

Supporting Information For:
Theoretical Study of the Mechanism for CO₂ Hydrogenation to Methanol Catalyzed by
***trans*-RuH₂(CO)(dpa)**

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Table S1. Calculated Gibbs free energies at 298.15 K and 1 atm of all the species. The energies are in Hartree.

Species	G298K
1	-2031.11879
2	-2219.72081
TS2/3	-2219.71339
3	-2219.72183
4	-2219.71729
5	-2029.93673
TS1/6	-2220.863216
6	-2220.863011
TS6/7	-2220.86065
7	-2220.86031
8	-2220.86735
TS8/9	-2220.86882
9	-2220.86944
10	-2106.36976
TS10/11	-2106.36267
11	-2106.36098
12	-2145.62385
TS12/13	-2145.62589
13	-2145.62825
14	-2031.09492
TS14/1	-2031.07759
15	-2107.52232
TS15/16	-2107.51413
16	-2107.5454

Table S2. Cartesian coordinates for the optimized geometries of all the species

1

Ru	0.00827100	0.14897900	0.03989200
H	0.01900500	1.80258700	0.13197400
P	-2.32103800	0.19435500	0.35249600
P	2.33775700	0.15394600	0.35454600
O	0.00988000	0.21526000	-2.95954000
N	0.00661500	0.16380000	2.26885500
C	0.00902900	0.17824400	-1.78861200
C	3.37349500	1.64081000	-0.07970900
C	-3.38476800	-1.19972400	-0.25104500
C	3.38299400	-1.23941100	-0.28053200
C	-3.33360700	1.68567900	-0.11958800
C	3.86969112	-2.27468364	0.53530317
C	-3.88605163	-2.20889098	0.58849780
C	-2.45665700	0.11831800	2.22430000
C	-3.69955354	-1.24060445	-1.62096415
C	-2.70158200	2.81856100	-0.65385300
C	3.69747093	-1.25266970	-1.65120750
C	2.46753800	0.03763300	2.22362900
C	4.76671100	1.64012100	0.11881700
C	2.76358300	2.78855000	-0.60754000
C	-4.50371749	-2.25973514	-2.13626755
C	1.25328600	0.72259500	2.84890600
C	3.52901000	3.91692900	-0.92552400
C	5.52806700	2.76849600	-0.19416800
C	-4.68466679	-3.23433346	0.06873825
C	-1.22081900	0.77046000	2.84224300
C	-4.83275000	3.96415300	-0.81614600
C	4.91057900	3.91056800	-0.71832300
C	4.96521052	-3.29931865	-1.37050390
C	-4.99685503	-3.26150247	-1.29297950
C	4.65341883	-3.29922596	-0.00850052
C	-4.72982200	1.70433600	0.05555800
C	-3.44797300	3.95118900	-1.00039400
C	-5.47225700	2.83703000	-0.28627300
C	4.48667994	-2.27114520	-2.19022928
H	-0.01378300	-0.83802900	2.49663300
H	-3.37656700	0.59764500	2.58941100
H	-2.49069300	-0.94682400	2.50413700
H	2.46350500	-1.03304400	2.48392000
H	3.40249200	0.47770600	2.60004000
H	1.26440000	1.80431500	2.64665200
H	1.26224500	0.58308100	3.94499600
H	-1.23481700	0.64304800	3.93980100
H	-1.19547300	1.84956600	2.62782900
H	3.64398685	-2.29718562	1.60285207
H	-3.66032917	-2.20967290	1.65629998
H	-3.30791402	-0.47424835	-2.29249445
H	-1.61863800	2.80485300	-0.78859000
H	3.31741120	-0.46524655	-2.30479380
H	5.26812000	0.75314200	0.51214700
H	1.68275600	2.78978300	-0.75910000
H	-4.73718696	-2.27598245	-3.20317888
H	3.04013400	4.80227500	-1.33885000
H	6.60853100	2.75391500	-0.03309100
H	-5.06313135	-4.01304424	0.73489054
H	-5.41545700	4.84737000	-1.08789800
H	5.50803500	4.79060700	-0.96741200
H	5.57609001	-4.09975512	-1.79374145
H	-5.61928874	-4.06267936	-1.69756764
H	5.02056682	-4.09858318	0.63927626

H	-5.24860800	0.82909800	0.45240200
H	-2.94169500	4.82446800	-1.41842500
H	-6.55538300	2.83721200	-0.14344400
H	4.72021653	-2.26591544	-3.25724262
H	0.00318900	-1.57372500	0.16908800

2

Ru	0.00028400	-0.23924700	0.01502200
H	0.00022500	-1.91156100	0.21459700
P	2.32383300	-0.21191300	0.32689000
P	-2.32198900	-0.21120000	0.33534700
O	-0.03027200	-0.43688300	-2.97690400
N	0.00512700	-0.11331400	2.25447400
C	-0.02180400	-0.35021900	-1.80592400
C	-3.38206100	-1.69946700	-0.04966500
C	3.36569600	1.16639200	-0.34946700
C	-3.36273700	1.17194200	-0.33864200
C	3.37894200	-1.70413900	-0.05157800
C	-4.31891700	1.86339600	0.42328800
C	4.32005700	1.86425100	0.41012400
C	2.46274000	-0.02578100	2.19445400
C	3.18382500	1.52266800	-1.69724700
C	2.77557800	-2.87782300	-0.52704600
C	-3.18072300	1.53680000	-1.68533100
C	-2.45924700	-0.02900700	2.19960200
C	-4.77854400	-1.66891600	0.12352000
C	-2.78341400	-2.87798300	-0.51933500
C	3.94236600	2.54408100	-2.27295600
C	-1.23529700	-0.66474400	2.85748000
C	-3.56207700	-4.00706900	-0.80194500
C	-5.55333900	-2.79773400	-0.15335900
C	5.07284400	2.89491400	-0.16545400
C	1.24200200	-0.66303000	2.85529600
C	4.93114900	-3.98578100	-0.61092500
C	-4.94680100	-3.97035700	-0.61852000
C	-4.88756600	3.24652400	-1.48631400
C	4.88925000	3.23447800	-1.50859300
C	-5.07144400	2.89789100	-0.14543800
C	4.77400200	-1.68372600	0.13350300
C	3.54797300	-4.01201500	-0.80548800
C	5.54258600	-2.81805800	-0.13903200
C	-3.93956700	2.56223900	-2.25474200
H	0.00469500	0.89556100	2.42977200
H	3.39126200	-0.46764200	2.58417800
H	2.48123900	1.05426900	2.41359700
H	-2.48075200	1.05068800	2.42012800
H	-3.38685200	-0.47303200	2.58961400
H	-1.22548400	-1.75346000	2.69841700
H	-1.25059200	-0.47920700	3.94683800
H	1.25836900	-0.47711900	3.94471200
H	1.23262700	-1.75183400	2.69688900
H	-4.48532500	1.61009400	1.47199700
H	4.48651900	1.61775800	1.46050700
H	2.43544300	1.00433700	-2.29919700
H	1.69255100	-2.89373100	-0.66409700
H	-2.43106800	1.02374300	-2.29026700
H	-5.27286900	-0.75825800	0.46814900
H	-1.69962800	-2.90198000	-0.64752200
H	3.78744800	2.80554200	-3.32224600
H	-3.08138100	-4.91653800	-1.16945100
H	-6.63617400	-2.75831900	-0.01204700
H	5.80783700	3.42907100	0.44065300
H	5.53412900	-4.87049500	-0.82857900
H	-5.55436400	-4.85131500	-0.83902000
H	-5.47499600	4.05395400	-1.92872200

H	5.47665600	4.03884600	-1.95654400
H	-5.80788300	3.42652600	0.46334800
H	5.27182300	-0.77765600	0.48440200
H	3.06339000	-4.91759000	-1.17810000
H	6.62439000	-2.78735900	0.01130700
H	-3.78423500	2.83114500	-3.30211700
H	0.00163800	1.44465400	0.09024000
C	-0.03521027	4.28947108	0.38222969
O	-0.07596584	4.50515160	1.52988988
O	0.00488926	4.11465226	-0.77005676

TS2/3

Ru	0.00000800	-0.01796200	0.04541200
H	0.00006100	1.63980100	0.13411500
P	-2.32600100	0.12039500	0.35571400
P	2.32603400	0.12024300	0.35569700
O	-0.00000900	-0.03524200	-2.96256500
N	0.00001300	-0.03122000	2.29372200
C	-0.00000600	-0.02500700	-1.79260800
C	3.16439900	1.71423600	-0.08784900
C	-3.53256000	-1.13818200	-0.28201200
C	3.53255500	-1.13827700	-0.28221100
C	-3.16435500	1.71433300	-0.08806300
C	3.51409515	-1.55081805	-1.62689083
C	-3.50074891	-1.56629545	-1.62156509
C	-2.46893700	-0.05579800	2.21540200
C	-4.51075894	-1.65866853	0.57910144
C	-2.36321809	2.74729775	-0.60858092
C	4.49735361	-1.67453456	0.58432761
C	2.46895000	-0.05622900	2.21534500
C	2.36530428	2.74292098	-0.61985400
C	4.53063736	1.95851655	0.11695856
C	-5.44629698	-2.58690230	0.10733881
C	1.23400700	0.53967700	2.88954600
C	5.08725069	3.20278216	-0.20623080
C	2.92248082	3.97930026	-0.94972935
C	-4.43783075	-2.49012159	-2.09049863
C	-1.23386900	0.53992700	2.88953700
C	-4.28759215	4.21445246	-0.74065491
C	4.28722562	4.21414598	-0.74192330
C	5.41253758	-3.00359001	-1.22568811
C	-5.41260904	-3.00301309	-1.22630975
C	4.45115430	-2.47491007	-2.09534930
C	-4.53289435	1.95443210	0.10605127
C	-2.92054164	3.98380555	-0.93773044
C	-5.08973476	3.19878812	-0.21638683
C	5.43288004	-2.60298468	0.11296989
H	-0.00008800	-1.03878100	2.49385500
H	-3.39512200	0.38051000	2.61710600
H	-2.51603000	-1.14099900	2.40190900
H	2.51579600	-1.14146900	2.40169300
H	3.39523700	0.37980700	2.61710800
H	1.19839400	1.63063400	2.74847400
H	1.26069300	0.34119000	3.97644300
H	-1.26056800	0.34150100	3.97644500
H	-1.19806000	1.63087000	2.74841000
H	2.76112007	-1.15583394	-2.31254218
H	-2.73734519	-1.18373588	-2.30271522
H	-4.54050457	-1.32972472	1.61877152
H	-1.29225601	2.58610525	-0.75371307
H	4.51671662	-1.35770912	1.62799912
H	1.29601537	2.57848431	-0.77344990
H	5.18078036	1.18681544	0.53174535
H	-6.20140366	-2.98605484	0.78839882
H	6.15271177	3.37589046	-0.03808456

