

Electronic Supplementary Information

Mechanistic insight into the dehydrogenation reaction catalyzed by the MLC catalyst with dual ancillary ligand sites

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Table of Contents

1. The comparison of free energy barriers using different functionals.	S2
2. The change in free energy introduced by the inclusion of water clusters	S3
3. Free energy diagram of the proton-shuttle transition state involving water molecules. S4	
4. The TDI and TDTS of the reaction pathway considering the energetic span model	S5
5. The IRC of transition states TS4 _a and TS4 _b	S6
6. Comparison of results calculated at the M06-L/def2-TZVP level and the B3LYP/LANL2DZ (for Ru)/6-31+G(d,p) (for non-metal atoms) level.....	S7
7. Rationale for choosing intermediate IM2 as the starting point	S8
8. Geometric structure diagrams.....	S9
9. The DFT calculated energies of all optimized structures.....	S11
10. The cartesian coordinates for all structures	S12

1. The comparison of free energy barriers using different functionals.

Table S1. The comparison of free energy barrier using different functionals (kcal/mol).

Functionals	M06-L	TPSSH	M06	PBE1PBE
IM2	0.0	0.0	0.0	0.0
TS6	19.9	22.2	21.8	22.4
TS4 _b	23.4	25.0	30.6	29.4

In order to select appropriate functional for our calculation, we compare a series of functionals which are widely used in the computational studies relevant to dehydrogenation reaction. The rate-determining transition states and intermediates were calculated using different functionals. The results are shown in Table S1. The relative reaction activation energy and mechanism selectivity calculated by different functionals is basically the same trend. Based on these results, we chose M06-L as the functional considering the computational expense and accuracy.

2. The change in free energy introduced by the inclusion of water clusters

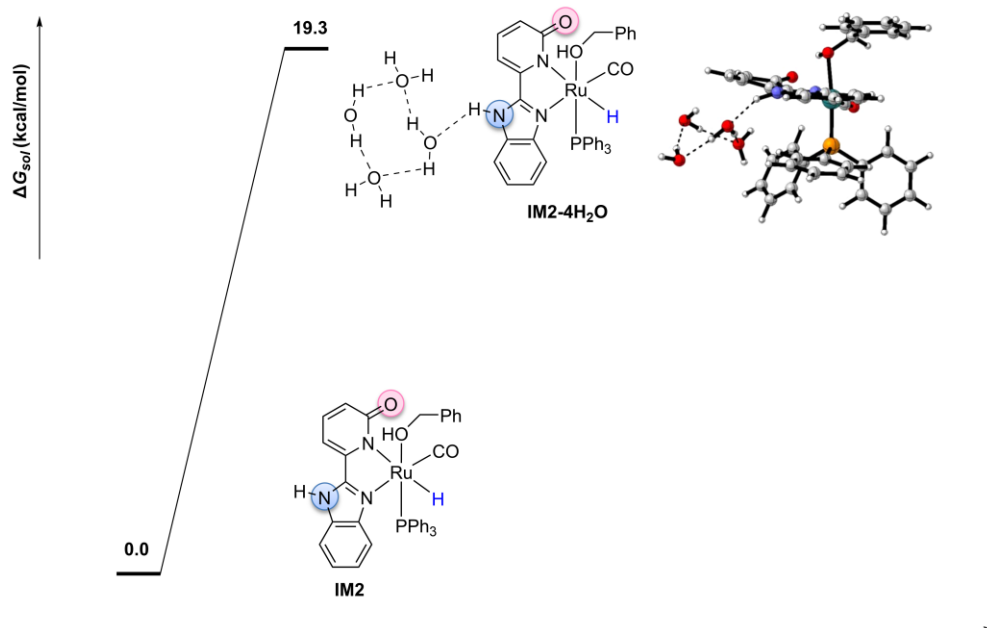


Figure S1. The free energy diagram of intermediate **IM2** with four water molecules

we explored the possibility of explicit water clusters binding to intermediate **IM2**. The computational results indicate that when **IM2** is bound to a water tetramer, the free energy increases by 19.3 kcal/mol, leading to a significant rise in the energy barrier compared to the transition state without water. Thus, this pathway was ruled out.

