300	-1.61918700
H	2.81818400	5.48241300	2.47945300
H	3.56433300	5.94338900	0.15401500
H	-0.66807400	2.22790400	1.43229600
N	1.49006900	0.12173700	0.61539500
C	2.81755100	-0.33400000	0.94024700
H	2.92241000	-0.65012600	2.00210700
H	3.57979800	0.46164300	0.80677400
C	3.19737700	-1.49914700	0.04783200
C	3.47880300	-2.76783100	0.56436100
C	3.24080200	-1.32141800	-1.34256700
C	3.78370500	-3.83850600	-0.28252600
H	3.44932100	-2.92028200	1.64086800
C	3.54505100	-2.38318900	-2.19265600
H	3.01784000	-0.33943200	-1.74853200
C	3.81441900	-3.65049300	-1.66435400
H	3.99362900	-4.81803500	0.13878900
H	3.57359600	-2.22540000	-3.26775800
H	4.04907800	-4.48036500	-2.32507800

TSN

Ru	0.0014240	0.4644790	-0.0183750
H	0.0054990	0.5952300	-1.6128520
N	-0.0290760	-1.7468430	0.1375690
P	-2.2926940	0.1138790	-0.1824770
P	2.2978940	0.0802010	-0.1582310

C	-3.2260180	-0.0079280	1.4002180
H	-3.4290580	1.0007950	1.7707570
H	-4.1705280	-0.5489300	1.2832170
H	-2.5765930	-0.5040300	2.1256670
C	3.5436430	0.8194580	0.9877510
H	4.5298420	0.3579160	0.8711000
H	3.6230760	1.8916490	0.7879610
H	3.2039940	0.6914540	2.0191880
C	-2.3249460	-1.6069280	-0.8758010
H	-3.3286000	-2.0499230	-0.8343090
H	-2.0337920	-1.5040880	-1.9270290
C	-1.2900650	-2.4703060	-0.1325890
H	-1.7279770	-2.8129160	0.8174490
H	-1.0953490	-3.3741300	-0.7250370
C	1.1690160	-2.4571870	-0.3174760
H	1.1974490	-2.5162220	-1.4179330
H	1.1775810	-3.4958640	0.0529370
C	2.4283620	-1.7445110	0.1934780
H	2.4859940	-1.8466610	1.2837570
H	3.3410190	-2.1756130	-0.2324930
C	-3.4109670	1.0671870	-1.2894330
H	-4.4052270	0.6124300	-1.3452840
H	-3.5040520	2.0894630	-0.9127820
H	-2.9678320	1.1084060	-2.2873710
C	3.1080800	0.2772250	-1.8015640
H	3.0812310	1.3315630	-2.0888220
H	4.1450790	-0.0743340	-1.7906550
H	2.5329300	-0.2864420	-2.5397920
C	0.0147940	2.3317170	0.0695030
O	0.0187270	3.4963190	0.1150230
H	0.0049730	-1.3004250	1.3630530
O	-0.1181560	-0.4072250	2.1635650
H	0.6972540	-0.2748390	2.6621780

TSO

Ru	1.5553850	0.0557490	-0.3949440
H	3.0054050	0.2202670	0.2839270
N	0.6661210	0.0091270	1.6641950
P	1.8289600	-2.2116150	0.0210710
P	1.3650770	2.3418820	-0.0025250
C	0.4401610	-3.3164460	-0.4787690
H	0.5295770	-3.5322690	-1.5470740
H	0.4268640	-4.2567950	0.0817810
H	-0.4920140	-2.7651480	-0.3375080
C	0.0410190	3.3677080	-0.7893100
H	-0.0603410	4.3482960	-0.3125960
H	0.2788560	3.5089230	-1.8477250
H	-0.9079650	2.8287720	-0.7214430
C	1.8021990	-2.2370540	1.8749820
H	1.6848720	-3.2523580	2.2758410
H	2.7697850	-1.8429980	2.2038620
C	0.6623050	-1.3091790	2.3261640
H	-0.2915380	-1.8038300	2.0918040
H	0.6863130	-1.1985180	3.4202640
C	1.2427790	1.0807980	2.4872490

H	2.3272040	0.9530600	2.6180840
H	0.7925220	1.0824290	3.4947760
C	0.9575760	2.4364510	1.8199330
H	-0.1097470	2.6693270	1.9019490
H	1.5095970	3.2494120	2.3031540
C	3.3346660	-3.1684000	-0.4312140
H	3.3205170	-4.1728930	0.0037930
H	3.3986010	-3.2479510	-1.5199180
H	4.2140910	-2.6260610	-0.0752710
C	2.8520410	3.4137500	-0.1948700
H	3.1397750	3.4460400	-1.2493510
H	2.6689450	4.4320650	0.1633640
H	3.6742600	2.9646680	0.3670310
C	2.3662580	0.1243010	-2.0776800
O	2.8997310	0.1655020	-3.1138360
H	-0.6104920	0.2831580	1.4100490
O	-0.5924090	-0.2727470	-1.1634980
H	-0.7219600	0.2706350	-1.9494730
N	-1.7521020	0.4575230	0.8924160
H	-2.0943940	1.4126680	0.9864000
H	-1.2452070	0.1626060	-0.2814280
C	-2.8144640	-0.4884240	1.2595550
H	-3.0897440	-0.4032940	2.3214080
H	-2.4020440	-1.4966690	1.1245880
C	-4.0559600	-0.3432950	0.4001480
C	-5.2799390	0.0509540	0.9496940
C	-3.9796840	-0.5821700	-0.9812910
C	-6.4106300	0.2053010	0.1420090
H	-5.3493980	0.2384490	2.0190980
C	-5.1056100	-0.4298950	-1.7882930
H	-3.0253830	-0.8766230	-1.4112180
C	-6.3259170	-0.0352110	-1.2292460
H	-7.3542670	0.5126650	0.5847560
H	-5.0349150	-0.6215750	-2.8557590
H	-7.2027810	0.0828450	-1.8597760

TSP

Ru	1.3434320	-0.2637450	0.6303870
H	1.0205140	1.1313750	1.3889390
N	-0.0211780	0.3718780	-1.1045080
P	-3.2965470	1.9962500	0.8623450
P	2.9351990	0.7921350	-0.6565020
C	-4.4116450	1.9955870	-0.6360150
H	-5.4347450	2.2280980	-0.3245240
H	-4.1005170	2.7265080	-1.3920950
H	-4.4189810	0.9980510	-1.0857620
C	4.5103400	-0.0515980	-1.1147640
H	5.0703940	0.5084590	-1.8707910
H	5.1295990	-0.1615310	-0.2200280
H	4.2770100	-1.0494570	-1.4946600
C	-1.6264290	1.9765040	0.0107580
H	-1.5124210	2.8774330	-0.6062030
H	-0.8618020	1.9957920	0.7948750
C	-1.4430710	0.7036080	-0.8148230
H	-1.8540000	-0.1470550	-0.2749050

H	-1.9962560	0.7850290	-1.7624520
C	0.6069320	1.3675420	-2.0070920
H	0.5525610	2.3414040	-1.5124510
H	0.0381010	1.4455740	-2.9463910
C	2.0668040	1.0111490	-2.2863950
H	2.1284080	0.0501120	-2.8099810
H	2.5428990	1.7732780	-2.9133720
C	-3.3698640	3.8107360	1.2848360
H	-3.1914560	4.4509080	0.4129070
H	-4.3523640	4.0509090	1.7025050
H	-2.6172970	4.0359160	2.0467160
C	3.5081090	2.4924170	-0.2303610
H	4.0505510	2.4537990	0.7182660
H	4.1564850	2.9165990	-1.0042240
H	2.6333680	3.1310850	-0.0855240
C	2.4684410	-0.6140820	2.0573760
O	3.1869740	-0.7875350	2.9589890
H	-0.0099270	-0.5333390	-1.5803830
C	0.2397070	-2.3675000	0.5736040
H	0.0444200	-1.0957270	1.3904220
H	0.4424640	-2.9724370	1.4656950
C	-1.2007520	-2.4680550	0.1284930
C	-2.2473670	-2.2895950	1.0440250
C	-1.5066630	-2.7313850	-1.2114350
C	-3.5740120	-2.3353370	0.6217000
H	-2.0152640	-2.0650240	2.0821330
C	-2.8372100	-2.7696980	-1.6379390
H	-0.6871440	-2.8984650	-1.9025320
C	-3.8734960	-2.5644320	-0.7261910
H	-4.3738340	-2.1742050	1.3383020
H	-3.0626750	-2.9637150	-2.6831670
H	-4.9077400	-2.5891250	-1.0576320
N	1.1944190	-2.2913630	-0.4055430
H	2.0514470	-2.7297080	-0.0745920

TSQ

Ru	0.8425530	0.5007330	0.3619690
H	1.8492770	1.7056310	-0.1420690
N	0.6351230	-0.2673140	-1.7140330
P	-0.7507840	2.0458590	-0.3541810
P	2.7537280	-0.8206540	0.2908070
C	-2.5753360	1.8871340	-0.1405580
H	-2.8225860	1.9431880	0.9217070
H	-3.1052830	2.6794980	-0.6800170
H	-2.9046960	0.9120140	-0.5019550
C	2.9213040	-2.4273380	1.1865950
H	3.8112700	-2.9817950	0.8712300
H	2.9810300	-2.2311690	2.2606100
H	2.0299150	-3.0307990	0.9988340
C	-0.5208840	1.9096150	-2.1968270
H	-1.3484590	2.3702950	-2.7498800
H	0.4006210	2.4471790	-2.4430730
C	-0.3854710	0.4248590	-2.5484570
H	-1.3362670	-0.0863450	-2.3628720
H	-0.1563310	0.2995880	-3.6153260

C	1.9543640	-0.4290610	-2.3706120
H	2.4099680	0.5568630	-2.4992200
H	1.8315890	-0.8794710	-3.3674040
C	2.8445570	-1.3337550	-1.5077540
H	2.4733890	-2.3622870	-1.5627920
H	3.8779270	-1.3334370	-1.8694070
C	-0.4746020	3.8320850	-0.0009150
H	-1.1355170	4.4675570	-0.5992220
H	-0.6621690	4.0202660	1.0599220
H	0.5699570	4.0698120	-0.2114170
C	4.3837340	-0.0278730	0.6240900
H	4.4259380	0.2709540	1.6751860
H	5.2175870	-0.7028490	0.4046150
H	4.4602930	0.8744580	0.0137030
C	0.9511340	1.0438440	2.1450640
O	1.0095680	1.3757810	3.2609140
N	-0.3820610	-2.6660420	-0.8642910
H	0.4300390	-3.2629150	-0.7001600
C	-0.8205520	-2.1845990	0.3105150
H	-0.1870970	-0.9286220	0.7036680
H	-0.5103270	-2.6639510	1.2494050
C	-2.2460740	-1.6995080	0.3754280
C	-2.7652790	-1.1804170	1.5687530
C	-3.0845830	-1.8055330	-0.7402230
C	-4.0952610	-0.7738620	1.6480640
H	-2.1091960	-1.0811710	2.4303930
C	-4.4149730	-1.3818440	-0.6677310
H	-2.6768640	-2.2420220	-1.6460180
C	-4.9255010	-0.8664630	0.5254330
H	-4.4851800	-0.3771470	2.5816520
H	-5.0561960	-1.4665720	-1.5413070
H	-5.9613470	-0.5440520	0.5841930
H	0.2447540	-1.2494540	-1.5432570