H	2.28728978	4.76501690	-1.36501538
H	-4.40419171	-2.81404312	-3.13335094
H	-4.72299277	5.18381638	-0.99311628
H	4.72246332	5.18343503	-0.99495738
H	6.14141796	-3.73000934	-1.59240852
H	-6.14152769	-3.72925041	-1.59331334
H	4.42795982	-2.78666312	-3.14218625
H	-5.18470573	1.17932864	0.51177730
H	-2.28371305	4.77289057	-1.34402465
H	-6.15702448	3.36858579	-0.05666699
H	6.17746109	-3.01450246	0.79824488
H	-0.00002300	-1.74482900	0.16876700
C	-0.00019200	-3.34268600	0.98844300
O	-0.00024500	-3.04572200	2.14192200
O	-0.00018300	-4.06436700	0.05098300

3

Ru	0.00003200	-0.13424500	0.04135400
H	0.00006500	1.45121500	-0.05273300
P	-2.34062900	0.07238900	0.35169500
P	2.34079800	0.07144600	0.35151000
O	-0.00056300	-0.21459500	-2.97208700
N	0.00005800	-0.07983800	2.26356800
C	-0.00021900	-0.19560800	-1.80759400
C	3.06500300	1.72167600	-0.07025800
C	-3.58584000	-1.12635800	-0.31264800
C	3.58509200	-1.12759000	-0.31401700
C	-3.06386800	1.72268300	-0.07152000
C	4.59536906	-1.65923637	0.50689710
C	-4.60184261	-1.64968458	0.50654870
C	-2.47066500	-0.11873500	2.20672700
C	-3.49736968	-1.54647827	-1.65019858
C	-4.45127411	1.89133165	0.09313442
C	3.50167177	-1.53943132	-1.65447598
C	2.47073000	-0.12132300	2.20636500
C	2.19644709	2.70940467	-0.57070310
C	4.42050794	2.03778994	0.10761988
C	-4.40755849	-2.48087474	-2.15587951
C	1.23360400	0.47858200	2.87408300
C	4.89841650	3.31550616	-0.20970552
C	2.67693584	3.97860847	-0.89632882
C	-5.50906803	-2.58173606	-0.00355198
C	-1.23281200	0.48013600	2.87402800
C	-4.29655848	4.16999230	-0.71658573
C	4.03060808	4.28651319	-0.71377735
C	5.41188943	-2.99997030	-1.33969465
C	-5.41407192	-2.99861522	-1.33596136
C	5.50187754	-2.59133522	-0.00438968
C	-2.30488041	2.79357886	-0.56756641
C	-5.06090663	3.10707597	-0.22005273
C	-2.92045806	4.00926246	-0.89135216
C	4.41111376	-2.47391070	-2.16133952
H	-0.00064500	-1.11095200	2.44041800
H	-3.39892600	0.30621200	2.61535000
H	-2.50487500	-1.20606000	2.38220500
H	2.50362600	-1.20881800	2.38102600
H	3.39949600	0.30216600	2.61534000
H	1.21218100	1.57309400	2.75277900
H	1.24931700	0.26415600	3.95772600
H	-1.24860600	0.26611900	3.95775200
H	-1.21019800	1.57457600	2.75233000
H	4.67974490	-1.34346753	1.54862383
H	-4.69011739	-1.32744428	1.54596654
H	-2.71365222	-1.15690762	-2.30150966
H	-5.06141544	1.06581204	0.46664075

H	2.72243695	-1.14330992	-2.30721179
H	1.13549371	2.48671790	-0.70502294
H	5.12195407	1.29736397	0.49439427
H	-4.32791099	-2.80045711	-3.19718540
H	5.95576674	3.54646950	-0.06233970
H	1.99030313	4.73228279	-1.28805633
H	-6.29422404	-2.98157103	0.64216873
H	-4.77477831	5.11915345	-0.96802570
H	4.40519891	5.28188398	-0.96225457
H	6.12360040	-3.72610118	-1.73896253
H	-6.12634521	-3.72468541	-1.73433560
H	6.28256071	-2.99766715	0.64269723
H	-1.22750788	2.69804171	-0.70896197
H	-6.13816175	3.22281835	-0.08197359
H	-2.31584915	4.83199782	-1.27943178
H	4.33541371	-2.78701361	-3.20490608
H	0.00299100	-2.01129800	0.30543200
C	-0.00072100	-3.04250200	0.94068000
O	-0.00119900	-2.87669800	2.17626300
O	-0.00265700	-4.02235200	0.20004000

4

Ru	-0.00000500	0.02369700	0.03095200
H	-0.00005700	1.61800700	0.09165600
P	-2.33890500	0.09683200	0.35375100
P	2.33888800	0.09700600	0.35371600
O	-0.00003800	0.28232300	-2.95865400
N	0.00002600	0.07416000	2.25283000
C	-0.00002300	0.14713100	-1.79697900
C	3.30791900	1.62416500	-0.07304800
C	-3.42014000	-1.25514500	-0.30298100
C	3.42015000	-1.25508000	-0.30277100
C	-3.30801000	1.62402400	-0.07270100
C	4.29860900	-2.00198000	0.49920100
C	-4.29825500	-2.00253600	0.49890700
C	-2.45848900	-0.02882300	2.21843100
C	-3.34670600	-1.54090700	-1.67850300
C	-4.69323100	1.68525300	0.16788700
C	3.34643100	-1.54141600	-1.67815800
C	2.45856100	-0.02827200	2.21843100
C	4.69317800	1.68546200	0.16730100
C	2.66599800	2.73675400	-0.63737900
C	-4.14003500	-2.54376400	-2.23931700
C	1.23394600	0.64950500	2.83416600
C	3.39290100	3.89130200	-0.95143700
C	5.41565800	2.83961300	-0.14257500
C	-5.08854100	-3.01127100	-0.06471000
C	-1.23402800	0.64915800	2.83424200
C	-4.76696100	3.94583500	-0.70322100
C	4.76668600	3.94598400	-0.70398600
C	5.01301500	-3.28323300	-1.43239200
C	-5.01288800	-3.28314600	-1.43303100
C	5.08895100	-3.01079400	-0.06420000
C	-2.66622100	2.73667100	-0.63705900
C	-5.41580300	2.83940200	-0.14177900
C	-3.39321800	3.89121800	-0.95091400
C	4.13982000	-2.54434400	-2.23875900
H	0.00018296	-1.04599793	2.46459920
H	-3.39112900	0.40878800	2.60314900
H	-2.44582400	-1.10107600	2.46874500
H	2.44622300	-1.10047300	2.46897600
H	3.39109500	0.40969300	2.60300500
H	1.24348600	1.73355700	2.63631200
H	1.24261400	0.51082600	3.93075500

H	-1.24265500	0.51034600	3.93081400
H	-1.24381200	1.73323300	2.63652100
H	4.37858000	-1.80784700	1.56993300
H	-4.37799700	-1.80884000	1.56973500
H	-2.65964600	-0.98010000	-2.31578900
H	-5.21771500	0.82617700	0.59234900
H	2.65909800	-0.98100500	-2.31549700
H	5.21776500	0.82643900	0.59174000
H	1.59230200	2.69376200	-0.82453800
H	-4.06980300	-2.75361900	-3.30891800
H	2.88008300	4.74863700	-1.39346800
H	6.49035200	2.87348300	0.05041200
H	-5.76541700	-3.58461600	0.57276000
H	-5.33425500	4.84629500	-0.94949800
H	5.33390900	4.84644400	-0.95042300
H	5.62944500	-4.07160600	-1.86995100
H	-5.62927400	-4.07146500	-1.87075100
H	5.76609100	-3.58375000	0.57334000
H	-1.59255400	2.69373000	-0.82440100
H	-6.49046500	2.87322200	0.05139300
H	-2.88050300	4.74860000	-1.39297100
H	4.06936600	-2.75464900	-3.30825800
C	0.11274663	-2.70895106	3.69156049
O	0.04590773	-2.28573764	2.49378897
O	0.20363999	-2.03798162	4.74599107
H	0.08469296	-3.82402575	3.78468776

5

Ru	-0.00001800	-0.01144500	0.03247300
H	-0.00010000	1.50803700	-0.31474800
P	-2.34109500	0.07638900	0.35577600
P	2.34098700	0.07704400	0.35583900
O	0.00012900	-0.46191100	-2.95772800
N	-0.00003900	0.11756000	2.12030100
C	0.00006800	-0.31225900	-1.79637600
C	3.29004400	1.61624700	-0.07312700
C	-3.44085900	-1.25611700	-0.31638200
C	3.44097300	-1.25586600	-0.31519200
C	-3.29047900	1.61581600	-0.07162100
C	4.27668800	-2.04093000	0.49633300
C	-4.27576600	-2.04264800	0.49455300
C	-2.45002800	-0.06544000	2.21208400
C	-3.42714900	-1.48940300	-1.70391500
C	-2.67467800	2.66445100	-0.77081900
C	3.42678700	-1.49087200	-1.70243100
C	2.45014300	-0.06321400	2.21224300
C	4.64245300	1.74399500	0.29357500
C	2.67416900	2.66373100	-0.77398300
C	-4.23434000	-2.48045200	-2.26628200
C	1.20712400	0.60516800	2.80172300
C	3.39306700	3.82080700	-1.09711500
C	5.35699900	2.90046900	-0.02529200
C	-5.08061300	-3.03869100	-0.07120400
C	-1.20763500	0.60377600	2.80191800
C	-4.73408600	3.94247600	-0.71808100
C	4.73311300	3.94253800	-0.72212900
C	5.06370200	-3.25986300	-1.44766400
C	-5.06291200	-3.25966200	-1.45059500
C	5.08186500	-3.03719700	-0.06855100
C	-4.64308200	1.74260600	0.29470700
C	-3.39384500	3.82171500	-1.09267900
C	-5.35790000	2.89925700	-0.02290200
C	4.23431100	-2.48214300	-2.26393500
H	-3.38287800	0.35988700	2.61015100
H	-2.41998200	-1.14102600	2.44638400

H	2.42110400	-1.13864700	2.44729200
H	3.38258400	0.36337800	2.60990500
H	1.29735400	1.71039100	2.73060100
H	1.15755400	0.37082300	3.88442500
H	-1.15787100	0.36901400	3.88452000
H	-1.29890900	1.70894800	2.73127700
H	4.30972500	-1.88609300	1.57567000
H	-4.30843300	-1.88912700	1.57408900
H	-2.77717200	-0.89673000	-2.35100700
H	-1.62763100	2.57145100	-1.06258500
H	2.77618600	-0.89938900	-2.34998000
H	5.14811000	0.93425000	0.82489000
H	1.62726200	2.56998400	-1.06601500
H	-4.21134600	-2.64838800	-3.34537200
H	2.90049800	4.62747500	-1.64481700
H	6.40590600	2.98687500	0.26740600
H	-5.72335700	-3.64230200	0.57365800
H	-5.29523300	4.84547300	-0.96901900
H	5.29404800	4.84539500	-0.97404300
H	5.69163800	-4.03846000	-1.88636200
H	-5.69058000	-4.03809200	-1.88996900
H	5.72523200	-3.63964700	0.57677500
H	-5.14867100	0.93197600	0.82473100
H	-2.90133600	4.62928400	-1.63910500
H	-6.40695800	2.98490400	0.26947500
H	4.21093700	-2.65141600	-3.34280800