3. Free energy diagram of the proton-shuttle transition state involving water molecules

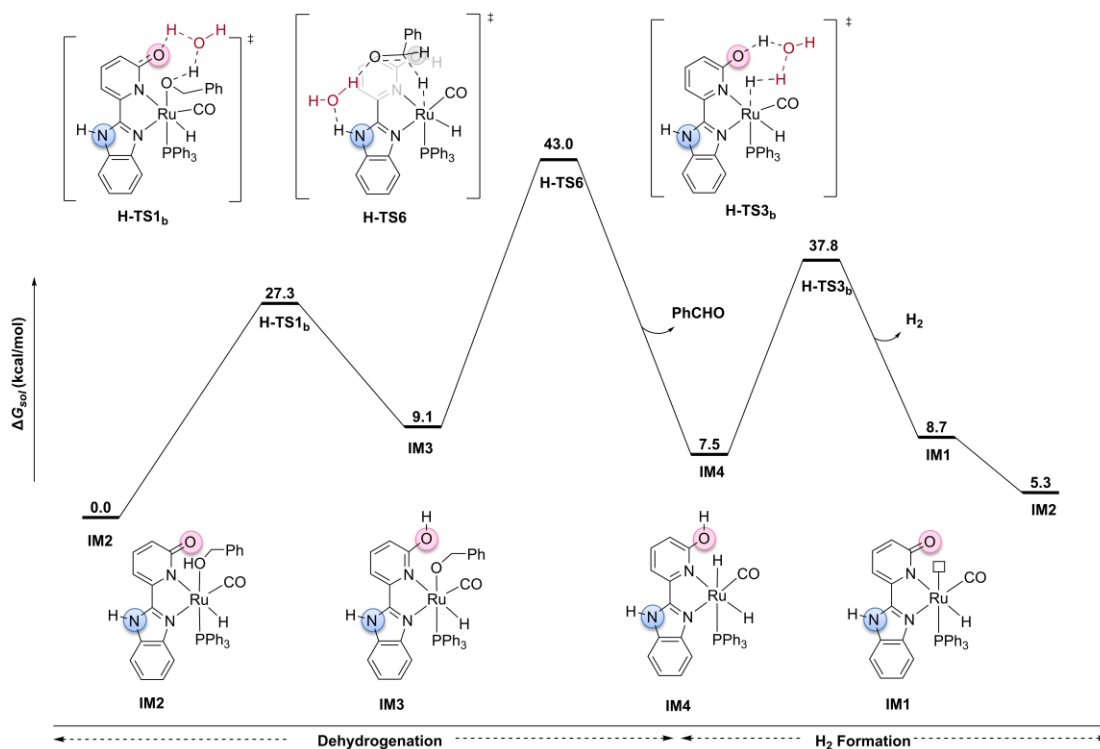


Figure S2. The free energy diagram of the reaction involving water

Additionally, we further considered the potential of a proton-shuttle transition state facilitated by water molecules. As shown in the figure, when water molecules participate in the reaction, the free energy barrier rises to 43.0 kcal/mol, indicating a substantial increase in energy. Therefore, although the ruthenium complex tends to coordinate with water molecules, in solution it is more likely to remain in its free state and is less prone to participate in proton transfer processes.