TSR

Ru	-1.35043000	-0.43907400	0.22829500
H	-2.12578000	-0.83452800	-1.11242300
N	0.24941000	0.46050000	-0.99861700
P	-0.17361200	-2.40958300	-0.25032300
P	-2.27912100	1.69682500	-0.15693500
C	1.15115300	-3.00936500	0.88634800
H	0.70061600	-3.34785600	1.82342100
H	1.72229800	-3.83141500	0.44199000
H	1.82742300	-2.17935000	1.10751600
C	-2.25979300	2.98356400	1.15348800
H	-2.62275300	3.94533900	0.77654800
H	-2.87886000	2.66517100	1.99670700
H	-1.21388500	3.06732000	1.46427400
C	0.75942900	-1.87746400	-1.75912400
H	1.56327400	-2.57933900	-2.01317400
H	0.04310900	-1.85113100	-2.58751200
C	1.29960200	-0.47145400	-1.45801400
H	2.05979300	-0.54134000	-0.67436100
H	1.81272600	-0.06741500	-2.34057500
C	-0.31942400	1.27526100	-2.08973300

H	-0.91397500	0.65597400	-2.77516600
H	0.49310900	1.73092400	-2.67733600
C	-1.18105300	2.39520200	-1.49023700
H	-0.52663800	3.11760000	-0.99482200
H	-1.76987700	2.90785100	-2.25756300
C	-1.04858000	-3.95604100	-0.72621800
H	-0.35227200	-4.70353500	-1.11924700
H	-1.56093800	-4.36747900	0.14781200
H	-1.79907900	-3.71682000	-1.48317200
C	-3.98816200	1.76055300	-0.84052700
H	-4.69127800	1.37957300	-0.09467100
H	-4.27137500	2.78158400	-1.11539700
H	-4.03880900	1.11319100	-1.71928700
C	-2.79466600	-1.16206400	1.20483300
O	-3.70988800	-1.61109200	1.76187100
H	0.67915700	1.26622600	-0.15451000
H	-0.34308500	0.50738000	1.58187200
O	0.85263100	2.17225200	0.72568700
H	-0.31138700	-0.24535700	1.83002400
C	1.89099400	1.94301300	1.61973700
H	2.25069500	2.90088800	2.04280200
H	1.58129300	1.33505300	2.49923300
C	3.07651300	1.23674300	0.97540100
C	3.62578800	0.06567700	1.50862000
C	3.59279200	1.72799200	-0.23221500
C	4.66321400	-0.60616100	0.85210700
H	3.23012200	-0.32844400	2.44266000
C	4.62920700	1.06712300	-0.88853000
H	3.14169300	2.61849100	-0.66085100
C	5.16609700	-0.10816200	-0.35063800
H	5.07285100	-1.51870100	1.27786000
H	5.01683000	1.46058500	-1.82488900
H	5.96844600	-0.62909600	-0.86579400

TSS

Ru	-1.71369800	0.13072600	-0.29563400
H	-3.01209000	0.31008500	0.60814600
N	-0.54093500	-0.16258300	1.58927900
P	-1.20232900	2.35956700	0.19245700
P	-1.91506900	-2.19204200	-0.13840600
C	-0.03936800	3.30008400	-0.89207500
H	-0.50964500	3.49092200	-1.86089400
H	0.25781700	4.25292000	-0.44223700
H	0.85153200	2.68412500	-1.04512600
C	-1.31311300	-3.23916600	-1.52749800
H	-1.18084500	-4.28381200	-1.22796800
H	-2.02660500	-3.18816600	-2.35479100
H	-0.36363200	-2.81569500	-1.86426800
C	-0.28222600	2.26526600	1.80861400
H	0.78290100	2.22690600	1.55889600
H	-0.46702400	3.14895400	2.42850500
C	-0.67127700	0.96498000	2.52183800
H	-0.01044800	0.82273900	3.39447700
H	-1.70058000	1.03705500	2.90949700
C	-0.80635000	-1.43531000	2.26743400

H	-1.79527000	-1.41895600	2.75765800
H	-0.06586700	-1.61179900	3.06706900
C	-0.75623600	-2.58948600	1.26209600
H	0.24735800	-2.65712900	0.82647700
H	-0.99188400	-3.55381000	1.72617700
C	-2.56163800	3.56735200	0.49015600
H	-2.17700800	4.53473800	0.82910400
H	-3.13348100	3.70398300	-0.43167100
H	-3.23226800	3.15169600	1.24615200
C	-3.50734300	-2.97600300	0.35324100
H	-4.25402500	-2.79266800	-0.42401300
H	-3.39721700	-4.05429600	0.50695500
H	-3.85619900	-2.50574800	1.27591000
C	-2.78446500	0.39978100	-1.81064800
O	-3.49169900	0.57290100	-2.72129700
H	0.75090000	-0.08348000	1.09357800
O	0.34549100	-0.32397700	-1.52430100
H	0.45438600	0.35718100	-2.19763500
O	1.72855300	0.11832900	0.54685300
H	1.04127000	-0.13699300	-0.79969400
C	2.75105700	-0.77223100	0.91907100
H	2.90369100	-0.73791600	2.01267200
H	2.48854400	-1.82025700	0.68319500
C	4.06610000	-0.44311100	0.23895800
C	4.28812400	0.81953600	-0.31881800
C	5.09162100	-1.39558700	0.18638900
C	5.51254100	1.12522400	-0.91736900
H	3.48852700	1.55144500	-0.27836900
C	6.31696000	-1.09184300	-0.40658400
H	4.92672600	-2.38458600	0.60972400
C	6.53155600	0.17232800	-0.96239700
H	5.67087900	2.11015700	-1.34900700
H	7.10177800	-1.84268300	-0.44187500
H	7.48357500	0.40945700	-1.42897900

TST

Ru	-0.84272000	0.50092700	-0.36188100
H	-1.84946700	1.70563200	0.14258800
N	-0.63481400	-0.26757800	1.71395500
P	0.75070100	2.04593800	0.35433600
P	-2.75360100	-0.82084900	-0.29071000
C	2.57521600	1.88727400	0.14037300
H	2.82229800	1.94386700	-0.92190500
H	3.10527200	2.67935500	0.68013800
H	2.90459200	0.91196200	0.50124000
C	-2.92068100	-2.42743700	-1.18676500
H	-3.81055600	-2.98216400	-0.87161600
H	-2.98029100	-2.23110700	-2.26075700
H	-2.02918000	-3.03072600	-0.99898100
C	0.52108700	1.90937800	2.19699500
H	1.34873900	2.36998800	2.74999100
H	-0.40039100	2.44689400	2.44344700
C	0.38576600	0.42457300	2.54843100
H	1.33660300	-0.08652700	2.36276200
H	0.15665200	0.29916500	3.61528800

C	-1.95392400	-0.42970800	2.37070000
H	-2.40962200	0.55612700	2.49967100
H	-1.83091700	-0.88038200	3.36734300
C	-2.84423500	-1.33423300	1.50778500
H	-2.47320400	-2.36282100	1.56268200
H	-3.87757300	-1.33383400	1.86953100
C	0.47433300	3.83221700	0.00146800
H	1.13571500	4.46762100	0.59933000
H	0.66105300	4.02051200	-1.05949700
H	-0.57006200	4.06993000	0.21281500
C	-4.38386500	-0.02853200	-0.62384000
H	-4.42615100	0.27052000	-1.67486900
H	-5.21749400	-0.70383800	-0.40453400
H	-4.46074000	0.87363200	-0.01324600
C	-0.95168500	1.04446300	-2.14481700
O	-1.01035000	1.37667200	-3.26057400
H	-0.24423800	-1.24959400	1.54287300
C	0.82055300	-2.18438800	-0.31112500
H	0.18729600	-0.92820400	-0.70383900
H	0.51025800	-2.66332100	-1.25020400
C	2.24612500	-1.69942200	-0.37581800
C	2.76547400	-1.18011500	-1.56898500
C	3.08452200	-1.80572500	0.73989300
C	4.09548700	-0.77361000	-1.64808000
H	2.10948300	-1.08065100	-2.43067000
C	4.41493500	-1.38207800	0.66762400
H	2.67669000	-2.24237300	1.64556100
C	4.92560800	-0.86647300	-0.52538300
H	4.48551700	-0.37671800	-2.58154600
H	5.05606400	-1.46701100	1.54124900
H	5.96147400	-0.54409700	-0.58397000
N	0.38197200	-2.66621200	0.86349500
H	-0.43023500	-3.26289200	0.69921300

heam-TS-1

C	-2.00690400	-1.04337600	1.00456900
O	-1.21552100	0.79361800	1.72362500
H	-2.27166800	-1.41262500	1.99510200
C	0.05607800	-2.20533700	1.27813900
H	-0.43842500	-3.00096100	1.85187700
H	0.44404900	-1.47747400	2.00581100
N	-0.93889200	-1.55293700	0.42127200
H	-0.43109800	-0.76041400	-0.22022700
H	-0.62503400	0.67940700	2.48153100
O	0.07560700	0.58792600	-0.34626400
H	-0.54228100	0.84231200	0.80063300
C	1.46719700	0.73924100	-0.32926000
H	1.90213500	0.32007600	-1.25258900
H	1.93847600	0.16622900	0.49436000
C	-3.09202500	-0.39201100	0.25878900
C	-4.35879100	-0.33391600	0.85834900
C	-2.90727400	0.15697200	-1.02178400
C	-5.43399500	0.24492300	0.18722500
H	-4.50011600	-0.74505800	1.85461900
C	-3.98235400	0.74232100	-1.68373400