TS1/6

Ru	-0.03035313	0.03559764	0.01612418
H	-0.01311499	1.63862714	-0.02435768
P	-2.37429447	0.07354745	0.30920544
P	2.29729830	0.21155466	0.33794309
O	0.00265342	0.04434830	-2.99249465
N	-0.05004845	0.07026078	2.20836149
C	-0.00926745	0.01792302	-1.82444738
C	3.14723998	1.77099032	-0.20236418
C	-3.42084927	-1.27181102	-0.41377747
C	3.47810294	-1.10492519	-0.20446687
C	-3.35967854	1.60142281	-0.07109836
C	4.38079993	-1.69473065	0.69991236
C	-4.27591680	-2.07900963	0.35464575
C	-2.50773684	-0.13245259	2.16244472
C	-3.34171007	-1.49308823	-1.80090781
C	-2.74031193	2.72110387	-0.64612992
C	3.48693648	-1.51772604	-1.54531265
C	2.42961833	0.18702591	2.21204162
C	2.42441349	2.76246614	-0.88985487
C	4.52295862	1.96042263	0.00604218
C	-4.10756221	-2.49163517	-2.40595731
C	1.13393909	0.69231956	2.84640028
C	5.15922035	3.11778813	-0.45665606
C	3.05894058	3.92251607	-1.34023066
C	-5.03898719	-3.08265931	-0.25387202
C	-1.31390559	0.56644391	2.81098769
C	-4.84451468	3.92587793	-0.62103853
C	4.42987759	4.10365117	-1.12613038
C	5.27750983	-3.08142168	-1.07355591
C	-4.95812243	-3.29040187	-1.63309357
C	5.27080554	-2.68063658	0.26804842
C	-4.73525233	1.65573372	0.22071579
C	-3.48065101	3.87752451	-0.91954838
C	-5.47077152	2.81155210	-0.04932656
C	4.38760603	-2.49730143	-1.97846697
H	-0.02372706	-0.96409967	2.38698299
H	-3.46028686	0.25024017	2.55661637

H	-2.43905661	-1.21181525	2.36669510
H	2.59107615	-0.86841763	2.48299224
H	3.29453292	0.76534835	2.56891055
H	1.04518985	1.78547458	2.74699998
H	1.14201688	0.46571367	3.92844720
H	-1.31516246	0.37090724	3.89879900
H	-1.36813823	1.65841645	2.67079423
H	4.39763895	-1.38262179	1.74643862
H	-4.35672952	-1.93567240	1.43307780
H	-2.67330051	-0.88462339	-2.41344911
H	-1.67400345	2.68206925	-0.87458909
H	2.78379370	-1.07574615	-2.25225776
H	1.35849276	2.63289532	-1.08468974
H	5.10672771	1.20506807	0.53443051
H	-4.03421686	-2.65027665	-3.48413028
H	6.23059931	3.24714860	-0.28717723
H	2.47921323	4.68561559	-1.86454995
H	-5.69811269	-3.70320816	0.35735069
H	-5.42208392	4.82788063	-0.83572526
H	4.92639819	5.00891615	-1.48236634
H	5.97630976	-3.85030362	-1.41074997
H	-5.55324952	-4.07496763	-2.10551764
H	5.96392463	-3.13437342	0.98001841
H	-5.24135596	0.79026289	0.65454982
H	-2.98606115	4.74109032	-1.37006255
H	-6.53774059	2.84086934	0.18316281
H	4.38539371	-2.80803773	-3.02543903
H	-0.05130561	-1.75936148	0.30536338
C	-0.33887687	-2.88614628	1.23529879
O	-0.33734016	-2.62279458	2.46746903
O	0.71038213	-3.71231528	0.75205379
H	-1.28591118	-3.14249090	0.70874976
H	1.47055813	-3.50821028	1.32342579

6

Ru	-0.02858700	0.08714100	0.02614400
H	-0.04442700	1.69086100	0.01062300
P	-2.36874700	0.10720300	0.34669800
P	2.30815500	0.20116300	0.34771000
O	-0.01689200	0.11473500	-2.98170000
N	-0.02510600	0.10931100	2.21858500
C	-0.02268300	0.08136100	-1.81334300
C	3.24651500	1.74178400	-0.09833500
C	-3.41179000	-1.25655400	-0.34680400
C	3.42146800	-1.13267100	-0.29639500
C	-3.37508500	1.62008800	-0.03860300
C	4.30566700	-1.86053600	0.51776400
C	-4.25482200	-2.05781400	0.44098700
C	-2.47832200	-0.08366000	2.20456900
C	-3.34278600	-1.49843900	-1.73095700
C	-2.76228700	2.76047600	-0.57875600
C	3.36944700	-1.42397900	-1.67154400
C	2.43287800	0.07866200	2.21113400
C	2.60018700	2.80250900	-0.75008200
C	4.61546500	1.85917600	0.20482400
C	-4.10577900	-2.51229100	-2.31381500
C	1.18568700	0.70656400	2.83060500
C	5.31720500	3.01973800	-0.12763300
C	3.30681900	3.96286200	-1.08796400
C	-5.01492500	-3.07679600	-0.14523900
C	-1.27509500	0.61426200	2.83708700
C	-4.89087300	3.92120800	-0.60207400
C	4.66386500	4.07486100	-0.77605700
C	5.06361800	-3.13564700	-1.40146700
C	-4.94340000	-3.30569300	-1.52156800

C	5.11971500	-2.85766000	-0.03361000
C	-4.75974300	1.64179800	0.21119200
C	-3.51783100	3.90525800	-0.85907100
C	-5.51071000	2.78611600	-0.06536400
C	4.18732800	-2.41372700	-2.21971500
H	0.01441510	-1.16986545	2.38059020
H	-3.42567800	0.30235800	2.60777000
H	-2.41516600	-1.16250900	2.41475100
H	2.44894400	-0.99433200	2.45771500
H	3.35155100	0.54227100	2.59822300
H	1.16682700	1.79631300	2.67003600
H	1.18508200	0.53105400	3.92190300
H	-1.26354000	0.42184900	3.92539700
H	-1.32743300	1.70562600	2.69384400
H	4.37428300	-1.65932000	1.58796000
H	-4.32918800	-1.89825400	1.51761600
H	-2.68458400	-0.89414400	-2.35858100
H	-1.68890200	2.74592900	-0.77408400
H	2.68020300	-0.87886400	-2.31990200
H	1.53874700	2.71546500	-0.98611000
H	5.14418000	1.03899400	0.69582200
H	-4.03994200	-2.68745800	-3.38988700
H	6.37919700	3.09865000	0.11575500
H	2.79130400	4.77981000	-1.59804200
H	-5.66418300	-3.69253600	0.48122600
H	-5.48042800	4.81412600	-0.82203600
H	5.21512200	4.98031300	-1.03976000
H	5.69821400	-3.91456900	-1.82966900
H	-5.53581900	-4.10243600	-1.97668300
H	5.80027400	-3.41577700	0.61329800
H	-5.26091500	0.75994200	0.61681600
H	-3.02812600	4.78533700	-1.28214000
H	-6.58464200	2.79016700	0.13451600
H	4.13310400	-2.62791100	-3.28934900
H	-0.03495446	-1.78237528	0.37997858
C	-0.06300493	-2.70876043	0.99081713
O	0.03121283	-2.43877166	2.33064140
O	0.96632707	-3.49574243	0.41251313
H	-1.01276293	-3.13694543	0.59697113
H	1.76679107	-3.28405343	0.92304313

TS6/7

Ru	0.03345800	0.04077800	-0.01969600
H	0.06013900	1.58437500	0.22070500
P	2.37822900	0.07425800	-0.34562000
P	-2.29790700	0.23135500	-0.34226000
O	0.03372000	-0.23533000	2.99065000
N	0.03092700	0.11687600	-2.12870000
C	0.03120600	-0.15711000	1.82328800
C	-3.18102900	1.79093000	0.14775000
C	3.44921000	-1.24036100	0.39921300
C	-3.45524700	-1.07994800	0.28044300
C	3.35458600	1.62052800	-0.01753000
C	-4.40112400	-1.72188600	-0.53889600
C	4.25702400	-2.09662700	-0.36700000
C	2.47827500	-0.16490700	-2.19224400
C	3.43616300	-1.38922200	1.79829300
C	2.72680100	2.77649000	0.46975800
C	-3.38422700	-1.43551800	1.64067100
C	-2.43010300	0.15607200	-2.20426200
C	-2.51987200	2.78155900	0.88893900
C	-4.52597800	1.99292900	-0.21258600
C	4.21862800	-2.36678600	2.41607500
C	-1.13499500	0.71609100	-2.79300000
C	-5.18816500	3.16729600	0.15080900

C	-3.18653700	3.95645800	1.25638800
C	5.03688500	-3.07927300	0.25465300
C	1.26588700	0.53139900	-2.81197200
C	4.83755000	3.96876200	0.43356200
C	-4.51903900	4.15298700	0.88635400
C	-5.18219100	-3.03391300	1.34558800
C	5.02041800	-3.21635100	1.64491600
C	-5.25664300	-2.69493400	-0.00743200
C	4.73835600	1.65216400	-0.27170300
C	3.46527600	3.94457100	0.69354600
C	5.47305000	2.81870700	-0.05013900
C	-4.24450100	-2.39992000	2.16881200
H	-0.05821190	-1.39120435	-2.33958411
H	3.42835800	0.20244100	-2.60722100
H	2.40469300	-1.24787800	-2.37536500
H	-2.52132300	-0.90699900	-2.47649600
H	-3.31813700	0.68691000	-2.57699700
H	-1.12609600	1.82340300	-2.70566100
H	-1.11499200	0.49361900	-3.87915800
H	1.21499000	0.26816200	-3.88805200
H	1.39995500	1.63368200	-2.77231600
H	-4.48443400	-1.46996200	-1.59730700
H	4.28784800	-2.00681100	-1.45375100
H	2.80628800	-0.73996100	2.40994000
H	1.65505700	2.75829600	0.67278700
H	-2.64758300	-0.96025300	2.29126100
H	-1.47851300	2.63035200	1.17600300
H	-5.06856100	1.22855500	-0.77359700
H	4.19700700	-2.46915600	3.50332900
H	-6.23163400	3.31171300	-0.13825600
H	-2.65877800	4.71851000	1.83427000
H	5.65927900	-3.73829200	-0.35487400
H	5.41396800	4.87977700	0.60959900
H	-5.03886100	5.07024500	1.17198500
H	-5.84979500	-3.79327600	1.75832900
H	5.62848200	-3.98451200	2.12774000
H	-5.98382400	-3.18560400	-0.65808500
H	5.25123300	0.76014000	-0.63856100
H	2.96267200	4.83639700	1.07472700
H	6.54651500	2.82876200	-0.25236100
H	-4.17595000	-2.66334300	3.22651600
H	0.16950695	-2.02437564	-0.26867803
C	-0.04141200	-2.96925000	-1.02737800
O	-0.04074700	-2.55107000	-2.34216400
O	-1.22327400	-3.62776000	-0.62753200
H	0.76866400	-3.69279500	-0.83494200
H	-1.96509900	-3.01134700	-0.74161900