4. The TDI and TDTS of the reaction pathway considering the energetic span model

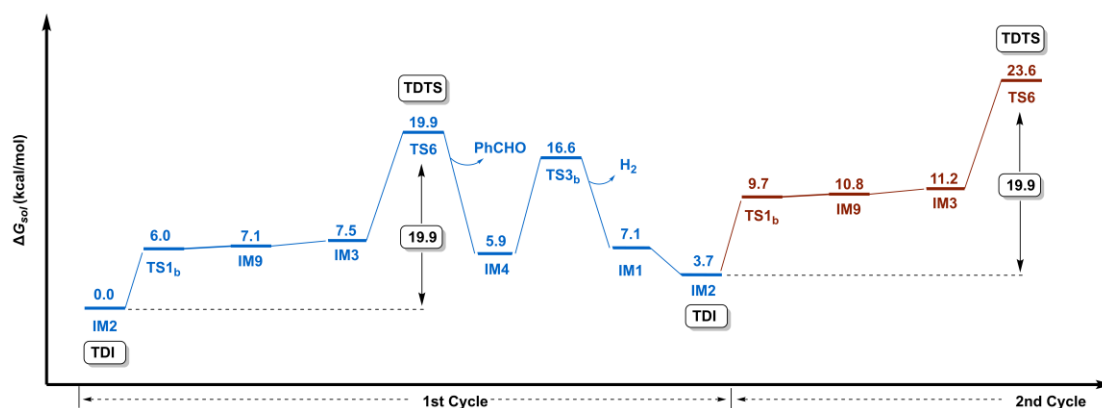


Figure S3. The potential energy diagram considering the energetic span model

As shown in the figure, the overall reaction has a free energy of 3.7 kcal/mol, making it an endothermic process. Therefore, the TOF-determining intermediate should be the lowest point on the free energy profile, which corresponds to **IM2**, while the TOF-determining transition state is **TS6**. The energy barrier calculation does not extend into the next catalytic cycle.