H	-1.91940000	0.16874100	-1.46808300
C	-5.24689500	0.78266600	-1.08729300
H	-6.41169800	0.27990100	0.65831200
H	-3.83316100	1.17452300	-2.66869600
H	-6.08133900	1.23833500	-1.61264500
C	1.90885100	2.18945400	-0.20221700
C	0.97677200	3.23041200	-0.20932200
C	3.27030300	2.49932100	-0.08174000
C	1.39789500	4.55832900	-0.09605300
H	-0.07533100	2.98325400	-0.30012500
C	3.69322100	3.82325200	0.02773800
H	4.00334000	1.69428500	-0.07356900
C	2.75507600	4.86035800	0.02132500
H	0.66192400	5.35829300	-0.10031000
H	4.75268300	4.04798600	0.12031400
H	3.08182400	5.89297700	0.10860600
C	1.20217000	-2.77337400	0.47082200
C	2.51010300	-2.70400900	0.96313000
C	0.97381400	-3.38543200	-0.76762100
C	3.57290600	-3.24403500	0.23720000
H	2.69941200	-2.21703200	1.91678700
C	2.03588400	-3.91930900	-1.49796100
H	-0.03719000	-3.42735000	-1.16165300
C	3.33796100	-3.85252600	-0.99693600
H	4.58339600	-3.17894600	0.63029100
H	1.84675300	-4.38578700	-2.46059900
H	4.16434100	-4.26600900	-1.56772600

heam-TS-2

C	0.60296900	-3.09685400	0.20402500
O	0.21439400	-2.15883100	2.11769100
H	0.91754800	-3.92105400	0.83459800
C	2.96610000	-2.58154900	-0.09480600
H	3.46333300	-3.07810000	-0.93694500
H	3.04588900	-3.26048600	0.76368500
N	1.54669700	-2.42958200	-0.41598200
H	1.26887700	-1.57457800	-0.96614700
H	1.06275800	-2.02416500	2.56279100
O	-0.10900100	-0.03426700	0.98529200
H	-0.01439800	-1.17601200	1.65785100
C	-0.79612100	1.01200500	1.60249700
H	-0.29903800	1.97692700	1.40179100
H	-0.78308400	0.88664300	2.70182000
C	-0.79900600	-3.09191100	-0.24546300
C	-1.78612400	-3.59217400	0.62066400
C	-1.16297200	-2.64993200	-1.52752800
C	-3.11578500	-3.63606900	0.21581200
H	-1.50137800	-3.88658100	1.62415600
C	-2.49706800	-2.70095900	-1.92782000
H	-0.41869000	-2.24258300	-2.19965800
C	-3.47410900	-3.19344100	-1.06104800
H	-3.87542800	-4.00436500	0.89817200
H	-2.77197100	-2.34798500	-2.91678600
H	-4.51311600	-3.22680100	-1.37565500
C	-2.24915100	1.14628100	1.16501100

C	-2.84115900	0.18523500	0.34315500
C	-3.01073900	2.25159500	1.56668500
C	-4.16624200	0.32684700	-0.07666000
H	-2.24628700	-0.66353100	0.03080600
C	-4.33459000	2.39569000	1.15291500
H	-2.55431600	3.01386300	2.19543800
C	-4.91881600	1.43163100	0.32413200
H	-4.60689200	-0.43081600	-0.71979600
H	-4.91070200	3.26139200	1.47032800
H	-5.94878000	1.54435400	-0.00386400
C	3.66618400	-1.26715300	0.20101700
C	3.02317200	-0.23544900	0.89676400
C	4.99384200	-1.09463900	-0.21012600
C	3.70794500	0.95009400	1.17255800
H	1.97225900	-0.30612200	1.16492900
C	5.67825700	0.08675200	0.07803800
H	5.49539100	-1.88579300	-0.76311300
C	5.03517300	1.11431500	0.77186600
H	3.18735400	1.75158000	1.68821600
H	6.70694200	0.20802100	-0.24907500
H	5.56253300	2.03901500	0.98839300
C	1.33683300	0.97203900	-1.83535500
H	2.37054400	0.88062200	-1.47256500
H	1.37742300	0.96176100	-2.93365500
C	0.74907000	2.28160000	-1.35322500
C	1.55529900	3.25980800	-0.76148300
C	-0.62689200	2.51390000	-1.47100400
C	0.99789300	4.45577100	-0.30219700
H	2.62039000	3.07458500	-0.64583500
C	-1.18738000	3.70210100	-1.00587900
H	-1.26064900	1.73555500	-1.88351000
C	-0.37543800	4.67846800	-0.42221800
H	1.63327600	5.20631000	0.16063600
H	-2.26044500	3.85182500	-1.07330700
H	-0.81270200	5.60202900	-0.05292900
O	0.54833100	-0.14487500	-1.43978100
H	0.20982700	0.00133400	-0.46647900

PNN

Ru	-0.4449040	-0.5586750	0.0879330
H	-0.4462440	-0.6863600	-1.4520430
P	1.7697010	0.1565260	-0.0503240
O	0.1351010	-3.5404300	0.1383780
N	-2.7433570	-0.4555070	0.1170490
N	-0.7826610	1.5134290	-0.0337770
C	1.5430490	1.8670400	-0.4783270
C	0.2534480	2.3760410	-0.3892760
C	-0.1046980	3.7510560	-0.6304270
H	0.6809930	4.4458980	-0.9091710
C	-1.4047700	4.1662040	-0.5191360
H	-1.6574460	5.2052320	-0.7152700
C	-2.4297990	3.2557240	-0.1412490
H	-3.4595590	3.5733530	-0.0258200
C	-2.0553160	1.9523610	0.1013630
C	-3.0081120	0.9167550	0.6527210

H	-2.8693460	0.8676800	1.7400150
H	-4.0478490	1.2191890	0.4714470
C	-0.1008680	-2.3964730	0.1416310
C	2.5907530	0.0952670	1.6867080
C	2.5776890	-1.3298790	2.2739510
H	2.9556310	-1.2999770	3.3040450
H	1.5644520	-1.7410560	2.2992280
H	3.2053930	-2.0270540	1.7170760
C	4.0215660	0.6577110	1.6967520
H	4.3754250	0.7495640	2.7318130
H	4.7227320	0.0035660	1.1719090
H	4.0655800	1.6520220	1.2410180
C	1.7043310	0.9891370	2.5828320
H	1.6700510	2.0185310	2.2186430
H	0.6735520	0.6183340	2.6345410
H	2.1042030	0.9910740	3.6043330
C	2.9186880	-0.5889190	-1.3755530
C	3.4751660	-1.9570390	-0.9444260
H	4.2129640	-1.8675360	-0.1425980
H	2.6825300	-2.6347980	-0.6141350
H	3.9797930	-2.4264850	-1.7978940
C	4.0793350	0.3641700	-1.7293640
H	4.6986380	-0.1012650	-2.5061580
H	3.7059830	1.3111820	-2.1275350
H	4.7282450	0.5804950	-0.8791670
C	2.0598430	-0.7791330	-2.6441850
H	1.3136390	-1.5651070	-2.5090820
H	1.5397560	0.1456890	-2.9119420
H	2.7111260	-1.0634020	-3.4801490
C	-3.2931350	-0.5336880	-1.2719350
H	-2.7569770	0.2210140	-1.8520010
H	-4.3528070	-0.2364420	-1.2557470
C	-3.1554230	-1.8973940	-1.9395990
H	-3.7817440	-2.6582760	-1.4642730
H	-3.4762620	-1.8142040	-2.9825670
H	-2.1185450	-2.2396030	-1.9248470
C	-3.3147070	-1.4930660	1.0254400
H	-2.9958850	-2.4651560	0.6457760
H	-2.8191380	-1.3634990	1.9936140
C	-4.8356720	-1.4732750	1.2128780
H	-5.1200780	-2.2648270	1.9130560
H	-5.1891190	-0.5239580	1.6258070
H	-5.3664490	-1.6570720	0.2745770
H	2.3701250	2.5294370	-0.7053900

PNP

Ru	0.0307210	-0.4372370	-0.0881540
H	0.0477580	-0.7018610	-1.6146910
C	0.0788190	-2.2899160	0.1450620
O	0.0870080	-3.4516240	0.2554980
P	2.3642640	0.0003500	-0.0258100
C	3.4558040	-0.6805430	-1.4280220
C	2.9891850	0.0487910	-2.7056230
H	3.1619650	1.1258520	-2.6393530
H	1.9212850	-0.1090620	-2.8851540

H	3.5429040	-0.3434200	-3.5678160
C	3.2181680	-2.1912670	-1.6158960
H	2.1607510	-2.4032160	-1.7939690
H	3.5410340	-2.7817170	-0.7560220
C	4.9522590	-0.3986580	-1.2080260
H	5.3628290	-0.9802190	-0.3780480
H	5.1401440	0.6623070	-1.0132440
H	5.5145690	-0.6748380	-2.1089910
C	3.0527020	-0.4547570	1.6984880
C	1.9011100	-0.0988720	2.6672870
H	1.0309520	-0.7503800	2.5128400
H	1.5910220	0.9441020	2.5429280
H	2.2275260	-0.2344310	3.7060830
C	4.2844660	0.3818920	2.0908090
H	4.5732210	0.1436110	3.1226540
H	4.0648530	1.4518860	2.0422400
H	5.1481030	0.1793000	1.4541150
C	3.3709100	-1.9530710	1.8232190
H	4.2503110	-2.2329190	1.2367890
H	2.5320160	-2.5779260	1.5040060
H	3.5890080	-2.1957790	2.8710390
P	-2.3021270	-0.1467560	-0.1144620
C	-2.9982650	0.1200590	1.6433230
C	-2.6491160	-1.1081760	2.5105020
H	-2.9699160	-0.9243060	3.5430270
H	-1.5709280	-1.2947900	2.5220530
H	-3.1411670	-2.0207510	2.1691050
C	-2.2597840	1.3449990	2.2325390
H	-2.5641210	1.4699640	3.2785460
H	-2.4942720	2.2718990	1.7029000
H	-1.1725260	1.2237550	2.2144560
C	-4.5119900	0.3871810	1.6982620
H	-4.8041850	1.2268850	1.0598550
H	-4.7977230	0.6430440	2.7260650
C	-3.4359250	-1.2505860	-1.1709490
C	-2.6387890	-1.5997250	-2.4480510
H	-3.2745610	-2.1994100	-3.1106360
H	-1.7412610	-2.1755850	-2.2147180
H	-2.3273780	-0.7100920	-3.0041220
C	-3.7400630	-2.5631780	-0.4236620
H	-4.4062120	-2.4104220	0.4295050
H	-2.8262190	-3.0510720	-0.0711870
H	-4.2429660	-3.2571590	-1.1076970
C	-4.7519490	-0.5619500	-1.5852600
H	-4.5733930	0.3397080	-2.1781980
H	-5.3750080	-0.2894180	-0.7326330
H	-5.3336630	-1.2500530	-2.2106930
N	-0.0287200	1.7103680	-0.3906760
C	2.3745230	1.7651690	-0.0974970
C	1.1664040	2.4319330	-0.2676580
C	1.0878050	3.8701360	-0.3136020
H	2.0061440	4.4341330	-0.1864690
C	-0.1071030	4.5034510	-0.5088380
H	-0.1503210	5.5894520	-0.5370430
C	-1.2917370	3.7459160	-0.6895770

H	-2.2439700	4.2236400	-0.8884570
C	-1.1957800	2.3696700	-0.6415310
C	-2.4144910	1.5208130	-0.9311350
H	-2.4396830	1.3118000	-2.0071660
H	-3.3379140	2.0534730	-0.6856280
H	3.7867340	-2.5418050	-2.4866710
H	3.2909320	2.3427300	-0.0386350
H	-5.0984630	-0.4878300	1.4076440