7

Ru	-0.03449700	0.03432300	-0.07710400
H	-0.04071000	1.52147400	-0.54257100
P	-2.37907200	0.13373000	0.23984600
P	2.30152400	0.14652200	0.23951600
O	0.05240900	-0.56919700	-3.03893300
N	-0.03877600	-0.01055600	1.98770300
C	0.00481200	-0.33205400	-1.89320100
C	3.15581400	1.78534600	0.05862900
C	-3.50830100	-1.11389600	-0.53109200
C	3.45472900	-1.01550000	-0.63363000
C	-3.27228900	1.74292000	-0.03249200
C	4.59506726	-1.51344868	0.02373297
C	-4.42420100	-1.87779400	0.21213000
C	-2.50194000	-0.14417600	2.08400200
C	-3.43503300	-1.30811300	-1.92263400
C	-2.56358528	2.84856970	-0.53284199

C	3.15081198	-1.49084030	-1.92145750
C	2.41857600	-0.26280800	2.05597600
C	2.57737200	2.80919600	-0.70758400
C	4.40498700	2.01488800	0.66477900
C	-4.26146000	-2.23946000	-2.55551300
C	1.18055500	0.31876400	2.74249000
C	5.05136700	3.24417500	0.51677900
C	3.22875700	4.03859800	-0.86104900
C	-5.24659400	-2.81525000	-0.42329600
C	-1.23440500	0.41606100	2.73314100
C	-4.54455701	4.23482198	-0.35652615
C	4.46398700	4.25983100	-0.24679000
C	5.11218975	-2.91570081	-1.89115828
C	-5.16822900	-2.99783500	-1.80658200
C	5.41773836	-2.45170605	-0.60774094
C	-4.62892986	1.90175060	0.30079367
C	-3.19453852	4.08686923	-0.68872880
C	-5.25960961	3.13874957	0.13696162
C	3.97364613	-2.43458268	-2.54413525
H	-0.21939600	-1.81307600	2.31234000
H	-3.41567300	0.30137500	2.50441500
H	-2.53030300	-1.23410500	2.23504700
H	2.40061400	-1.36075800	2.13626100
H	3.35214900	0.10558700	2.50608400
H	1.29236800	1.41817000	2.86018700
H	1.11560800	-0.09220500	3.77048400
H	-1.18338900	0.05422800	3.77998200
H	-1.29221100	1.52345300	2.79576800
H	4.85524553	-1.18144871	1.03084059
H	-4.50719500	-1.74883700	1.29221200
H	-2.72348800	-0.73142700	-2.51652500
H	-1.51455826	2.73273433	-0.81083815
H	2.26891932	-1.12261309	-2.44857332
H	1.61100200	2.63985300	-1.18471500
H	4.88677900	1.22893500	1.25050600
H	-4.19111000	-2.37794300	-3.63668900
H	6.01886000	3.40828600	0.99675200
H	2.76574100	4.82396500	-1.46274500
H	-5.95176300	-3.40271200	0.16908000
H	-5.03974545	5.19984124	-0.48610474
H	4.97117700	5.22029400	-0.36320700
H	5.75711966	-3.64999972	-2.37918981
H	-5.80987400	-3.73103400	-2.30027900
H	6.30414235	-2.82244988	-0.08734509
H	-5.20210481	1.05700579	0.68673703
H	-2.62883050	4.93584759	-1.07949869
H	-6.31597306	3.24400565	0.39500494
H	3.72234271	-2.79132803	-3.54571761
H	0.15675100	-3.35987600	0.72135100
C	0.20305500	-3.64854000	1.78830900
O	-0.44844900	-2.73867700	2.61606300
O	1.59554700	-3.75297000	2.06926000
H	-0.29197500	-4.62662100	1.92422300
H	1.67776800	-3.99638600	3.00565900

8

Ru	-0.02863400	0.08729200	0.02611600
H	-0.04486000	1.69100600	0.01081000
P	-2.36880600	0.10725500	0.34666700
P	2.30809600	0.20108800	0.34777500
O	-0.01633800	0.11595800	-2.98172200
N	-0.02523200	0.10916500	2.21857600
C	-0.02248000	0.08202300	-1.81338600
C	3.24642800	1.74180500	-0.09807200
C	-3.41169300	-1.25667600	-0.34675400

C	3.42151700	-1.13260400	-0.29636900
C	-3.37517800	1.62008700	-0.03878900
C	4.30506700	-1.86114500	0.51788800
C	-4.25515500	-2.05751800	0.44103600
C	-2.47851400	-0.08360800	2.20455100
C	-3.34213000	-1.49918400	-1.73075600
C	-2.76250300	2.76037700	-0.57927500
C	3.37010500	-1.42321800	-1.67169100
C	2.43271900	0.07840900	2.21119700
C	2.60004300	2.80287600	-0.74918200
C	4.61549900	1.85890900	0.20470600
C	-4.10500500	-2.51320900	-2.31349800
C	1.18556100	0.70630300	2.83068700
C	5.31728600	3.01951300	-0.12750600
C	3.30672100	3.96327000	-1.08683300
C	-5.01510600	-3.07667100	-0.14505600
C	-1.27522200	0.61409600	2.83717100
C	-4.89112500	3.92105800	-0.60255000
C	4.66388000	4.07497300	-0.77531600
C	5.06363100	-3.13550800	-1.40161000
C	-4.94303700	-3.30617100	-1.52126900
C	5.11911100	-2.85821700	-0.03358600
C	-4.75980400	1.64183200	0.21119700
C	-3.51812000	3.90507200	-0.85974400
C	-5.51084800	2.78607200	-0.06549600
C	4.18797300	-2.41292500	-2.21995000
H	-0.17359840	-1.37807725	2.77587210
H	-3.42580700	0.30261800	2.60768700
H	-2.41559700	-1.16248300	2.41465000
H	2.44866100	-0.99463500	2.45761000
H	3.35144600	0.54183200	2.59838400
H	1.16673900	1.79607200	2.67021600
H	1.18491800	0.53070400	3.92197100
H	-1.26363200	0.42149100	3.92544400
H	-1.32748600	1.70548400	2.69410200
H	4.37322200	-1.66048100	1.58821400
H	-4.32993400	-1.89753000	1.51757500
H	-2.68359800	-0.89524400	-2.35837300
H	-1.68914500	2.74586000	-0.77473600
H	2.68135000	-0.87754700	-2.32011200
H	1.53851700	2.71607300	-0.98491700
H	5.14425600	1.03845300	0.69520500
H	-4.03871800	-2.68884300	-3.38946600
H	6.37936600	3.09819800	0.11557400
H	2.79115300	4.78047100	-1.59645200
H	-5.66467500	-3.69209000	0.48140200
H	-5.48072500	4.81392100	-0.82261700
H	5.21516700	4.98046100	-1.03883700
H	5.69820600	-3.91441400	-1.82987200
H	-5.53534100	-4.10306200	-1.97627500
H	5.79918300	-3.41685600	0.61338400
H	-5.26094100	0.76007500	0.61707300
H	-3.02848900	4.78506200	-1.28308700
H	-6.58474800	2.79012300	0.13455500
H	4.13423600	-2.62655100	-3.28972000
H	1.03605429	-3.35448946	2.00028484
C	0.65606967	-2.30400001	1.79661267
O	-0.13549743	-2.42914938	2.90776484
O	0.18336041	-2.32505232	0.45884370
H	1.60939668	-1.72937291	1.75928700
H	-0.74316101	-2.61488955	0.52011607

TS8/9

Ru	-0.00973200	0.02993300	0.04231300
H	0.01337100	1.60106700	0.16411900

P	-2.33683300	0.13909300	0.38469900
P	2.32865700	0.09339000	0.37209700
O	-0.01524400	0.40236900	-2.95069200
N	-0.00572100	-0.04114300	2.21443000
C	-0.01242400	0.20934600	-1.79466100
C	3.27216700	1.64951700	-0.01073900
C	-3.40322300	-1.21622500	-0.30603300
C	3.43736400	-1.20708800	-0.35132600
C	-3.29151500	1.66673800	-0.06494000
C	4.37436000	-1.92897500	0.40777100
C	-4.31006400	-1.95874400	0.47061000
C	-2.47267200	-0.00946800	2.24038100
C	-3.28287600	-1.51724100	-1.67642300
C	-2.63454500	2.76516000	-0.63975100
C	3.33040400	-1.47563500	-1.72792200
C	2.46073600	-0.10742000	2.22493800
C	2.63697300	2.72696400	-0.64602500
C	4.63447100	1.76255500	0.32196300
C	-4.05496700	-2.52803500	-2.25525100
C	1.20119100	0.49841100	2.84568100
C	5.34021500	2.93289500	0.03488700
C	3.34696600	3.89762200	-0.93845700
C	-5.07959700	-2.97282300	-0.11068600
C	-1.18699800	0.56116300	2.84319100
C	-4.72186000	3.99509000	-0.73411000
C	4.69738500	4.00417100	-0.59721500
C	5.07581200	-3.14948400	-1.56745600
C	-4.95502800	-3.25964400	-1.47295800
C	5.18666400	-2.89468100	-0.19793800
C	-4.67680100	1.74584000	0.16793100
C	-3.34713200	3.92332100	-0.97234000
C	-5.38560100	2.90302500	-0.16204600
C	4.14619200	-2.43529900	-2.33172300
H	-0.13909245	-1.25935223	2.31968365
H	-3.37188900	0.49209100	2.62724000
H	-2.53846500	-1.08380400	2.46866400
H	2.49219500	-1.18868900	2.43285700
H	3.37880800	0.34754600	2.62562000
H	1.24584800	1.60733000	2.75722800
H	1.20307500	0.28083100	3.93457700
H	-1.19063900	0.36000400	3.93531600
H	-1.18559300	1.66908000	2.73787900
H	4.48199900	-1.74702400	1.47844700
H	-4.42669700	-1.75356800	1.53585400
H	-2.58076700	-0.95632200	-2.29689400
H	-1.56050200	2.70819900	-0.82098900
H	2.60144700	-0.93248900	-2.33296300
H	1.58101500	2.64492700	-0.90547400
H	5.15562100	0.93095700	0.80173900
H	-3.94816200	-2.74679600	-3.32002300
H	6.39700300	3.00718600	0.30161600
H	2.83902100	4.72735700	-1.43543400
H	-5.77931500	-3.53960800	0.50767300
H	-5.27819000	4.89818300	-0.99537800
H	5.25125200	4.91783100	-0.82483100
H	5.70985100	-3.90401900	-2.03830900
H	-5.55543000	-4.05280600	-1.92385300
H	5.90907100	-3.44767000	0.40683600
H	-5.21186700	0.89871200	0.60317600
H	-2.82270400	4.76987700	-1.42146800
H	-6.46092100	2.95098800	0.02453200
H	4.05005900	-2.63043500	-3.40218300
H	0.10534500	-4.16658000	1.01110600
C	0.29976600	-3.09167600	1.16722900
O	-0.38026700	-2.65228800	2.27616000
O	-0.08811700	-2.36953400	-0.03506100