5. The IRC of transition states TS4_a and TS4_b

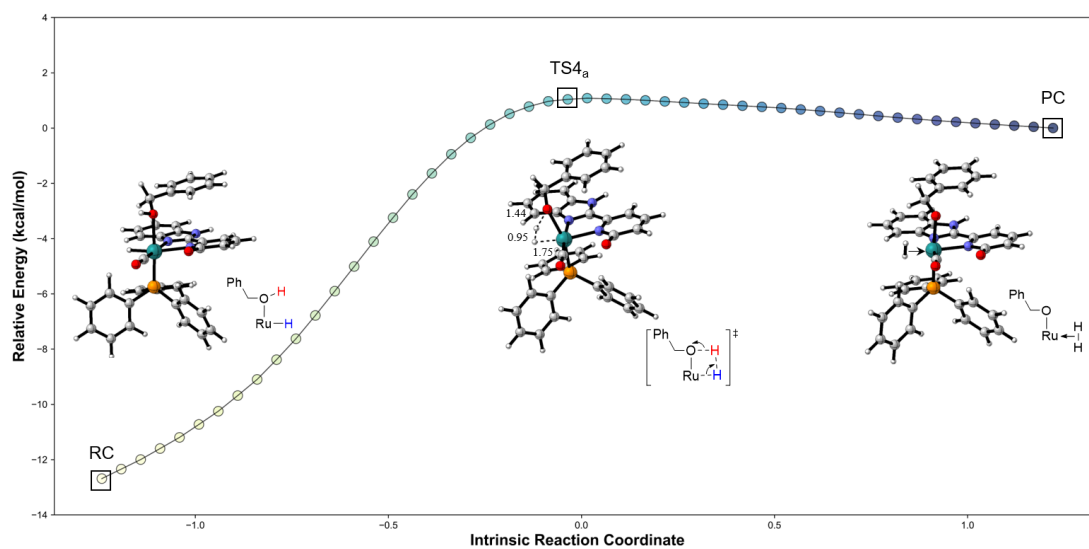


Figure S4. Schematic diagram of the IRC curve for transition state TS4_a

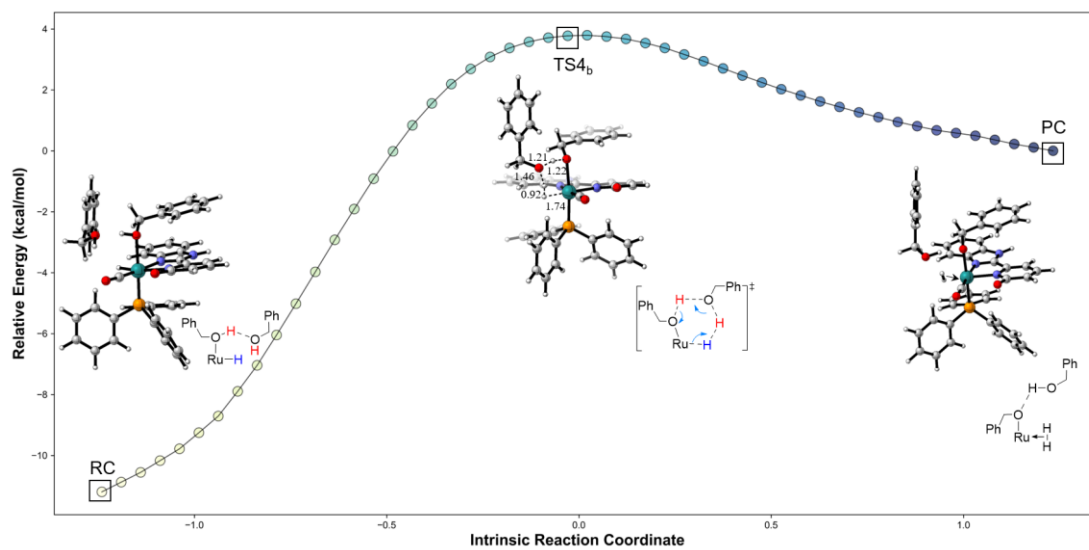


Figure S5. Schematic diagram of the IRC curve for the proton shuttle transition state TS4_b

6. Comparison of results calculated at the M06-L/def2-TZVP level and the B3LYP/LANL2DZ (for Ru)/6-31+G(d,p) (for non-metal atoms) level

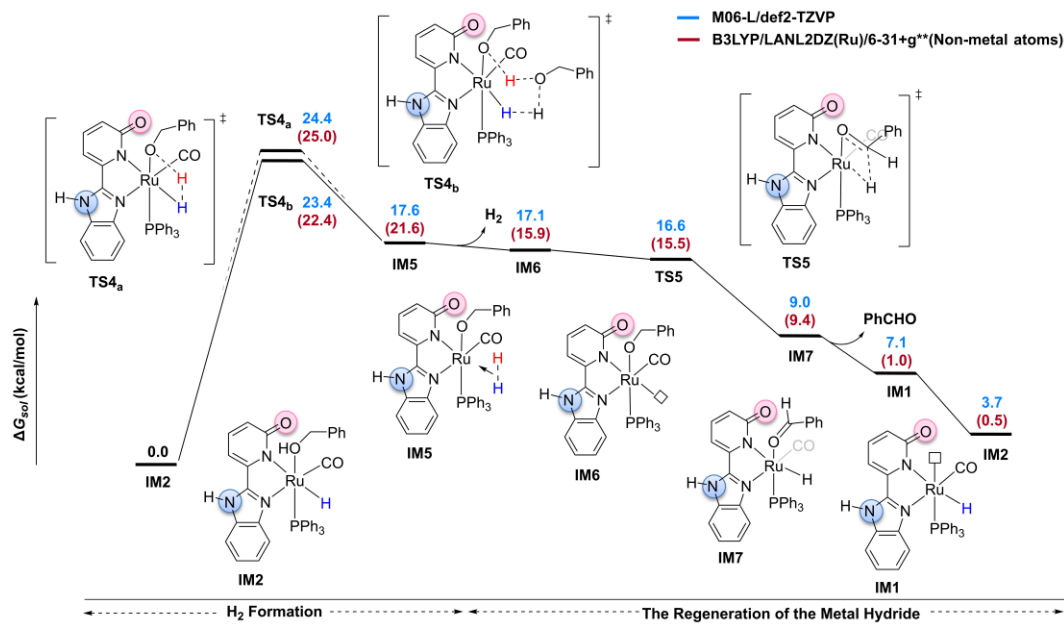


Figure S6. The Free energy diagram for the inner-sphere mechanism.