PNN-TSM

Ru	1.5063850	-0.8115610	-0.4675270
H	2.2724260	-2.0987450	0.0266190
P	-0.4389800	-2.0437020	-0.1667050
O	2.0672010	-1.7611670	-3.2881540
N	3.4392210	0.3920600	0.1275250
N	1.0876850	-0.2481130	1.5534810
C	-1.1424910	-1.0679780	1.2234870
C	-0.0916450	-0.6017190	2.1357530
C	-0.2785110	-0.3409880	3.5071270
H	-1.2111070	-0.6302190	3.9789520
C	0.7233470	0.2902470	4.2280290
H	0.5924360	0.4795240	5.2896540
C	1.8901050	0.7236770	3.5786470
H	2.6552600	1.2829750	4.1058800
C	2.0206370	0.4583420	2.2224700
C	3.0533350	1.1440160	1.3538520
H	2.5862790	2.0803150	1.0252970
H	3.9343630	1.4191170	1.9485260
C	1.8569340	-1.3787130	-2.2053860
C	-1.7802190	-2.1186880	-1.5200540
C	-1.7191920	-0.7839220	-2.2887180
H	-2.5272930	-0.7595800	-3.0291530
H	-1.8508770	0.0609090	-1.6169020
H	-0.7687110	-0.6800340	-2.8210040
C	-1.4855140	-3.2459860	-2.5281610
H	-2.1870030	-3.1566970	-3.3663230
H	-0.4727430	-3.1730290	-2.9370040
H	-1.6187240	-4.2410220	-2.0998000
C	-3.1965160	-2.2792770	-0.9320180
H	-3.3330180	-3.2290780	-0.4141750
H	-3.4482650	-1.4686950	-0.2470280
H	-3.9266590	-2.2444070	-1.7489270
C	-0.1223470	-3.8118860	0.5244520
C	0.7900790	-4.6114670	-0.4289770
H	0.3293060	-4.8032460	-1.3988870
H	1.7333570	-4.0873400	-0.5982600
H	1.0155250	-5.5849320	0.0243400
C	-1.4224800	-4.5957000	0.7901890
H	-1.1751830	-5.5342870	1.3015550
H	-2.1065080	-4.0394090	1.4390970
H	-1.9537870	-4.8583230	-0.1264770
C	0.6121180	-3.6661560	1.8759440
H	1.5190550	-3.0647670	1.7849390
H	-0.0251980	-3.2169430	2.6416770
H	0.8992190	-4.6644470	2.2279230

C	4.5589860	-0.5325860	0.4807370
H	4.1658400	-1.2046950	1.2482870
H	5.3724600	0.0487070	0.9422610
C	5.1169030	-1.3448600	-0.6809940
H	4.3245900	-1.8994700	-1.1857760
H	5.6295630	-0.7164160	-1.4151480
H	5.8487050	-2.0607940	-0.2937520
C	3.7842580	1.3396900	-0.9767570
H	3.9696610	0.7356520	-1.8671600
H	2.8755670	1.9133620	-1.1741410
C	4.9718440	2.2725850	-0.7183840
H	5.0977890	2.9354870	-1.5800530
H	4.8151180	2.9054790	0.1605700
H	5.9099630	1.7256540	-0.5830150
H	-2.0044070	-1.5081930	1.7283270
C	-0.3129350	2.0852700	0.0874550
O	0.5386850	1.3321700	-0.9938900
N	-1.5529600	1.5158970	0.3312630
H	-1.4654260	0.0829470	0.7275500
C	-2.6938910	2.0346070	-0.4099570
H	-2.8996820	3.0881430	-0.1481080
H	-2.5645340	2.0471440	-1.5101990
H	0.3447280	1.9274270	0.9430980
H	-0.0700460	1.1604040	-1.7243740
C	-3.9371080	1.2253330	-0.0954480
C	-4.8700760	0.9115970	-1.0900030
C	-4.1762170	0.7747070	1.2109100
C	-6.0098790	0.1597120	-0.7954180
H	-4.6923190	1.2460830	-2.1095310
C	-5.3101860	0.0192290	1.5089870
H	-3.4431550	1.0070120	1.9767970
C	-6.2316500	-0.2948020	0.5053360
H	-6.7171780	-0.0815370	-1.5845500
H	-5.4756780	-0.3292250	2.5254590
H	-7.1116920	-0.8889850	0.7355240
C	-0.2775820	3.5679220	-0.2629480
C	0.2085900	4.0778490	-1.4703620
C	-0.7736180	4.4654660	0.6956830
C	0.1959420	5.4541580	-1.7176400
H	0.6083740	3.3959160	-2.2123630
C	-0.7802730	5.8376810	0.4547340
H	-1.1660860	4.0661460	1.6273470
C	-0.2959760	6.3383960	-0.7578640
H	0.5759210	5.8336210	-2.6626470
H	-1.1671340	6.5175780	1.2091630
H	-0.3026690	7.4076770	-0.9500630

PNP -TSM

Ru	1.0991300	-0.9003220	-0.4707930
H	1.8174600	-2.2415420	-0.0417860
P	-0.9353360	-2.0949120	-0.0840920
O	1.6270570	-1.6872720	-3.3446110
N	0.7451390	-0.4443000	1.6597760
C	-1.5928590	-1.0087530	1.2430040
C	-0.5305880	-0.5395850	2.1439280

C	-0.8062460	-0.0980450	3.4539410
H	-1.8248010	-0.1541920	3.8227580
C	0.2127030	0.4154980	4.2374080
H	0.0032390	0.7704590	5.2430320
C	1.5206310	0.4604290	3.7360370
H	2.3424060	0.8278520	4.3411630
C	1.7565460	0.0026440	2.4450220
C	3.1582960	-0.0919410	1.8848770
H	3.8372270	0.5979820	2.3959020
H	3.5246530	-1.1073660	2.0827770
C	1.4114940	-1.3663380	-2.2438800
C	-2.3130500	-2.2204050	-1.3994730
C	-2.2452420	-0.9377240	-2.2520880
H	-3.0468360	-0.9614400	-3.0010790
H	-2.3964000	-0.0541440	-1.6341640
H	-1.2890860	-0.8597610	-2.7811930
C	-2.0689300	-3.4135010	-2.3427750
H	-2.7805030	-3.3530080	-3.1763150
H	-1.0590860	-3.3982540	-2.7681250
H	-2.2259670	-4.3776070	-1.8534900
C	-3.7205030	-2.3099180	-0.7757810
H	-3.8635730	-3.2162350	-0.1848160
H	-3.9436480	-1.4454920	-0.1476780
H	-4.4676780	-2.3194010	-1.5793590
C	-0.6455860	-3.8277860	0.7057390
C	0.2045010	-4.7144820	-0.2288270
H	-0.3133930	-4.9803910	-1.1521970
H	1.1428270	-4.2195820	-0.4953170
H	0.4484370	-5.6514030	0.2899580
C	-1.9572450	-4.5506160	1.0675830
H	-1.7222080	-5.4647340	1.6289760
H	-2.6013090	-3.9314650	1.7020200
H	-2.5288740	-4.8510010	0.1865480
C	0.1501500	-3.6306620	2.0157260
H	1.0943240	-3.1082500	1.8456130
H	-0.4210590	-3.0748640	2.7651390
H	0.3781830	-4.6180830	2.4384920
C	4.7782890	-0.8917790	-0.4687940
C	4.4739620	-2.4039250	-0.3790550
H	4.1281530	-2.7076820	0.6148150
H	3.7156750	-2.7100520	-1.1016690
H	5.3975000	-2.9580950	-0.5926180
C	3.4682550	1.9572510	-0.2856610
C	4.8897340	2.4932720	-0.0463400
H	4.8745390	3.5845800	-0.1668650
H	5.2449530	2.2842870	0.9692570
H	5.6195510	2.0996920	-0.7581890
H	-2.4563030	-1.3992750	1.7898910
C	-0.9246430	1.9968460	0.1192740
O	-0.0780640	1.2512480	-0.9644980
N	-2.1966650	1.4808620	0.2852840
H	-2.0035320	0.0831460	0.6950150
C	-3.2713940	2.0186590	-0.5322070
H	-3.4567860	3.0831760	-0.2970140
H	-3.0740250	2.0059290	-1.6234490

H	-0.3185700	1.7611990	0.9976190
H	-0.7233820	0.9913920	-1.6392130
C	-4.5483770	1.2404380	-0.2786880
C	-5.4078240	0.8875510	-1.3246560
C	-4.8852410	0.8467840	1.0247120
C	-6.5718750	0.1533290	-1.0826320
H	-5.1539280	1.1777070	-2.3421510
C	-6.0444070	0.1112690	1.2713750
H	-4.2071730	1.1066220	1.8319060
C	-6.8923280	-0.2421920	0.2169120
H	-7.2215450	-0.1185130	-1.9111240
H	-6.2870250	-0.1914460	2.2875180
H	-7.7923850	-0.8211920	0.4074460
C	-0.8159090	3.4890050	-0.1589720
C	-1.2325330	4.3639230	0.8551020
C	-0.3435930	4.0262400	-1.3591410
C	-1.1661220	5.7448920	0.6784130
H	-1.6168410	3.9436920	1.7814340
C	-0.2815240	5.4110270	-1.5417770
H	-0.0080580	3.3564480	-2.1424250
C	-0.6883050	6.2750430	-0.5244030
H	-1.4883870	6.4089860	1.4767700
H	0.0903360	5.8131520	-2.4812350
H	-0.6352390	7.3515770	-0.6652260
P	3.2064090	0.0879100	0.0171400
C	2.5200600	2.6965950	0.6791330
H	1.5112830	2.2965930	0.6350760
H	2.8677950	2.6499590	1.7167590
H	2.4627450	3.7532020	0.3923110
C	3.0243200	2.2490090	-1.7353910
H	1.9838060	1.9503930	-1.8825250
H	3.1019910	3.3275420	-1.9256610
H	3.6479610	1.7345600	-2.4731820
C	5.9887560	-0.6066530	0.4463340
H	6.3237020	0.4295790	0.4092170
H	5.7799510	-0.8610580	1.4912250
H	6.8312510	-1.2325740	0.1245930
C	5.1307340	-0.5732690	-1.9361660
H	5.9473620	-1.2306790	-2.2615460
H	4.2787290	-0.7496280	-2.6015040
H	5.4678340	0.4573470	-2.0723450

PNP –TSI2

Ru	0.8506340	-0.6438560	0.5907020
H	1.2980130	-2.1890930	0.6296100
P	2.8255100	-0.4094340	-0.6977200
O	2.0346880	-0.1842930	3.3353420
N	-0.0519770	-0.8166390	-1.4056280
C	2.0721600	-0.0043070	-2.3442810
C	0.6892270	-0.5753760	-2.5143990
C	0.1563240	-0.7687530	-3.7915570
H	0.7783430	-0.5846690	-4.6604680
C	-1.1680790	-1.1683100	-3.9283440
H	-1.5979160	-1.3251720	-4.9133960
C	-1.9448940	-1.3337930	-2.7845290