H	1.39170600	-2.92290700	1.21210500
H	-1.00838300	-2.60851400	-0.23779600
9			
Ru	-0.02863400	0.08729200	0.02611600
H	-0.04486000	1.69100600	0.01081000
P	-2.36880600	0.10725500	0.34666700
P	2.30809600	0.20108800	0.34777500
O	-0.01633800	0.11595800	-2.98172200
N	-0.02523200	0.10916500	2.21857600
C	-0.02248000	0.08202300	-1.81338600
C	3.24642800	1.74180500	-0.09807200
C	-3.41169300	-1.25667600	-0.34675400
C	3.42151700	-1.13260400	-0.29636900
C	-3.37517800	1.62008700	-0.03878900
C	4.30506700	-1.86114500	0.51788800
C	-4.25515500	-2.05751800	0.44103600
C	-2.47851400	-0.08360800	2.20455100
C	-3.34213000	-1.49918400	-1.73075600
C	-2.76250300	2.76037700	-0.57927500
C	3.37010500	-1.42321800	-1.67169100
C	2.43271900	0.07840900	2.21119700
C	2.60004300	2.80287600	-0.74918200
C	4.61549900	1.85890900	0.20470600
C	-4.10500500	-2.51320900	-2.31349800
C	1.18556100	0.70630300	2.83068700
C	5.31728600	3.01951300	-0.12750600
C	3.30672100	3.96327000	-1.08683300
C	-5.01510600	-3.07667100	-0.14505600
C	-1.27522200	0.61409600	2.83717100
C	-4.89112500	3.92105800	-0.60255000
C	4.66388000	4.07497300	-0.77531600
C	5.06363100	-3.13550800	-1.40161000
C	-4.94303700	-3.30617100	-1.52126900
C	5.11911100	-2.85821700	-0.03358600
C	-4.75980400	1.64183200	0.21119700
C	-3.51812000	3.90507200	-0.85974400
C	-5.51084800	2.78607200	-0.06549600
C	4.18797300	-2.41292500	-2.21995000
H	-0.13548958	-0.93395406	2.37136966
H	-3.42580700	0.30261800	2.60768700
H	-2.41559700	-1.16248300	2.41465000
H	2.44866100	-0.99463500	2.45761000
H	3.35144600	0.54183200	2.59838400
H	1.16673900	1.79607200	2.67021600
H	1.18491800	0.53070400	3.92197100
H	-1.26363200	0.42149100	3.92544400
H	-1.32748600	1.70548400	2.69410200
H	4.37322200	-1.66048100	1.58821400
H	-4.32993400	-1.89753000	1.51757500
H	-2.68359800	-0.89524400	-2.35837300
H	-1.68914500	2.74586000	-0.77473600
H	2.68135000	-0.87754700	-2.32011200
H	1.53851700	2.71607300	-0.98491700
H	5.14425600	1.03845300	0.69520500
H	-4.03871800	-2.68884300	-3.38946600
H	6.37936600	3.09819800	0.11557400
H	2.79115300	4.78047100	-1.59645200
H	-5.66467500	-3.69209000	0.48140200
H	-5.48072500	4.81392100	-0.82261700
H	5.21516700	4.98046100	-1.03883700
H	5.69820600	-3.91441400	-1.82987200
H	-5.53534100	-4.10306200	-1.97627500
H	5.79918300	-3.41685600	0.61338400
H	-5.26094100	0.76007500	0.61707300

H	-3.02848900	4.78506200	-1.28308700
H	-6.58474800	2.79012300	0.13455500
H	4.13423600	-2.62655100	-3.28972000
H	1.16609218	-3.20283768	0.88514395
C	0.69398657	-2.26827670	1.32458771
O	-0.03675784	-2.58667062	2.35154336
O	0.13907357	-2.23304413	-0.10355444
H	1.51859274	-1.56578313	1.58333342
H	-0.78773739	-2.52820063	-0.09326107

10

Ru	0.04161200	0.09121600	0.17839000
H	0.04507900	1.68823700	-0.05323500
P	-2.29359800	0.21019800	0.49341700
P	2.37124100	0.23371800	0.46216700
O	-0.01473300	-0.09961000	-2.81311600
N	0.05277300	0.48186300	2.36542000
C	0.01287600	-0.08029100	-1.64155900
C	3.35205200	1.61692600	-0.29842900
C	-3.43127200	-1.17040100	0.00887400
C	3.43240100	-1.25297200	0.12865300
C	-3.24867900	1.69693600	-0.09109400
C	4.29531778	-1.81823397	1.08454197
C	-4.30394900	-1.80781200	0.90570300
C	-2.40723300	0.30000800	2.36134800
C	-3.41332800	-1.58742700	-1.33424600
C	-2.61412646	2.69787468	-0.84159435
C	3.36308691	-1.83395055	-1.15005415
C	2.52284000	0.48952800	2.31776900
C	2.71881250	2.53421690	-1.15080587
C	4.72787440	1.76148143	-0.04259558
C	-4.25702200	-2.61068400	-1.77144800
C	1.26663800	1.17887500	2.84894200
C	5.45005000	2.80769155	-0.62069500
C	3.44567325	3.57890254	-1.73386351
C	-5.14332800	-2.83876300	0.46691200
C	-1.19953500	1.06755000	2.89719400
C	-4.68946575	3.94461536	-0.98108386
C	4.81020868	3.71921229	-1.46923719
C	5.00794149	-3.49672598	-0.51378166
C	-5.12320300	-3.24130300	-0.87101200
C	5.07747572	-2.93267538	0.76379271
C	-4.61824001	1.83124932	0.20306832
C	-3.33231676	3.81472799	-1.28563805
C	-5.33150344	2.94940422	-0.23400618
C	4.14914308	-2.94478139	-1.46947681
H	0.09572400	-0.51133700	2.63787500
H	-3.34550800	0.76364000	2.69943200
H	-2.38127600	-0.73602800	2.73525300
H	2.61609300	-0.51103000	2.76971400
H	3.42218000	1.06453400	2.58191900
H	1.21335100	2.22105300	2.49830700
H	1.28899200	1.19808000	3.95374000
H	-1.19762800	1.04581900	4.00198100
H	-1.23639100	2.12323500	2.58592200
H	4.36652532	-1.39750142	2.08935512
H	-4.34238800	-1.50900000	1.95426800
H	-2.72862900	-1.11682700	-2.04286300
H	-1.55226152	2.59593087	-1.06962384
H	2.68043008	-1.42489037	-1.89683783
H	1.65151895	2.42570189	-1.34798047
H	5.24831693	1.05144389	0.60358271
H	-4.22813400	-2.92415100	-2.81726800
H	6.51757839	2.90852339	-0.41187677
H	2.93986264	4.28325395	-2.39824273

H	-5.81533700	-3.32598000	1.17717700
H	-5.24942671	4.81654934	-1.32690855
H	5.37741334	4.53422972	-1.92457353
H	5.61763214	-4.36844143	-0.76177850
H	-5.77833400	-4.04617000	-1.21177500
H	5.74209681	-3.36073879	1.51769417
H	-5.13928443	1.05502591	0.76844020
H	-2.82531071	4.58440593	-1.87221646
H	-6.39369985	3.04141024	0.00427848
H	4.07972476	-3.38524442	-2.46642231
O	0.02376100	-1.93446400	0.99867900
H	0.90585700	-2.30980300	0.86494400

TS10/11

Ru	0.00719000	-0.11149200	0.11227200
H	-0.00512500	1.43751100	-0.16698300
P	-2.33218200	-0.02491100	0.43357700
P	2.33564600	0.05421400	0.43246900
O	-0.00043100	-0.45878100	-2.88635800
N	0.00956000	0.09075100	2.24899800
C	0.00533700	-0.36129400	-1.71773100
C	3.27903600	1.52386000	-0.20355300
C	-3.43421900	-1.38037900	-0.19087500
C	3.44030500	-1.35910600	-0.05631800
C	-3.28995300	1.49675200	-0.04290900
C	4.41053000	-1.90742500	0.80059200
C	-3.36981600	-1.71007400	-1.55687200
C	-2.44832100	-0.10162300	2.29563700
C	-4.32535400	-2.08684800	0.63386800
C	-4.64874200	1.62372000	0.29981400
C	3.29551900	-1.89978700	-1.34731800
C	2.47246000	0.14544800	2.29702700
C	2.64335900	2.47388700	-1.01689100
C	4.63855800	1.69896800	0.11329600
C	-5.13527800	-3.09780900	0.10320300
C	1.17539100	0.74466700	2.84345500
C	5.34164900	2.80614700	-0.36607800
C	3.35066800	3.58105700	-1.50054400
C	-4.18276400	-2.71529600	-2.08558800
C	-1.21535600	0.60053000	2.86838400
C	-4.73984100	3.79792200	-0.76707500
C	4.69863000	3.75064500	-1.17537300
C	5.06939900	-3.49349500	-0.91174400
C	-5.06747300	-3.41368300	-1.25617600
C	5.21809600	-2.96823300	0.37477000
C	-2.67098600	2.53327300	-0.75735900
C	-5.36672000	2.76736300	-0.05605400
C	-3.39311100	3.67730200	-1.11791500
C	4.10675400	-2.95496200	-1.77257900
H	0.08518765	-1.23709477	2.25146160
H	-3.38516600	0.33596600	2.67131700
H	-2.42902900	-1.16857200	2.57003400
H	2.58300500	-0.88845400	2.66114900
H	3.35772100	0.71630000	2.61407100
H	1.16855200	1.84307500	2.66071900
H	1.17111700	0.62320800	3.94718300
H	-1.19385500	0.43884700	3.96662300
H	-1.31950300	1.70069600	2.72713000
H	4.54768200	-1.51359800	1.80892000
H	-2.67587100	-1.18103300	-2.21332200
H	-4.39874800	-1.85792900	1.69813400
H	-5.15730100	0.82287300	0.84154900
H	2.54026200	-1.49666600	-2.02486600
H	1.58935200	2.34260200	-1.26518800
H	5.16030200	0.96479200	0.73141000