H	-2.9972380	-1.5836420	-2.8497700
C	-1.3649640	-1.1335400	-1.5315680
C	-2.2111280	-1.1605650	-0.2867260
H	-2.5447190	-0.1296000	-0.1312490
H	-3.1028370	-1.7781560	-0.4239830
C	1.5852790	-0.3781090	2.2758220
C	4.0832250	0.9973570	-0.4081700
C	3.2637370	2.2043820	0.0804760
H	3.9402940	3.0486630	0.2622160
H	2.5186540	2.5183110	-0.6523160
H	2.7378790	1.9859120	1.0105380
C	5.0642790	0.5929700	0.7086880
H	5.6587620	1.4696240	0.9924740
H	4.5356720	0.2511420	1.6045110
H	5.7636660	-0.1875650	0.3990100
C	4.8534770	1.4289140	-1.6736920
H	5.5042880	0.6532040	-2.0772730
H	4.1748360	1.7574320	-2.4662550
H	5.4881270	2.2864850	-1.4188760
C	3.7567060	-2.0573920	-1.0214220
C	4.1428570	-2.7143490	0.3196150
H	4.8605220	-2.1181360	0.8868150
H	3.2611880	-2.8712280	0.9454910
H	4.6062900	-3.6891060	0.1226010
C	5.0126180	-1.8964200	-1.8977240
H	5.4132630	-2.8904550	-2.1319990
H	4.7925180	-1.4023440	-2.8495300
H	5.8050260	-1.3395440	-1.3945420
C	2.7883930	-3.0028860	-1.7646670
H	1.8524470	-3.1294180	-1.2198720
H	2.5559860	-2.6500600	-2.7737460
H	3.2592710	-3.9884780	-1.8623390
C	-1.2994490	-3.4726500	1.3257580
C	-0.2685220	-3.9808280	2.3540030
H	0.7308810	-3.6072850	2.1176880
H	-0.5114080	-3.6828260	3.3758770
H	-0.2435500	-5.0772800	2.3283610
C	-2.3069750	-0.8269990	2.6513360
C	-3.8259540	-0.9499070	2.4118420
H	-4.3524580	-0.4781580	3.2510770
H	-4.1406850	-0.4322140	1.5023240
H	-4.1713390	-1.9822380	2.3532270
H	2.7152280	-0.2477110	-3.1946030
C	-0.1673620	2.3040280	-0.4586810
H	0.2640660	1.1133530	0.2941350
O	0.3438780	2.2775230	-1.6166390
N	-1.6360270	2.1946730	-0.3736630
H	-1.9832260	2.9094100	0.2562750
C	-2.3357340	2.2167950	-1.6545960
H	-2.3788660	3.2324130	-2.0853410
H	-1.7350770	1.6353960	-2.3560380
H	1.9109140	1.0807830	-2.3100470
C	-3.7419500	1.6527430	-1.5907930
C	-4.3218780	1.1278490	-2.7546520
C	-4.4991240	1.6416720	-0.4122410

C	-5.6118440	0.5965140	-2.7418520
H	-3.7448950	1.1252680	-3.6762690
C	-5.7906060	1.1080520	-0.3927610
H	-4.0704760	2.0303300	0.5058390
C	-6.3516660	0.5802330	-1.5564320
H	-6.0378020	0.1894210	-3.6551070
H	-6.3555810	1.1036410	0.5354460
H	-7.3542150	0.1624870	-1.5415270
C	0.3174980	3.3821970	0.5226570
C	0.6085070	4.6392630	-0.0228240
C	0.4412580	3.1947600	1.8997660
C	1.0021310	5.6938670	0.8008690
H	0.5404670	4.7605490	-1.0995250
C	0.8349720	4.2482260	2.7274530
H	0.2762960	2.2063400	2.3082990
C	1.1122030	5.5031950	2.1811320
H	1.2313280	6.6632660	0.3657470
H	0.9389440	4.0831580	3.7966480
H	1.4240410	6.3224520	2.8232670
P	-1.2390570	-1.5558350	1.2433920
C	-1.9427410	0.6674280	2.7260630
H	-2.6088030	1.1679470	3.4402940
H	-0.9170630	0.7937910	3.0745240
H	-2.0277890	1.1649350	1.7583080
C	-1.9255380	-1.4675690	3.9999420
H	-2.4068630	-0.9031570	4.8076500
H	-2.2553990	-2.5049160	4.0862620
H	-0.8450820	-1.4309390	4.1732350
C	-0.9027250	-4.0146620	-0.0649160
H	-1.6491200	-3.7833380	-0.8304190
H	0.0601290	-3.6207640	-0.3911750
H	-0.8199300	-5.1066320	-0.0082550
C	-2.6940250	-4.0364860	1.6587240
H	-2.6638690	-5.1299470	1.5763940
H	-3.0172690	-3.7997310	2.6740700
H	-3.4591760	-3.6805720	0.9612310

PNN-TSI2

Ru	0.7851410	-0.4301400	0.9214340
H	1.3193910	-1.7880590	1.6462920
P	2.5974090	-0.6711320	-0.4917850
O	2.1569680	1.3096840	2.9848340
N	-1.2136490	-0.9311740	1.9548140
N	-0.1937120	-1.5505840	-0.6027800
C	1.6907090	-1.0994690	-2.0694770
C	0.3940780	-1.8102540	-1.7901270
C	-0.2423460	-2.6302250	-2.7252350
H	0.2413300	-2.8380860	-3.6733370
C	-1.4994900	-3.1525350	-2.4295570
H	-2.0043960	-3.7987420	-3.1415390
C	-2.1196130	-2.8130610	-1.2259740
H	-3.1232060	-3.1496130	-0.9921180
C	-1.4404930	-1.9830870	-0.3367910
C	-2.1194330	-1.3542800	0.8515400
H	-2.5788030	-0.4456190	0.4612460

H	-2.9282480	-1.9985980	1.2180480
C	1.6283810	0.6250710	2.2002770
C	3.7151180	0.7936830	-0.9882530
C	2.8142320	2.0420240	-0.9984740
H	3.4126320	2.9109870	-1.2990870
H	1.9822640	1.9431090	-1.6974600
H	2.3917890	2.2462090	-0.0139770
C	4.8142600	0.9965630	0.0730630
H	5.3296220	1.9428370	-0.1302240
H	4.3939500	1.0627090	1.0816960
H	5.5688740	0.2061500	0.0599710
C	4.3416800	0.6507990	-2.3910930
H	5.0208380	-0.1966160	-2.4839550
H	3.5761040	0.5668940	-3.1678980
H	4.9197180	1.5574030	-2.6077860
C	3.6670830	-2.2284440	-0.1445690
C	4.2131560	-2.1695660	1.2967300
H	4.9097940	-1.3426700	1.4476250
H	3.3966760	-2.0662920	2.0147790
H	4.7530090	-3.0996300	1.5142290
C	4.8342860	-2.4121400	-1.1322330
H	5.3235800	-3.3728970	-0.9298780
H	4.4985080	-2.4339810	-2.1742900
H	5.5954580	-1.6358920	-1.0314020
C	2.7483790	-3.4651040	-0.2638010
H	1.8765890	-3.3787230	0.3885100
H	2.4057520	-3.6295840	-1.2900820
H	3.3143760	-4.3549320	0.0374440
C	-1.0647330	-2.0764430	2.9074950
H	-0.6036180	-2.8850340	2.3357410
H	-2.0662990	-2.4178360	3.2120890
C	-0.2317050	-1.7810290	4.1479120
H	0.7566120	-1.4120430	3.8693740
H	-0.7129780	-1.0503720	4.8048560
H	-0.1092410	-2.7062340	4.7202280
C	-1.7791710	0.2911920	2.6091140
H	-1.0420340	0.6396900	3.3350010
H	-1.8395080	1.0414650	1.8190260
C	-3.1480560	0.1270270	3.2788160
H	-3.4559420	1.0922750	3.6940400
H	-3.9171430	-0.1833850	2.5650040
H	-3.1273330	-0.5931110	4.1021670
H	2.3038970	-1.6339850	-2.7999010
C	-0.6419030	1.7504500	-1.0755930
H	0.0359290	0.9365760	0.0050790
O	-0.2220370	1.3368410	-2.1904810
N	-2.0558500	1.5402930	-0.7527510
H	-2.4659500	2.4179110	-0.4533740
C	-2.8399480	0.8935160	-1.8007620
H	-3.0360440	1.5731300	-2.6472550
H	-2.2212250	0.0960880	-2.2172310
H	1.3921100	-0.1288180	-2.4875560
C	-4.1560980	0.3183720	-1.3117870
C	-4.7537290	-0.7259800	-2.0322850
C	-4.8079180	0.7882330	-0.1641150

C	-5.9601940	-1.2902050	-1.6170650
H	-4.2561740	-1.1055800	-2.9214480
C	-6.0142660	0.2237500	0.2587150
H	-4.3579650	1.5823190	0.4230650
C	-6.5948890	-0.8188720	-0.4647640
H	-6.4019210	-2.1022380	-2.1884790
H	-6.4982950	0.6003560	1.1557440
H	-7.5313040	-1.2599360	-0.1355930
C	-0.1951820	3.1174610	-0.5533110
C	0.1585860	4.0853580	-1.4988250
C	-0.1711960	3.4468470	0.8050420
C	0.5335940	5.3664040	-1.0908520
H	0.1528540	3.8035780	-2.5470720
C	0.1996430	4.7278000	1.2151460
H	-0.3925690	2.6790350	1.5385490
C	0.5528800	5.6924090	0.2671940
H	0.8169180	6.1087860	-1.8324640
H	0.2311320	4.9675350	2.2745820
H	0.8519650	6.6870590	0.5863140

PNN-TSR

Ru	0.75733600	1.17819700	-0.28126600
H	1.34823600	1.93842700	0.97690400
P	2.08992800	-0.67663100	0.16670400
O	2.79958700	2.71949000	-1.91551200
N	-0.57571100	0.12227800	1.00099200
C	0.72729200	-1.86260400	0.57114700
C	-0.40603300	-1.19944600	1.24806600
C	-1.36088400	-1.87904000	2.02234600
H	-1.24202600	-2.94209800	2.19687900
C	-2.46276600	-1.19465600	2.51110000
H	-3.22408100	-1.72309000	3.07523800
C	-2.60273900	0.17585400	2.25661700
H	-3.45486800	0.73413200	2.62767000
C	-1.62480700	0.80597300	1.50328700
C	-1.59293000	2.29419600	1.25064300
H	-2.57923300	2.73190000	1.44540300
H	-0.88903800	2.73890500	1.96343300
C	1.99803500	2.12803300	-1.31413900
C	3.09315400	-1.50646600	-1.23541500
C	2.42089200	-1.18548300	-2.58919800
H	3.01414300	-1.66386000	-3.37936600
H	1.40012500	-1.57247300	-2.63892900
H	2.40941100	-0.11098400	-2.78804100
C	4.52835500	-0.94574200	-1.28362800
H	5.03236900	-1.35902000	-2.16492300
H	4.53222900	0.14396000	-1.38817500
H	5.12912500	-1.21383600	-0.41249800
C	3.10974900	-3.04049400	-1.06856400
H	3.53588900	-3.36731300	-0.11761700
H	2.10081900	-3.44922800	-1.16501500
H	3.71974800	-3.47512200	-1.86973300
C	3.14111900	-0.53831000	1.76267100
C	4.12014200	0.64891600	1.66166400
H	4.88619800	0.50658800	0.89865000

H	3.58527700	1.57611600	1.44088700
H	4.63441300	0.77212900	2.62286800
C	3.90075900	-1.83878300	2.09110000
H	4.39815300	-1.72654200	3.06235600
H	3.22301100	-2.69517400	2.16912200
H	4.67256300	-2.07881700	1.35773400
C	2.17486600	-0.25361400	2.93473500
H	1.57877200	0.64410500	2.75917400
H	1.49555800	-1.08929300	3.12241000
H	2.76574800	-0.09752500	3.84540600
C	-0.62588000	4.04867800	-0.19207000
C	-2.06825900	2.24031700	-1.17037100
C	-3.41518100	2.97035400	-1.23352900
H	-4.05640100	2.44181300	-1.94662400
H	-3.93669800	2.97692300	-0.27174600
H	-3.31874600	4.00077500	-1.58290500
H	1.04721700	-2.78196200	1.06607800
O	-0.43239900	-2.04796200	-1.83049600
H	0.26118000	-2.09634700	-0.50961700
H	-0.10042400	0.44461700	-1.94541400
H	-0.28590700	-0.33067100	-1.81253800
C	-1.53036100	5.13885600	0.40033000
H	-1.04167400	6.10752500	0.25308600
H	-2.51577800	5.18988100	-0.06390900
H	-1.66900500	5.00945800	1.47788900
C	-1.44446000	-2.98945900	-1.88490900
H	-1.72624200	-3.22081800	-2.93398000
H	-1.12988000	-3.96520500	-1.45446400
C	-2.72385900	-2.57093100	-1.16274800
C	-3.22876400	-1.27763200	-1.35239300
C	-3.42170000	-3.43368300	-0.31124600
C	-4.38891500	-0.85366400	-0.70723000
H	-2.68981600	-0.61497300	-2.02202700
C	-4.58817600	-3.01819800	0.33880900
H	-3.04292900	-4.44112000	-0.14996700
C	-5.07420200	-1.72415800	0.14732700
H	-4.76378000	0.15438000	-0.86976400
H	-5.11341100	-3.70386700	0.99945100
H	-5.97823400	-1.39698100	0.65401700
N	-1.08922000	2.62880500	-0.11002800
H	-2.25169700	1.17562900	-1.02801600
H	-1.54861000	2.34421700	-2.12647900
H	-0.43263500	4.24518800	-1.25076100
H	0.33956400	4.08574900	0.31790400

PNP-TSR

Ru	-0.68197100	-0.87876000	-0.33889900
H	-1.33554900	-1.84985800	0.73328600
P	-2.51499000	0.61393600	-0.02428100
O	-1.93666500	-2.66088300	-2.44439300
N	0.07054100	0.28192200	1.36905900
C	-1.56286600	1.97391500	0.76529100
C	-0.53045700	1.46904000	1.67618900
C	-0.09427300	2.20503800	2.79472300
H	-0.58362400	3.14451700	3.02714100

C	0.95431800	1.73513700	3.56677400
H	1.30393600	2.30489900	4.42300700
C	1.55359500	0.51470100	3.24003200
H	2.36489200	0.10865600	3.83365800
C	1.07140500	-0.19777900	2.14694900
C	1.59874900	-1.57762300	1.83577400
H	2.64164100	-1.67773900	2.15050000
H	1.01518200	-2.29668100	2.42230300
C	-1.44229700	-1.95804400	-1.66005300
C	-3.38593200	1.39905400	-1.53811500
C	-2.39351900	1.40785000	-2.72219300
H	-2.88547300	1.89160700	-3.57600600
H	-1.48024300	1.95776500	-2.48152200
H	-2.12446800	0.39202500	-3.02473800
C	-4.61027600	0.56810700	-1.96852900
H	-4.99752100	0.98082100	-2.90760200
H	-4.34245100	-0.47600400	-2.15896100
H	-5.42763500	0.59170400	-1.24510000
C	-3.79678600	2.85745300	-1.24903200
H	-4.48051300	2.95229100	-0.40258200
H	-2.91739500	3.47845700	-1.06004200
H	-4.30569400	3.26492500	-2.13121800
C	-3.80555100	0.03867700	1.27099700
C	-4.43071500	-1.30361800	0.83869500
H	-5.03256000	-1.22145600	-0.06700100
H	-3.65615800	-2.05617000	0.66841500
H	-5.08948600	-1.66757600	1.63707600
C	-4.90259100	1.08748300	1.53321200
H	-5.54026200	0.74432600	2.35746900
H	-4.47537700	2.05087800	1.83001500
H	-5.55027400	1.25088100	0.67004400
C	-3.05813700	-0.19948900	2.60220000
H	-2.22504600	-0.89498200	2.47910800
H	-2.67350300	0.72920100	3.03086900
H	-3.75979600	-0.63212600	3.32567100
C	1.29237700	-3.97337000	0.13406700
C	1.43986000	-4.54506500	-1.28963900
H	0.71837400	-4.10024600	-1.98175700
H	2.44451000	-4.39846000	-1.69283300
H	1.25221300	-5.62496700	-1.26414800
C	2.88952700	-1.42301500	-0.83655500
C	4.17988400	-2.18682800	-0.48821800
H	5.03038100	-1.66717600	-0.94531500
H	4.36491300	-2.22053000	0.59026900
H	4.17936900	-3.20953000	-0.87305200
H	-2.16320700	2.77310600	1.20485300
O	0.08029800	2.51134500	-1.18914400
H	-0.84332900	2.39838400	-0.18191000
P	1.32733800	-2.06509300	0.05360900
H	0.17390400	0.06031600	-1.73402200
H	0.15517500	0.80627800	-1.43387000
C	3.06693700	0.04971300	-0.40683300
H	2.17763600	0.65971000	-0.56761900
H	3.35370800	0.14420400	0.64355400
H	3.87244200	0.50078200	-0.99505100

C	2.66525500	-1.46708600	-2.36234200
H	1.78239100	-0.89591300	-2.65582800
H	3.53243400	-1.01796800	-2.86049100
H	2.55617600	-2.48485000	-2.74400000
C	-0.08823600	-4.39846500	0.68151500
H	-0.89841600	-4.10905100	0.01164600
H	-0.10097600	-5.49000000	0.78904200
H	-0.30236000	-3.96511400	1.66301800
C	2.37485200	-4.57393000	1.05610100
H	2.27258500	-5.66580100	1.05652700
H	3.38950200	-4.34264800	0.73380200
H	2.26149700	-4.24156500	2.09217600
C	0.80157200	3.69591800	-1.30523300
H	0.80679100	4.07143200	-2.34650200
H	0.33669800	4.50187900	-0.69896800
C	2.24406500	3.54646500	-0.84270100
C	3.31004400	3.51377500	-1.74729000
C	2.52322500	3.37562000	0.52025200
C	4.62320500	3.32182100	-1.30568100
H	3.10775700	3.63772300	-2.80885400
C	3.82782600	3.17930500	0.96899100
H	1.70178500	3.38653900	1.22945400
C	4.88637000	3.15285700	0.05475600
H	5.43932600	3.30347400	-2.02369000
H	4.02055600	3.04665900	2.03089800
H	5.90559000	3.00289600	0.40077300

PNN-TSS

Ru	0.90225300	1.08169500	-0.29877000
H	1.59908600	1.70062200	0.98315200
P	1.88028900	-0.95565300	0.22138600
O	3.22182400	2.20729300	-1.88784500
N	-0.61470300	0.27528000	0.98159600
C	0.35188100	-1.90025000	0.60554300
C	-0.66042900	-1.05828200	1.24427200
C	-1.70840400	-1.55315700	2.04799600
H	-1.76960200	-2.61831500	2.23934400
C	-2.65620300	-0.68292800	2.55846700
H	-3.47773800	-1.06662600	3.15509700
C	-2.56072200	0.69218200	2.29912000
H	-3.28316500	1.39546400	2.69773900
C	-1.50956500	1.13339300	1.51084200
C	-1.21002900	2.59227300	1.25989200
H	-2.09056200	3.21123400	1.47908400
H	-0.42212100	2.88435400	1.95904400
C	2.30841800	1.77881200	-1.29913800
C	2.82453600	-1.96355600	-1.10818700
C	2.25868600	-1.61437000	-2.50200700
H	2.82660400	-2.17772700	-3.25331300
H	1.21041900	-1.89583800	-2.59727900
H	2.38244700	-0.55151100	-2.72425900
C	4.31876800	-1.58527900	-1.12484900
H	4.79690300	-2.08165000	-1.97775000
H	4.45735600	-0.50703500	-1.25274300
H	4.85341200	-1.90190100	-0.22812800

C	2.64725300	-3.48087200	-0.89701900
H	3.00952400	-3.82481300	0.07316200
H	1.59686600	-3.76571400	-0.99781200
H	3.21218100	-4.01774400	-1.66933300
C	2.90825500	-0.92744800	1.85142000
C	4.05153800	0.10366200	1.76113600
H	4.81554900	-0.16939300	1.03273300
H	3.66537000	1.09154100	1.49769500
H	4.54432500	0.17873100	2.73880800
C	3.46338900	-2.31269900	2.23445200
H	3.93198000	-2.25040700	3.22447700
H	2.66879100	-3.06325200	2.29715200
H	4.22410700	-2.67478300	1.54052400
C	1.96000000	-0.48015700	2.98719300
H	1.50530100	0.48992400	2.77608600
H	1.16235900	-1.20564800	3.16628200
H	2.54094500	-0.39028200	3.91327100
C	-0.17561900	4.22667400	-0.25536300
C	-1.77018700	2.58943500	-1.12536700
C	-2.98920700	3.51984000	-1.09340500
H	-3.69463700	3.18300400	-1.86007300
H	-3.51712200	3.49020800	-0.13516500
H	-2.73985100	4.56127400	-1.31449400
H	0.49827800	-2.86048700	1.10529000
O	-0.77241500	-2.17636600	-1.75289800
H	-0.23141400	-2.14303700	-0.61007300
H	-0.64220000	-0.83614300	-2.00128600
C	1.07351000	4.57199300	0.55104200
H	1.91775300	3.94186400	0.27256100
H	1.33270600	5.61777400	0.35383000
H	0.91720400	4.47266700	1.62884600
N	-0.69343700	2.83508500	-0.11512900
H	-2.09355100	1.56012100	-0.99068300
H	-1.29250700	2.62166900	-2.10586000
H	0.03661100	4.36108600	-1.32066600
H	-0.97278400	4.93827700	0.00815200
O	-0.37277600	0.24407100	-2.12355700
H	0.21369800	0.25537700	-2.88853100
C	-1.99065200	-2.88030100	-1.80737800
H	-2.28683000	-2.99465700	-2.86292900
H	-1.84777100	-3.90071200	-1.41680400
C	-3.13601500	-2.22355400	-1.05333100
C	-3.96528300	-2.96665200	-0.20730800
C	-3.39664800	-0.85585500	-1.21767800
C	-5.03380800	-2.36304500	0.46160600
H	-3.77113900	-4.02784000	-0.06668200
C	-4.45448000	-0.24772300	-0.54431700
H	-2.75520600	-0.27146500	-1.86901800
C	-5.27948100	-0.99961200	0.29775000
H	-5.66739500	-2.95650300	1.11561700
H	-4.63642300	0.81589700	-0.67531300
H	-6.10432000	-0.52505200	0.82218500

PNP-TSS

Ru	-0.87967200	0.82082700	-0.26399700
----	-------------	------------	-------------