H	-5.82166100	-3.63836500	0.75905900
H	6.39648000	2.92995000	-0.11027600
H	2.84252300	4.31167400	-2.13407500
H	-4.11954900	-2.95802800	-3.14877300
H	-5.30315100	4.69073400	-1.04809100
H	5.25043300	4.61465900	-1.55259300
H	5.69933100	-4.32233500	-1.24225300
H	-5.69943400	-4.20333100	-1.66868900
H	5.96600100	-3.38318100	1.05438500
H	-1.61766000	2.44034100	-1.02538100
H	-6.42055800	2.85261400	0.21902300
H	-2.89748200	4.47531300	-1.67562800
H	3.98044600	-3.36201900	-2.77831700
O	-0.03297300	-2.29167100	1.14457500
H	0.82484600	-2.74126000	1.09145500

11

Ru	0.00490200	-0.10675200	0.09611700
H	0.00157500	1.44024900	-0.24535600
P	-2.33467300	-0.01432500	0.42376300
P	2.33698900	0.04342400	0.41442600
O	-0.01168800	-0.54067500	-2.88386100
N	0.00861700	0.13174000	2.25623300
C	-0.00221600	-0.40533300	-1.71955400
C	3.28614700	1.51585200	-0.20572400
C	-3.42967500	-1.38586600	-0.17374700
C	3.44190200	-1.37037200	-0.07036000
C	-3.30236300	1.49633800	-0.06622100
C	4.45575900	-1.86996200	0.76582100
C	-3.37515900	-1.72732400	-1.53729300
C	-2.44739800	-0.06855300	2.28943100
C	-4.30675100	-2.09219900	0.66578700
C	-4.66563300	1.61108500	0.26315800
C	3.25788000	-1.95689100	-1.33532400
C	2.47282100	0.11487100	2.28238200
C	2.67657700	2.42926000	-1.07885900
C	4.62506800	1.72393200	0.17218800
C	-5.11206900	-3.11549300	0.15207900
C	1.19956300	0.74453900	2.85125200
C	5.33350900	2.82822800	-0.30596600
C	3.38981400	3.53269400	-1.56212800
C	-4.18340100	-2.74501500	-2.04890600
C	-1.22207600	0.64033100	2.87156400
C	-4.76504000	3.78464000	-0.80431200
C	4.71687000	3.73577400	-1.17574000
C	5.08065000	-3.49935500	-0.91799000
C	-5.05378800	-3.44365200	-1.20473900
C	5.26809900	-2.92815000	0.34394200
C	-2.68526100	2.53822200	-0.77441700
C	-5.38997400	2.74843900	-0.09976700
C	-3.41389900	3.67596300	-1.14179500
C	4.07420600	-3.00986500	-1.75715700
H	0.02397763	-1.27489220	1.98474521
H	-3.38495600	0.37178900	2.65909700
H	-2.42797200	-1.13229100	2.57345900
H	2.56037700	-0.92635000	2.63199200
H	3.37211400	0.65772500	2.60776000
H	1.20809700	1.83895100	2.67175400
H	1.19834300	0.61007600	3.95208800
H	-1.20331300	0.47842000	3.96842600
H	-1.31224000	1.73565800	2.71990000
H	4.62273500	-1.44080800	1.75525000
H	-2.69227900	-1.19847400	-2.20538600
H	-4.37277700	-1.85439100	1.72846700
H	-5.17261200	0.80565500	0.79952200

H	2.46770200	-1.59301000	-1.99442500
H	1.63758600	2.27311300	-1.37208700
H	5.12741800	1.01856900	0.83788100
H	-5.78716600	-3.65613500	0.81943100
H	6.37185700	2.97855700	-0.00169000
H	2.90252000	4.23463700	-2.24269200
H	-4.12758500	-2.99721800	-3.11027000
H	-5.33339700	4.67248200	-1.09084200
H	5.27290300	4.59756500	-1.55180200
H	5.71458200	-4.32636800	-1.24541300
H	-5.68199800	-4.24309900	-1.60385200
H	6.04971100	-3.30583400	1.00711800
H	-1.62851500	2.45374000	-1.03198100
H	-6.44724300	2.82427600	0.16463600
H	-2.91988700	4.47833900	-1.69464700
H	3.91696700	-3.45362100	-2.74278100
O	-0.06320000	-2.11174100	1.29179200
H	0.77983600	-2.59003200	1.27098700

12

Ru	-0.00000100	-0.00639400	0.03242200
H	0.00000432	1.68004575	-0.07721819
P	-2.34103800	0.06287200	0.35509900
P	2.34103400	0.06286100	0.35509500
O	0.00001300	-0.08791100	-2.97768800
N	-0.00000500	0.07772800	2.20569400
C	0.00000000	-0.08313600	-1.80873400
C	3.31198100	1.58361200	-0.08539600
C	-3.41456400	-1.29736900	-0.29836600
C	3.41454600	-1.29736500	-0.29842200
C	-3.31198100	1.58361300	-0.08544000
C	4.25303300	-2.07377300	0.51823600
C	-4.25306200	-2.07373300	0.51832200
C	-2.44995200	-0.06493500	2.21598800
C	-3.37422900	-1.56375600	-1.67924100
C	-2.68932500	2.66301300	-0.72956100
C	3.37420400	-1.56370100	-1.67930600
C	2.44994000	-0.06501800	2.21597900
C	4.68279200	1.66916100	0.22027700
C	2.68932200	2.66304300	-0.72946100
C	-4.16057400	-2.57751500	-2.23038900
C	1.22968100	0.63090400	2.81886100
C	3.42093800	3.81085600	-1.05696700
C	5.40978000	2.81671500	-0.10278500
C	-5.03677100	-3.09259300	-0.03620700
C	-1.22966700	0.63095500	2.81885400
C	-4.77978800	3.89089900	-0.74316800
C	4.77979300	3.89091600	-0.74304400
C	4.99347200	-3.34628200	-1.40949600
C	-4.99352700	-3.34630000	-1.40936300
C	5.03672400	-3.09262600	-0.03633100
C	-4.68278700	1.66918400	0.22024800
C	-3.42093800	3.81081600	-1.05710700
C	-5.40977200	2.81673000	-0.10285300
C	4.16053000	-2.57745300	-2.23049300
H	-0.00004281	-0.95226789	2.40967552
H	-3.39065400	0.34555600	2.61019000
H	-2.39420700	-1.13734500	2.45954400
H	2.39414400	-1.13743400	2.45949600
H	3.39065800	0.34542000	2.61019800
H	1.26819200	1.72052000	2.65295600
H	1.21461800	0.46399800	3.91194400
H	-1.21460600	0.46406300	3.91193900
H	-1.26813300	1.72057000	2.65293100
H	4.30441600	-1.89535500	1.59322000

H	-4.30443800	-1.89527800	1.59330000
H	-2.72071200	-0.97861300	-2.32979300
H	-1.62707400	2.60026100	-0.97007700
H	2.72069400	-0.97852500	-2.32983600
H	5.19226100	0.83411600	0.70673100
H	1.62706700	2.60030900	-0.96996300
H	-4.11745200	-2.77153000	-3.30443400
H	2.92368100	4.64291600	-1.56067800
H	6.47298300	2.87090400	0.14208100
H	-5.68238800	-3.68876700	0.61257800
H	-5.35060000	4.78645500	-0.99892600
H	5.35060700	4.78648000	-0.99877200
H	5.60454400	-4.14266200	-1.83994900
H	-5.60461400	-4.14268500	-1.83978600
H	5.68233300	-3.68883300	0.61243100
H	-5.19225500	0.83416400	0.70674400
H	-2.92368300	4.64285100	-1.56086200
H	-6.47297100	2.87093600	0.14202500
H	4.11740200	-2.77142900	-3.30454400
H	0.00007367	-1.68656593	0.35041932
C	0.00428379	-3.31368347	1.16581539
O	0.03365575	-3.21820746	2.37168505
H	-0.97084038	-3.31579660	0.57528310
H	0.95683561	-3.42901546	0.53190406

TS12/13

Ru	0.01911200	-0.10310700	0.04474300
H	0.09893300	1.46259300	-0.13233600
P	-2.32023600	0.08048000	0.34657100
P	2.35385700	-0.01276500	0.37414700
O	0.05108600	-0.30014600	-2.96429000
N	0.00300100	-0.00116500	2.19938000
C	0.03623300	-0.24863400	-1.79656300
C	3.20080300	1.57019200	-0.08243600
C	-3.45692800	-1.22904600	-0.30645200
C	3.51590700	-1.29763200	-0.28094200
C	-3.20541100	1.64435200	-0.12243600
C	4.35986126	-2.02229879	0.57975203
C	-4.33192002	-1.96331318	0.51120302
C	-2.45587600	-0.01932400	2.20632800
C	-3.43444937	-1.49515664	-1.68783522
C	-2.52110095	2.68132026	-0.77373255
C	3.54823588	-1.56756946	-1.65768579
C	2.45937000	-0.18125800	2.22771300
C	2.43151003	2.56656540	-0.71151233
C	4.55141575	1.83057301	0.19471099
C	-4.27467959	-2.46518940	-2.23852997
C	1.23513600	0.48912600	2.85258500
C	5.12249916	3.06137589	-0.15347264
C	3.00467287	3.78894914	-1.06551165
C	-5.16954583	-2.93865651	-0.04272393
C	-1.19873700	0.60613600	2.81125200
C	-4.54378728	4.01716022	-0.82141467
C	4.35338889	4.04086353	-0.78527664
C	5.23641977	-3.26998700	-1.30443998
C	-5.14451584	-3.19092247	-1.41667514
C	5.21167866	-3.00482669	0.07020237
C	-4.57271887	1.80509664	0.16838889
C	-3.18836725	3.86195665	-1.12152610
C	-5.23537213	2.98512775	-0.17531743
C	4.40579077	-2.54964110	-2.16669830
H	-0.06602600	-1.19360200	2.43423400
H	-3.37241800	0.45620700	2.58418900
H	-2.47177900	-1.08965700	2.46377200
H	2.41315900	-1.26551700	2.41552700

H	3.40357000	0.19556700	2.64685500
H	1.29951300	1.58858400	2.76140900
H	1.20529900	0.25788800	3.93482100
H	-1.19687000	0.42862300	3.90392300
H	-1.19199200	1.70131800	2.66333000
H	4.36020452	-1.81527409	1.65240440
H	-4.37008147	-1.78545814	1.58684590
H	-2.75280570	-0.94463229	-2.33964537
H	-1.46187319	2.56012661	-1.00516359
H	2.90200476	-1.00510181	-2.33398245
H	1.37498161	2.38643417	-0.92454626
H	5.17560664	1.08148340	0.68377757
H	-4.24516143	-2.65860177	-3.31317271
H	6.17507148	3.24887398	0.07053298
H	2.39476508	4.54994589	-1.55750945
H	-5.84329041	-3.50176976	0.60700464
H	-5.06420984	4.93856385	-1.09239668
H	4.80064798	4.99926043	-1.05795774
H	5.90646470	-4.03582904	-1.70154894
H	-5.79816396	-3.95288353	-1.84690507
H	5.86179849	-3.56283543	0.74790203
H	-5.13006143	1.00360590	0.65895947
H	-2.64323768	4.66064914	-1.62964981
H	-6.29647724	3.09802841	0.05843514
H	4.42387469	-2.74819551	-3.24059732
H	-0.09160700	-2.05636000	0.44412000
C	-0.17257300	-2.91353400	1.25087500
O	-0.15882800	-2.46690200	2.52890200
H	-1.11139400	-3.42282700	0.93423300
H	0.68617600	-3.56268500	0.96435800