H	-1.52953500	1.50706100	0.99211500
P	1.04324500	2.16991100	0.17154900
O	-2.49296000	2.74575200	-1.95030600
N	0.26257100	-0.51320800	1.09608800
C	2.22300800	0.83151800	0.56089300
C	1.60316900	-0.29708600	1.25225100
C	2.36282000	-1.21074800	2.01415300
H	3.43212000	-1.05990700	2.09940300
C	1.75117400	-2.30183900	2.59993900
H	2.34204000	-3.02248000	3.15627000
C	0.36654700	-2.47261800	2.47229500
H	-0.14609100	-3.30020600	2.94955600
C	-0.34970800	-1.54762300	1.72475100
C	-1.85850100	-1.60237700	1.64946600
H	-2.22714100	-2.61720700	1.82543100
H	-2.25421200	-0.97290100	2.45520400
C	-1.85796300	1.99624500	-1.31940500
C	1.85462100	3.21491000	-1.21589400
C	1.53031400	2.56692700	-2.58030700
H	1.94849800	3.20115100	-3.37230800
H	1.98598500	1.58039300	-2.67005700
H	0.45033700	2.50450300	-2.74330100
C	1.27183800	4.64134800	-1.24402000
H	1.66938400	5.16604900	-2.12094800
H	0.18090300	4.63044200	-1.33596100
H	1.53958500	5.23241300	-0.36703400
C	3.38939400	3.25884300	-1.06746000
H	3.71324300	3.68604600	-0.11627600
H	3.81542700	2.25762300	-1.16770900
H	3.80877200	3.88069000	-1.86849800
C	0.89437000	3.22804400	1.77239400
C	-0.29313100	4.20755600	1.67786600
H	-0.13803000	5.00007000	0.94523800
H	-1.21406000	3.67887600	1.41818200
H	-0.44028800	4.68999300	2.65239500
C	2.19351900	3.98407000	2.11178400
H	2.08353800	4.47057000	3.08907600
H	3.04852900	3.30332300	2.18020900
H	2.43461200	4.76489600	1.38786000
C	0.60578700	2.25641400	2.93937000
H	-0.29607400	1.66662800	2.76275600
H	1.43609300	1.56876300	3.11811500
H	0.45673400	2.84265700	3.85449700
C	-4.29424500	-0.30735800	0.57439300
C	-2.59752300	-2.33003000	-1.14014000
C	-3.70147600	-3.36370700	-0.86252700
H	-3.56632700	-4.21440100	-1.54189300
H	-3.65439900	-3.75419000	0.15908800
H	-4.70399900	-2.96664900	-1.03742200
H	3.15611100	1.15264500	1.03048300
O	2.78243300	-0.21100600	-1.77004400
H	2.57590900	0.30098000	-0.64097200
H	1.26769500	-0.43700600	-1.98734900
C	-4.17942900	0.99183700	1.40299100
H	-3.77520300	1.81611300	0.81443200

H	-5.18096500	1.27344200	1.75081900
H	-3.54322700	0.87172700	2.28512400
P	-2.53001500	-0.85406100	0.07065400
C	-1.23026000	-3.03788000	-1.03087400
H	-0.40792100	-2.33450400	-1.14430200
H	-1.11268800	-3.56841500	-0.08187600
H	-1.15214400	-3.78093300	-1.83436900
C	-2.74698500	-1.77355800	-2.57170600
H	-2.74687600	-2.60878400	-3.28302200
H	-3.67896800	-1.22117100	-2.71306300
H	-1.90923800	-1.12005200	-2.81813100
C	-5.04361800	-1.34683400	1.43519000
H	-6.02618400	-0.94045300	1.70417200
H	-5.21430400	-2.29082300	0.91969800
H	-4.51770800	-1.55884200	2.37087900
C	-5.10695700	0.01263300	-0.69608300
H	-5.34273800	-0.88151400	-1.27779000
H	-6.05887400	0.47427700	-0.40742100
H	-4.57948200	0.71984300	-1.34344000
O	0.25695400	-0.38450400	-2.10709400
H	0.14429100	0.19534700	-2.86918300
C	3.85520400	-1.11329500	-1.75799500
H	4.09856100	-1.39764600	-2.79594500
H	4.76450200	-0.63248800	-1.35546400
C	3.59045400	-2.38248000	-0.96192600
C	4.53551400	-2.89435900	-0.06678900
C	2.37928600	-3.06797900	-1.12175800
C	4.28113100	-4.06435000	0.65447600
H	5.47817700	-2.36872800	0.07147900
C	2.11716600	-4.23137400	-0.40108000
H	1.64062900	-2.67728100	-1.81321200
C	3.06825600	-4.73498600	0.49177400
H	5.02680800	-4.44635000	1.34705400
H	1.16927100	-4.74509000	-0.53428600
H	2.86396800	-5.64131000	1.05532500

PNN-26

Ru	0.71890600	0.99659100	-0.35709700
H	1.42083000	2.00224400	0.78791700
P	2.29937900	-0.63129100	0.00039700
O	2.15385200	2.43353600	-2.60615400
N	-0.23782000	-0.00990000	1.25895100
C	1.24226200	-1.90573400	0.89940000
C	0.13000700	-1.24324700	1.66989400
C	-0.52244200	-1.84875400	2.74593000
H	-0.21691500	-2.83788700	3.06932900
C	-1.56728300	-1.17764900	3.38012800
H	-2.09226900	-1.64187300	4.20939600
C	-1.93277800	0.09456900	2.93799700
H	-2.73834300	0.64614300	3.41046600
C	-1.23153700	0.66002600	1.87704100
C	-1.42506100	2.07876900	1.40613700
H	-2.40418500	2.46269400	1.72209800
H	-0.64983600	2.67696500	1.89388000
C	1.59052700	1.88813600	-1.74154100

C	3.04919000	-1.62888400	-1.45021800
C	1.98375400	-1.72990600	-2.56265700
H	2.41073200	-2.30257300	-3.39599500
H	1.07676600	-2.23926000	-2.23026500
H	1.68978600	-0.74529600	-2.92702600
C	4.25799300	-0.85937200	-2.01889300
H	4.58772800	-1.34602100	-2.94451600
H	3.99676000	0.17449700	-2.26416100
H	5.10916000	-0.84991500	-1.33460900
C	3.46511200	-3.06351100	-1.06360400
H	4.23792600	-3.09870100	-0.29657100
H	2.61162600	-3.65500400	-0.71995800
H	3.86444100	-3.56548600	-1.95336700
C	3.66051900	-0.20871400	1.28777900
C	4.40265300	1.06528900	0.83297300
H	4.97711800	0.91422000	-0.08364400
H	3.69538700	1.88135500	0.66789200
H	5.10821000	1.36850500	1.61660500
C	4.67280700	-1.33839000	1.55272000
H	5.33029100	-1.03977800	2.37849800
H	4.18556100	-2.27330100	1.84962700
H	5.31208400	-1.54161100	0.69083300
C	2.94401100	0.11065400	2.61982800
H	2.18201600	0.88159500	2.48372600
H	2.48126200	-0.77512000	3.06609300
H	3.68542100	0.48381300	3.33661700
C	-1.17691100	3.65289100	-0.46606700
C	-2.32336100	1.52187900	-0.81035000
C	-3.75022400	2.05014400	-0.62429400
H	-4.42203400	1.39028400	-1.17972300
H	-4.07777400	2.01965100	0.41908300
H	-3.88599600	3.06754900	-1.00169600
H	1.82825900	-2.56957400	1.54214600
O	-1.08817300	-2.22903000	-1.12878000
H	0.77691900	-2.52008400	0.12097000
H	-0.11845700	0.01147700	-1.49258500
H	-0.73097000	-1.30188600	-1.21150800
C	-0.03552500	4.49255100	0.10020900
H	0.93422200	4.05183300	-0.12877100
H	-0.09420700	5.49204200	-0.34433400
H	-0.10448400	4.61510000	1.18520500
N	-1.21904900	2.21463600	-0.06135800
H	-2.29241100	0.47537600	-0.51608200
H	-2.03915400	1.55221800	-1.86379000
H	-1.11248100	3.64722400	-1.55815300
H	-2.13121500	4.12959800	-0.19855100
C	-2.27685500	-2.32163100	-1.88333900
H	-2.40753500	-3.37928200	-2.15153600
H	-2.19391200	-1.76663100	-2.83082000
C	-3.51366200	-1.84950900	-1.13347100
C	-3.50408400	-1.75428700	0.26188900
C	-4.68464800	-1.51755800	-1.82622200
C	-4.64023600	-1.32683600	0.95140000
H	-2.59114800	-1.99917000	0.79224700
C	-5.82699700	-1.10415200	-1.13803200

H	-4.70098600	-1.57813500	-2.91259300
C	-5.80700600	-1.00363300	0.25586400
H	-4.60984500	-1.24608500	2.03468700
H	-6.72799900	-0.84896100	-1.68935200
H	-6.69159100	-0.67144400	0.79194000

PNP-26

Ru	-0.74817200	0.52985800	-0.48904000
H	-1.61860800	1.92162200	-0.20374200
P	1.23146100	1.71248000	-0.05934200
O	-0.84981000	0.91337700	-3.48702100
N	-0.65537400	0.27139900	1.69048700
C	1.71893700	0.87922400	1.54313300
C	0.51349100	0.46203900	2.34806300
C	0.60750500	0.25006300	3.72447000
H	1.55784500	0.40427500	4.22376900
C	-0.51319400	-0.17455500	4.42971600
H	-0.45527000	-0.35880500	5.49832000
C	-1.71380200	-0.35143300	3.74672000
H	-2.61245600	-0.66475900	4.26712400
C	-1.76295100	-0.10660600	2.37453600
C	-3.06314700	-0.18750200	1.61261300
H	-3.76491800	-0.86707600	2.10528300
H	-3.51318600	0.81245400	1.62149800
C	-0.81282000	0.76370000	-2.32923000
C	2.77753600	1.49652600	-1.16402700
C	2.72350500	0.07638100	-1.76182300
H	3.63788800	-0.09682300	-2.34201100
H	2.67509600	-0.69337800	-0.99367100
H	1.86014900	-0.05636700	-2.41457600
C	2.72529300	2.50194800	-2.33084400
H	3.51865100	2.25481600	-3.04631700
H	1.77144900	2.44835500	-2.86501100
H	2.88583800	3.53308000	-2.00850800
C	4.10812100	1.63637900	-0.39494100
H	4.23347700	2.60819200	0.08300300
H	4.21808200	0.85657500	0.36311300
H	4.93797500	1.50693400	-1.10033400
C	1.02389900	3.55524900	0.43223500
C	0.30428900	4.29903700	-0.71181100
H	0.90961800	4.36485500	-1.61827100
H	-0.63567900	3.79967800	-0.95909100
H	0.08111800	5.32412900	-0.39047100
C	2.33849500	4.27408800	0.78423600
H	2.10853200	5.28602900	1.14048200
H	2.88604300	3.76663000	1.58552900
H	3.00391900	4.37798300	-0.07534100
C	0.10674800	3.59673500	1.67487000
H	-0.82778800	3.06124700	1.49301100
H	0.59019300	3.17603200	2.56202100
H	-0.13409200	4.64263900	1.90054600
C	-4.37373800	0.14644900	-1.02600200
C	-2.82629100	-2.48573900	-0.28937200
C	-4.21349500	-3.14153800	-0.17304700
H	-4.08661500	-4.23073200	-0.13821500

H	-4.73125200	-2.84661100	0.74531300
H	-4.86158500	-2.92109400	-1.02401000
H	2.40404100	1.47549700	2.15386100
O	1.28365700	-2.22878900	1.14415300
H	2.24585900	-0.03503700	1.25082300
H	0.15213200	-0.92807600	-0.65501900
H	0.86962900	-1.66501800	0.43814100
C	-4.24226800	1.68353500	-1.08974900
H	-3.38126500	1.99366400	-1.68099600
H	-5.15381300	2.08980300	-1.54640800
H	-4.13240500	2.13585600	-0.10004800
P	-2.79845200	-0.56865500	-0.20198200
C	-1.96557000	-3.00692700	0.88108800
H	-0.97667500	-2.55145200	0.91934800
H	-2.45308500	-2.85558200	1.84965700
H	-1.82482800	-4.08816800	0.75911000
C	-2.15731900	-2.90747900	-1.61403800
H	-2.08683500	-4.00192200	-1.65078700
H	-2.72630500	-2.58390000	-2.48994600
H	-1.15113100	-2.48758200	-1.68670700
C	-5.68086800	-0.17681600	-0.27058800
H	-6.51482700	0.32392500	-0.77745500
H	-5.91389800	-1.23995000	-0.24044000
H	-5.66023900	0.19806100	0.75762900
C	-4.44860100	-0.37732200	-2.47489900
H	-4.64720000	-1.45011300	-2.52312200
H	-5.26623100	0.13047000	-3.00055100
H	-3.52396700	-0.17172600	-3.02302100
C	1.92722500	-3.32040200	0.50768700
H	1.97431000	-4.13219100	1.24595000
H	1.33619700	-3.69300500	-0.34192900
C	3.32965500	-2.97258100	0.04333500
C	3.79690000	-3.34394200	-1.22032700
C	4.17168500	-2.23246400	0.88513900
C	5.07768800	-2.97757700	-1.64275900
H	3.14679300	-3.90419500	-1.88815600
C	5.44844900	-1.86120000	0.46625300
H	3.80209000	-1.93414700	1.86197600
C	5.90478500	-2.23089300	-0.80291700
H	5.42250500	-3.26334900	-2.63267600
H	6.08852300	-1.28139000	1.12595400
H	6.89663100	-1.93623400	-1.13381100

PNN-28

Ru	-1.29912300	0.65252900	-0.38902500
H	-2.15348400	1.48539000	0.69732300
P	0.63829100	1.68934900	0.24651600
O	-2.12629900	2.71959000	-2.43675100
N	-0.68612100	-0.74051400	1.14208500
C	1.54875900	0.17876200	0.88696800
C	0.60057100	-0.79551100	1.53680200
C	1.00888800	-1.74107900	2.47861500
H	2.04636400	-1.77070900	2.79040600
C	0.08052000	-2.65621300	2.96474700
H	0.38344100	-3.41262500	3.68270000

C	-1.23894600	-2.60670500	2.51341200
H	-1.98030300	-3.31698100	2.86326100
C	-1.59539900	-1.61875000	1.60134000
C	-3.01391200	-1.39193400	1.13067900
H	-3.62967500	-2.27662100	1.34388600
H	-3.41726400	-0.56220300	1.71805800
C	-1.81447800	1.90447000	-1.65956300
C	1.82856200	2.43137100	-1.04978100
C	1.65228200	1.63129100	-2.35969600
H	2.41695900	1.96547400	-3.07267900
H	1.73122200	0.55426200	-2.21202100
H	0.67050300	1.81727900	-2.80051600
C	1.45384300	3.89751900	-1.34368100
H	2.04465200	4.24407300	-2.20002600
H	0.39775300	3.99964400	-1.61209300
H	1.66988700	4.56773100	-0.50865500
C	3.30729300	2.33783100	-0.61748900
H	3.52650300	2.89030100	0.29686600
H	3.62519200	1.30207700	-0.48053900
H	3.93060900	2.76497200	-1.41301300
C	0.49175900	2.84863500	1.76340200
C	-0.51044200	3.97910000	1.44890600
H	-0.15748600	4.65318700	0.66633200
H	-1.47278500	3.56561900	1.13839000
H	-0.66595100	4.57943600	2.35378000
C	1.83416600	3.44713400	2.22271100
H	1.67392800	4.00995600	3.15057000
H	2.57955700	2.67421500	2.43700300
H	2.25687600	4.14143500	1.49404500
C	-0.08471600	2.01966400	2.93340100
H	-1.03086200	1.54695600	2.66228200
H	0.60780300	1.24532900	3.27633300
H	-0.26780000	2.69158300	3.78057800
C	-4.46101200	-0.50336600	-0.63762400
C	-2.73795800	-2.14331100	-1.19580800
C	-3.70505700	-3.33433500	-1.21840700
H	-3.27073400	-4.11133800	-1.85517900
H	-3.84647000	-3.77826000	-0.22774800
H	-4.68948400	-3.08603800	-1.62508600
H	2.39474700	0.41363800	1.53762700
O	0.35005400	-3.03205000	-0.53121400
H	1.93991500	-0.30917100	-0.01184800
H	0.20513900	-2.12561300	-1.00175400
C	-4.88880600	0.81823700	-0.00548800
H	-4.22814800	1.63248300	-0.30132200
H	-5.90805400	1.04464000	-0.33727200
H	-4.90261500	0.77729400	1.08748000
N	-3.09546800	-0.99663900	-0.30036400
H	-1.74759000	-2.49199000	-0.91189900
H	-2.64166400	-1.72487700	-2.20138800
H	-4.47928800	-0.39761700	-1.72697500
H	-5.20034300	-1.27593500	-0.37686500
O	-0.02761800	-0.78795200	-1.61934000
H	-0.35380700	-0.81378600	-2.52581500
C	1.46789700	-3.64705200	-1.12148100

H	1.34134600	-3.78526200	-2.21053200
H	1.57367600	-4.64952900	-0.68401900
C	2.73745500	-2.85116500	-0.87356500
C	3.41969200	-2.95737000	0.34558900
C	3.19147300	-1.91832600	-1.81347500
C	4.52742600	-2.15416900	0.62114100
H	3.06921800	-3.67365400	1.08449200
C	4.30427700	-1.11694700	-1.54882400
H	2.65315100	-1.80792100	-2.75015600
C	4.97372500	-1.22942200	-0.32776900
H	5.04855100	-2.25310800	1.57007500
H	4.64086300	-0.39722000	-2.28966100
H	5.83786000	-0.60479800	-0.11903900

PNP-28

Ru	-0.84266500	-0.78272500	-0.32686800
H	-1.60824200	-1.70715100	0.74391200
P	-2.52910600	0.84331400	0.00432900
O	-2.12954900	-2.39311100	-2.53335200
N	0.02893000	0.31318500	1.37824000
C	-1.51051500	2.15740300	0.85008000
C	-0.40069200	1.56205600	1.67759500
C	0.17264800	2.28646700	2.72637000
H	-0.18767000	3.28632900	2.94165800
C	1.20905300	1.72243900	3.46200100
H	1.67857900	2.27841900	4.26798800
C	1.62972300	0.43089300	3.15635700
H	2.42197300	-0.04794500	3.72114000
C	1.00610500	-0.26319600	2.11934900
C	1.33829000	-1.70882800	1.84583400
H	2.35673200	-1.94368800	2.16745100
H	0.65670700	-2.32104800	2.44816300
C	-1.62790100	-1.76036300	-1.68980800
C	-3.35561000	1.78312100	-1.44257600
C	-2.32873100	1.87073800	-2.59224500
H	-2.79020200	2.41786900	-3.42408700
H	-1.41734600	2.39829100	-2.30362100
H	-2.06125400	0.87495900	-2.95467700
C	-4.56809800	0.98151600	-1.95405600
H	-4.93132200	1.43905200	-2.88201700
H	-4.29954500	-0.05531100	-2.18116700
H	-5.40045600	0.97703500	-1.24734000
C	-3.77851300	3.22091600	-1.07755600
H	-4.50767400	3.26416800	-0.26844200
H	-2.91745300	3.83570700	-0.80172300
H	-4.23779700	3.68739700	-1.95778100
C	-3.84041600	0.36936000	1.32040700
C	-4.55153300	-0.92893300	0.88309400
H	-5.15544400	-0.79687600	-0.01662300
H	-3.82569500	-1.72381200	0.69549700
H	-5.22497800	-1.25688700	1.68462200
C	-4.88275900	1.46697300	1.60568600
H	-5.51794300	1.14752400	2.44104200
H	-4.41689600	2.41400400	1.89777000
H	-5.54163500	1.65545700	0.75551400

C	-3.09314300	0.07568500	2.64174000
H	-2.31623800	-0.67904200	2.50445700
H	-2.63886900	0.97331900	3.07160200
H	-3.81499500	-0.30500000	3.37431400
C	0.69633600	-4.08900500	0.21005400
C	2.64929700	-1.84666600	-0.82608300
C	3.79545700	-2.82287000	-0.51222500
H	4.70848000	-2.45150000	-0.99347600
H	4.00310400	-2.89196200	0.56102100
H	3.61386800	-3.82930400	-0.89717900
H	-2.11888800	2.83269800	1.46027200
O	0.62436000	3.06132500	-1.14866400
H	-1.04175900	2.75966000	0.06326500
H	0.53877800	2.03824900	-1.28933000
C	-0.72201000	-4.32263000	0.77433100
H	-1.49342500	-3.92697100	0.11393600
H	-0.87743900	-5.40293400	0.88661400
H	-0.86508600	-3.86208000	1.75656300
P	1.00114500	-2.20505000	0.07185300
C	3.08034000	-0.42853000	-0.39499700
H	2.29152700	0.29771000	-0.58743200
H	3.37961500	-0.37898900	0.65576800
H	3.95370300	-0.12660400	-0.98426400
C	2.37525200	-1.81963700	-2.34487900
H	3.31324900	-1.59658100	-2.86889000
H	2.00155400	-2.77220100	-2.72912700
H	1.65822600	-1.02838500	-2.56900600
C	1.69336200	-4.81382500	1.13940000
H	1.43291800	-5.87865900	1.17570200
H	2.72635600	-4.74356800	0.80285800
H	1.64268200	-4.43712400	2.16561900
C	0.74752900	-4.70354600	-1.20395500
H	1.75056500	-4.67542500	-1.63560300
H	0.44295400	-5.75570900	-1.15019700
H	0.06068100	-4.19534300	-1.88799800
O	0.36752100	0.60102700	-1.58454800
H	0.01863000	0.56808700	-2.48092700
C	1.82839000	3.46961400	-1.74394500
H	1.79555800	4.56381600	-1.86126600
H	1.94148600	3.05344200	-2.75996400
C	3.06499200	3.10498400	-0.93349700
C	2.97188700	2.94373400	0.45218800
C	4.31059000	2.93444500	-1.54801500
C	4.09676500	2.61738900	1.20955700
H	1.99980400	3.05364800	0.91724200
C	5.44073000	2.61093300	-0.79411300
H	4.39448200	3.04221900	-2.62762600
C	5.33751400	2.44961400	0.58993000
H	4.00156300	2.48532000	2.28455900
H	6.39964200	2.47447400	-1.28743900
H	6.21430200	2.18944500	1.17681000