13

Ru	-0.00001100	-0.00659800	0.03245200
H	0.00004000	1.57817600	-0.07070700
P	-2.34105100	0.06285900	0.35513800
P	2.34102500	0.06276500	0.35515900
O	0.00012200	-0.08846100	-2.97765300
N	-0.00001000	0.07758300	2.20565900
C	0.00009600	-0.08353700	-1.80869400
C	3.31177700	1.58367000	-0.08522000
C	-3.41465500	-1.29727400	-0.29843400
C	3.41475000	-1.29726900	-0.29841100
C	-3.31184600	1.58370000	-0.08530900
C	4.25299600	-2.07388700	0.51829800
C	-4.25316300	-2.07367000	0.51822100
C	-2.44994000	-0.06512200	2.21599300
C	-3.37438400	-1.56355000	-1.67932700
C	-2.68926800	2.66272500	-0.73013200
C	3.37481800	-1.56324700	-1.67937300
C	2.44993200	-0.06522000	2.21600500
C	4.68235900	1.66972600	0.22134000
C	2.68927700	2.66263400	-0.73021900
C	-4.16079000	-2.57723600	-2.23053300
C	1.22967600	0.63066600	2.81894600
C	3.42081500	3.81048600	-1.05776400
C	5.40926200	2.81732800	-0.10173700
C	-5.03693500	-3.09244800	-0.03636400
C	-1.22967900	0.63077400	2.81889900
C	-4.77946700	3.89106500	-0.74315400
C	4.77942800	3.89106000	-0.74293300
C	4.99402900	-3.34587800	-1.40955300
C	-4.99375400	-3.34604500	-1.40954500
C	5.03686200	-3.09258400	-0.03630700
C	-4.68248300	1.66967800	0.22101600
C	-3.42079200	3.81056800	-1.05774000

C	-5.40937300	2.81726900	-0.10213200
C	4.16131800	-2.57684800	-2.23059400
H	-0.00019663	-1.23534010	2.42604870
H	-3.39065600	0.34524400	2.61028900
H	-2.39402900	-1.13755600	2.45940000
H	2.39411300	-1.13765500	2.45944300
H	3.39065400	0.34514300	2.61029300
H	1.26820400	1.72030300	2.65318000
H	1.21456100	0.46359700	3.91199800
H	-1.21458100	0.46378200	3.91196700
H	-1.26816100	1.72040300	2.65306600
H	4.30404800	-1.89577800	1.59334800
H	-4.30448200	-1.89532800	1.59322000
H	-2.72085300	-0.97840200	-2.32986000
H	-1.62713900	2.59966500	-0.97110200
H	2.72148400	-0.97792200	-2.32994400
H	5.19172500	0.83503800	0.70851500
H	1.62719200	2.59952800	-0.97136700
H	-4.11770500	-2.77116300	-3.30459400
H	2.92368700	4.64218200	-1.56220300
H	6.47227800	2.87192400	0.14384900
H	-5.68254800	-3.68865200	0.61239700
H	-5.35020400	4.78665800	-0.99895000
H	5.35017200	4.78666500	-0.99867300
H	5.60524100	-4.14213600	-1.84003400
H	-5.60489100	-4.14236800	-1.84001200
H	5.68227600	-3.68896400	0.61249200
H	-5.19190300	0.83494500	0.70805600
H	-2.92360800	4.64231400	-1.56204200
H	-6.47243500	2.87180800	0.14326300
H	4.11851000	-2.77053800	-3.30470900
H	-0.00032284	-1.94503065	0.42969992
C	-0.00012708	-2.80180089	1.16579860
O	-0.00065762	-2.44462324	2.46769101
H	-0.90468208	-3.34390989	0.79685460
H	0.90501992	-3.34328189	0.79738960

14

Ru	-0.00001800	-0.01144500	0.03247300
H	-0.00010000	1.50803700	-0.31474800
P	-2.34109500	0.07638900	0.35577600
P	2.34098700	0.07704400	0.35583900
O	0.00012900	-0.46191100	-2.95772800
N	-0.00003900	0.11756000	2.12030100
C	0.00006800	-0.31225900	-1.79637600
C	3.29004400	1.61624700	-0.07312700
C	-3.44085900	-1.25611700	-0.31638200
C	3.44097300	-1.25586600	-0.31519200
C	-3.29047900	1.61581600	-0.07162100
C	4.27668800	-2.04093000	0.49633300
C	-4.27576600	-2.04264800	0.49455300
C	-2.45002800	-0.06544000	2.21208400
C	-3.42714900	-1.48940300	-1.70391500
C	-2.67467800	2.66445100	-0.77081900
C	3.42678700	-1.49087200	-1.70243100
C	2.45014300	-0.06321400	2.21224300
C	4.64245300	1.74399500	0.29357500
C	2.67416900	2.66373100	-0.77398300
C	-4.23434000	-2.48045200	-2.26628200
C	1.20712400	0.60516800	2.80172300
C	3.39306700	3.82080700	-1.09711500
C	5.35699900	2.90046900	-0.02529200
C	-5.08061300	-3.03869100	-0.07120400
C	-1.20763500	0.60377600	2.80191800
C	-4.73408600	3.94247600	-0.71808100

C	4.73311300	3.94253800	-0.72212900
C	5.06370200	-3.25986300	-1.44766400
C	-5.06291200	-3.25966200	-1.45059500
C	5.08186500	-3.03719700	-0.06855100
C	-4.64308200	1.74260600	0.29470700
C	-3.39384500	3.82171500	-1.09267900
C	-5.35790000	2.89925700	-0.02290200
C	4.23431100	-2.48214300	-2.26393500
H	-3.38287800	0.35988700	2.61015100
H	-2.41998200	-1.14102600	2.44638400
H	2.42110400	-1.13864700	2.44729200
H	3.38258400	0.36337800	2.60990500
H	1.29735400	1.71039100	2.73060100
H	1.15755400	0.37082300	3.88442500
H	-1.15787100	0.36901400	3.88452000
H	-1.29890900	1.70894800	2.73127700
H	4.30972500	-1.88609300	1.57567000
H	-4.30843300	-1.88912700	1.57408900
H	-2.77717200	-0.89673000	-2.35100700
H	-1.62763100	2.57145100	-1.06258500
H	2.77618600	-0.89938900	-2.34998000
H	5.14811000	0.93425000	0.82489000
H	1.62726200	2.56998400	-1.06601500
H	-4.21134600	-2.64838800	-3.34537200
H	2.90049800	4.62747500	-1.64481700
H	6.40590600	2.98687500	0.26740600
H	-5.72335700	-3.64230200	0.57365800
H	-5.29523300	4.84547300	-0.96901900
H	5.29404800	4.84539500	-0.97404300
H	5.69163800	-4.03846000	-1.88636200
H	-5.69058000	-4.03809200	-1.88996900
H	5.72523200	-3.63964700	0.57677500
H	-5.14867100	0.93197600	0.82473100
H	-2.90133600	4.62928400	-1.63910500
H	-6.40695800	2.98490400	0.26947500
H	4.21093700	-2.65141600	-3.34280800
H	0.44079329	-1.95393304	0.18494190
H	-0.26896621	-1.93891852	0.17417044

TS14/1

Ru	0.00289100	-0.24209100	0.15664300
H	-0.00650200	1.32277400	-0.25917100
P	-2.33080300	-0.06727500	0.44862500
P	2.33223700	-0.03449500	0.45737100
O	0.00895800	-0.88075900	-2.79139600
N	-0.00414600	0.03880100	2.34235200
C	0.00841900	-0.64571100	-1.64657600
C	3.16949100	1.47757800	-0.20441500
C	-3.49462100	-1.41591600	-0.06564500
C	3.51006700	-1.38804700	-0.00855300
C	-3.17515500	1.46054700	-0.16829800
C	3.50050815	-1.95183046	-1.29731663
C	-3.47516109	-1.94353690	-1.36906654
C	-2.46701600	-0.06403400	2.31243000
C	-4.44542327	-1.89353980	0.85031241
C	-2.37771443	2.46301796	-0.75054038
C	4.46089787	-1.83181031	0.92379909
C	2.46299800	0.02740100	2.32233200
C	2.38945960	2.42457705	-0.89298214
C	4.53055462	1.74577214	0.00616444
C	-5.36628756	-2.87547090	0.46819526
C	1.19129800	0.64879300	2.90530800
C	5.10104244	2.93448220	-0.46526384
C	2.96083721	3.60698265	-1.36643930
C	-4.39606549	-2.92330653	-1.74847941

C	-1.22280200	0.60096300	2.90603800
C	-4.33154152	3.85391906	-1.09683580
C	4.32000888	3.86636710	-1.15273306
C	5.37712126	-3.36971376	-0.71053224
C	-5.34389271	-3.39103273	-0.83069696
C	4.43017577	-2.93461092	-1.64542534
C	-4.55620756	1.67721914	-0.05016090
C	-2.95177063	3.64662280	-1.21665522
C	-5.12969174	2.86925576	-0.51065937
C	5.39024315	-2.81791400	0.57333165
H	-3.39856300	0.39927100	2.66957200
H	-2.50142300	-1.12905100	2.59382600
H	2.54698500	-1.02687500	2.63205700
H	3.37255600	0.54467100	2.66220900
H	1.19734500	1.74782800	2.71930800
H	1.21190500	0.52495300	4.00882900
H	-1.24203100	0.46975200	4.00867800
H	-1.27122700	1.69998900	2.72544800
H	2.76161452	-1.62662960	-2.03322369
H	-2.73566725	-1.59234656	-2.09217449
H	-4.46158835	-1.49302097	1.86565497
H	-1.29813430	2.31879257	-0.83839687
H	4.47112970	-1.40120129	1.92675323
H	1.32626075	2.23757525	-1.06253514
H	5.16056311	1.03529594	0.54304041
H	-6.09934446	-3.24048851	1.19118829
H	6.16230231	3.12779671	-0.29287004
H	2.34145940	4.32994979	-1.90213956
H	-4.37173654	-3.32501111	-2.76413060
H	-4.78021209	4.78241359	-1.45684319
H	4.76647097	4.79281880	-1.52063877
H	6.10093559	-4.14099456	-0.98349993
H	-6.06074268	-4.15975957	-1.12814131
H	4.41387715	-3.36424849	-2.64974057
H	-5.20067559	0.92372518	0.40452935
H	-2.31879008	4.41295288	-1.66972262
H	-6.20643040	3.02315259	-0.40923286
H	6.12310761	-3.15679517	1.30910983
H	0.01227200	-1.29550300	1.69591600
H	0.01389500	-1.91614300	0.95851900

15

Ru	0.01260300	-0.02497400	0.11035700
H	0.00522500	1.59002800	-0.03628800
P	-2.32535800	-0.00257000	0.42769000
P	2.33637800	0.05562200	0.42680700
O	-0.00016700	-0.15241000	-2.88432400
N	0.00940500	0.17387200	2.31628900
C	0.00663400	-0.12617400	-1.71071700
C	3.35478300	1.48233200	-0.19211300
C	-3.38020900	-1.41889500	-0.13726100
C	3.37248900	-1.41196900	-0.04110200
C	-3.34487600	1.46693100	-0.08268100
C	4.35420800	-1.96719000	0.79718400
C	-4.32652000	-2.05217400	0.68509200
C	-2.44668700	-0.03661500	2.29779900
C	-3.22721700	-1.86452200	-1.46201900
C	-2.77421200	2.46666500	-0.88506100
C	3.15654400	-1.98882700	-1.30533500
C	2.47383000	0.14096200	2.29800500
C	2.74938600	2.48740300	-0.96170800
C	4.72971500	1.57545800	0.09131600
C	-4.01131600	-2.91009600	-1.95559500
C	1.22507600	0.80742500	2.87531900
C	5.47852000	2.65697300	-0.37781400

C	3.50289100	3.56777200	-1.43604700
C	-5.10654300	-3.10388300	0.19092500
C	-1.24754600	0.69959700	2.89537000
C	-4.86877500	3.68857800	-0.89518900
C	4.86623800	3.65624700	-1.14400100
C	4.88884200	-3.63085500	-0.88449700
C	-4.95302800	-3.53368000	-1.12989400
C	5.10634300	-3.06983100	0.37713400
C	-4.69203900	1.58978700	0.30380400
C	-3.53412800	3.57028400	-1.29085800
C	-5.44658900	2.69521900	-0.09519400
C	3.91223300	-3.08684400	-1.72533500
H	0.05680800	-0.84383300	2.48091100
H	-3.38962400	0.39520800	2.66337000
H	-2.41701200	-1.09664400	2.59668300
H	2.53603300	-0.89810200	2.65838100
H	3.38242600	0.66959200	2.62049500
H	1.19564600	1.87818100	2.62103100
H	1.23297200	0.72513300	3.97756700
H	-1.24502500	0.58455900	3.99457500
H	-1.29795300	1.77704200	2.67382100
H	4.54242300	-1.54911800	1.78760100
H	-4.46617800	-1.73610800	1.72020700
H	-2.48390600	-1.39781500	-2.11132500
H	-1.72816700	2.37570700	-1.18181400
H	2.38680800	-1.58075600	-1.96345900
H	1.68254900	2.41766400	-1.17980600
H	5.22812600	0.79736800	0.67377100
H	-3.87878400	-3.24425600	-2.98709200
H	6.54489900	2.71737100	-0.14836600
H	3.01881200	4.34159800	-2.03633800
H	-5.83616200	-3.58745500	0.84458500
H	-5.46098000	4.55087000	-1.21012600
H	5.45389000	4.49961100	-1.51384200
H	5.47550300	-4.49276000	-1.21004300
H	-5.56186700	-4.35514800	-1.51410000
H	5.86410600	-3.49077000	1.04195200
H	-5.16484500	0.81616600	0.91335500
H	-3.07727300	4.33964100	-1.91768400
H	-6.49066800	2.77900800	0.21525700
H	3.73043200	-3.52298700	-2.71013600
O	-0.01665214	-2.07707972	0.81527279
H	0.60280186	-2.60798572	0.29474779
H	0.32034041	-1.72078534	-0.21830557
H	-0.56965959	-1.72078534	-0.21830557

TS15/16

Ru	0.00300400	-0.03907300	0.02186500
H	0.02280400	1.56168100	0.13028500
P	-2.33783600	0.06452300	0.35553700
P	2.34352800	-0.01818500	0.35380000
O	0.00939200	0.25658300	-2.98275700
N	-0.00781400	-0.07954200	2.21700600
C	0.00530200	0.11550600	-1.82619600
C	3.32782900	1.51302800	0.02231100
C	-3.37153800	-1.35436700	-0.24169000
C	3.36457600	-1.39173000	-0.36153200
C	-3.29071700	1.57787000	-0.12164900
C	4.15435872	-2.16960499	0.50647006
C	-3.19963695	-1.92641317	-1.51255596
C	-2.46903400	-0.01401000	2.22284400
C	-4.29491000	-1.93129577	0.65279431
C	-4.61418288	1.76491223	0.32088222
C	3.30880458	-1.73926832	-1.72095720
C	2.44955900	-0.26592400	2.20615600

C	2.74005253	2.59567812	-0.64996829
C	4.66635303	1.61861683	0.44528211
C	-5.04821868	-3.04104238	0.26061762
C	1.23312300	0.39822000	2.84910200
C	5.39657005	2.78405950	0.20236004
C	3.47530006	3.76038659	-0.89815121
C	-3.95179608	-3.04336009	-1.89411915
C	-1.18800500	0.55677600	2.82910800
C	-4.71673375	3.90187837	-0.81718194
C	4.80219658	3.85752110	-0.47158036
C	4.83517821	-3.58566361	-1.34035249
C	-4.88183637	-3.59954686	-1.01215875
C	4.88953203	-3.25167383	0.01775303
C	-2.69355174	2.56977191	-0.91444087
C	-5.32050083	2.91948376	-0.02313302
C	-3.40438304	3.72444947	-1.26199299
C	4.03990488	-2.83003985	-2.20534140
H	-0.10924112	-1.23745631	2.35059859
H	-3.36199300	0.52001200	2.57824500
H	-2.56602300	-1.07543700	2.49194100
H	2.42331000	-1.35116700	2.38512400
H	3.39328700	0.12420300	2.61388500
H	1.30770200	1.49838700	2.75783800
H	1.22199200	0.16707400	3.93259200
H	-1.19258200	0.37413200	3.92181300
H	-1.14675500	1.65289300	2.68683800
H	4.19129003	-1.94073827	1.57433435
H	-2.47854769	-1.50313857	-2.21353120
H	-4.41283271	-1.52987340	1.66538610
H	-5.10368258	1.00346193	0.93247856
H	2.69490469	-1.15934209	-2.41161850
H	1.69823924	2.52915010	-0.96549867
H	5.14960663	0.78660007	0.96258136
H	-5.76647319	-3.47648060	0.95948092
H	6.43337748	2.85345097	0.53901285
H	3.00470616	4.59477501	-1.42284410
H	-3.80777946	-3.47643354	-2.88674865
H	-5.27035297	4.80428699	-1.08627742
H	5.37455586	4.76825707	-0.66169353
H	5.40755976	-4.43483849	-1.72008935
H	-5.47150119	-4.46889486	-1.31209344
H	5.50274969	-3.84037467	0.70376687
H	-1.66284965	2.44194790	-1.24677441
H	-6.34606535	3.05185641	0.32885316
H	-2.92603060	4.48781181	-1.87968054
H	3.98520014	-3.08605730	-3.26591847
O	-0.34301800	-2.56713500	2.23539300
H	0.40219300	-3.05399200	2.62089200
H	0.02266200	-1.85351700	-0.31050500
H	-0.07394100	-1.94970500	0.50863200

16

Ru	0.01538500	-0.07592300	0.05905500
H	0.08555100	1.58564400	0.24611800
P	-2.31117700	0.01236000	0.36084000
P	2.33297200	-0.01929600	0.38488400
O	0.06178000	0.05534800	-2.93679900
N	0.00109100	-0.09621600	2.31211700
C	0.04052800	0.00316200	-1.76627800
C	3.25604000	1.50576500	-0.13246700
C	-3.42397600	-1.30751600	-0.31840800
C	3.48230600	-1.36362000	-0.18774600
C	-3.27682200	1.55293700	-0.05040700
C	4.38669505	-1.98022706	0.69592674
C	-4.44204621	-1.92472060	0.42691475

C	-2.46510500	-0.13922600	2.22399800
C	-3.22914930	-1.70238534	-1.65417986
C	-2.66407463	2.59264985	-0.76519058
C	3.43473067	-1.78928067	-1.52366397
C	2.46824700	-0.12010200	2.25249100
C	4.58985472	1.76633560	0.21541090
C	2.55101151	2.46926979	-0.87749332
C	-4.03801579	-2.68315601	-2.23225377
C	1.22795100	0.49844000	2.89602100
C	3.17046167	3.65472685	-1.27660716
C	5.20851859	2.95966240	-0.17914531
C	-5.24694222	-2.91353830	-0.15163004
C	-1.23739600	0.49815500	2.87338900
C	-4.71063693	3.89119180	-0.68096049
C	4.50344323	3.90437711	-0.92783052
C	5.16072585	-3.43413749	-1.08281912
C	-5.04906114	-3.29372589	-1.48134248
C	5.21653474	-3.01233618	0.25122019
C	-4.62120063	1.69485123	0.34040122
C	-3.37864857	3.75496839	-1.07984816
C	-5.33064518	2.85775341	0.03200541
C	4.27138039	-2.81980071	-1.96863415
H	-0.00438100	-1.09560600	2.56345000
H	-3.39014500	0.32272700	2.59923300
H	-2.49480700	-1.21403700	2.46372700
H	2.51943400	-1.19614100	2.48541300
H	3.39096600	0.33486800	2.64118500
H	1.19405200	1.58345700	2.71538600
H	1.24789600	0.33753400	3.98954100
H	-1.27030000	0.35177900	3.96844500
H	-1.21066400	1.58123200	2.67863100
H	4.45067740	-1.65124304	1.73570806
H	-4.62021378	-1.64546213	1.46667326
H	-2.43304081	-1.24576513	-2.24590578
H	-1.61945039	2.48479746	-1.06212364
H	2.73405977	-1.30682366	-2.20836452
H	5.16478480	1.04740441	0.80100560
H	1.50534953	2.29573657	-1.14311534
H	-3.87194859	-2.97735548	-3.27108342
H	2.60809059	4.38945962	-1.85735921
H	6.24771596	3.14583262	0.10183235
H	-6.03174959	-3.38587158	0.44374110
H	-5.26813658	4.79814360	-0.92631968
H	4.98721111	4.83376830	-1.23638432
H	5.81426709	-4.23775739	-1.43006410
H	-5.67746259	-4.06564473	-1.93117866
H	5.91274283	-3.48618744	0.94725022
H	-5.12589380	0.89210410	0.88280125
H	-2.88880456	4.55500926	-1.63996280
H	-6.37296470	2.95528657	0.34464077
H	4.22810888	-3.13924501	-3.01254267
O	0.01933083	-2.89966428	2.28495618
H	0.05667952	-3.82371581	1.99269197
H	0.03841566	-2.38887991	1.43131685
H	-0.06342500	-1.78751400	-0.00955000