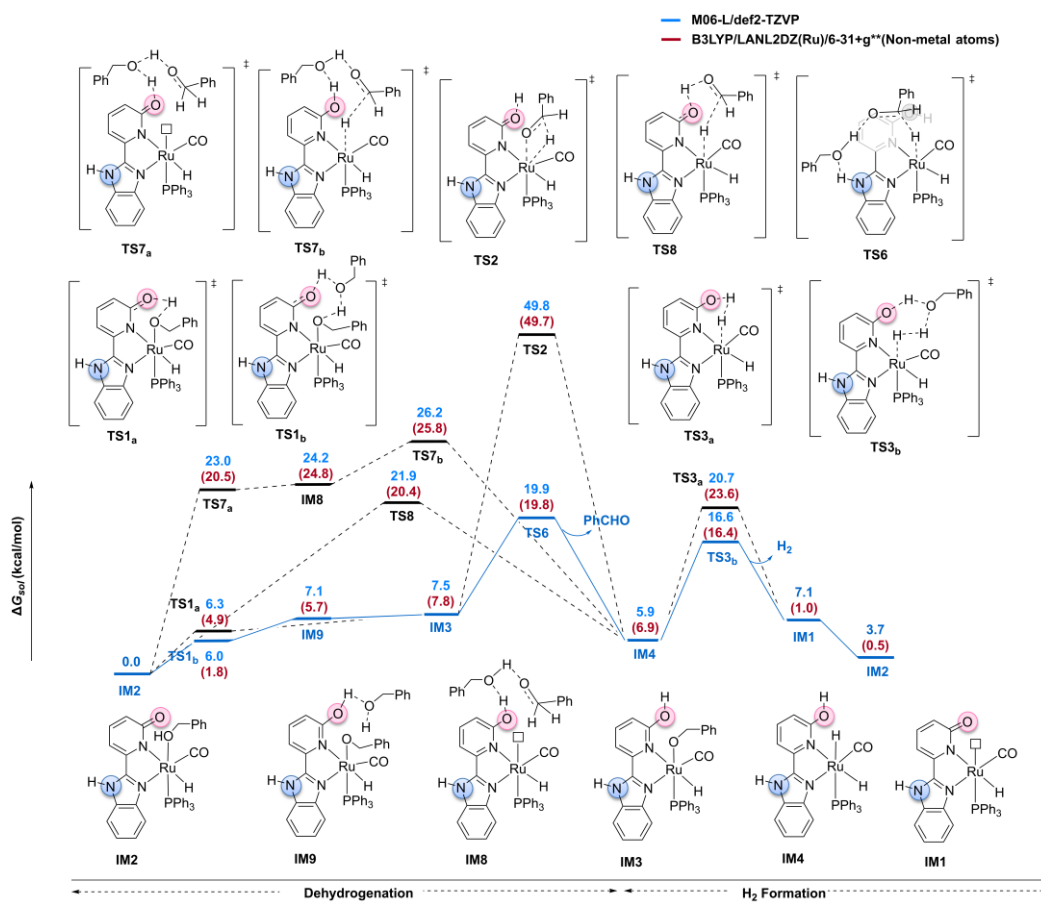


Figure S7. The Free energy diagram for the outer-sphere mechanism.

7. Rationale for choosing intermediate IM2 as the starting point

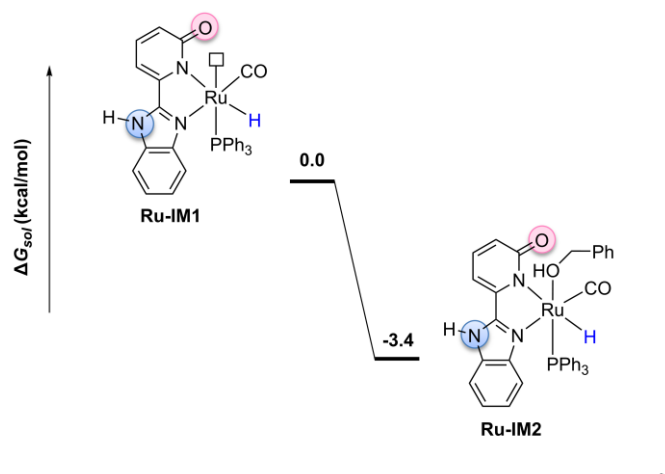


Figure S8. The free energy diagram to examine the stability of intermediate IM2 as the starting point

The reaction free energy for the coordination of the alcohol molecule was calculated to be -3.4 kcal/mol, indicating that this process is exothermic and stabilizes intermediate IM2.

8. Geometric structure diagrams

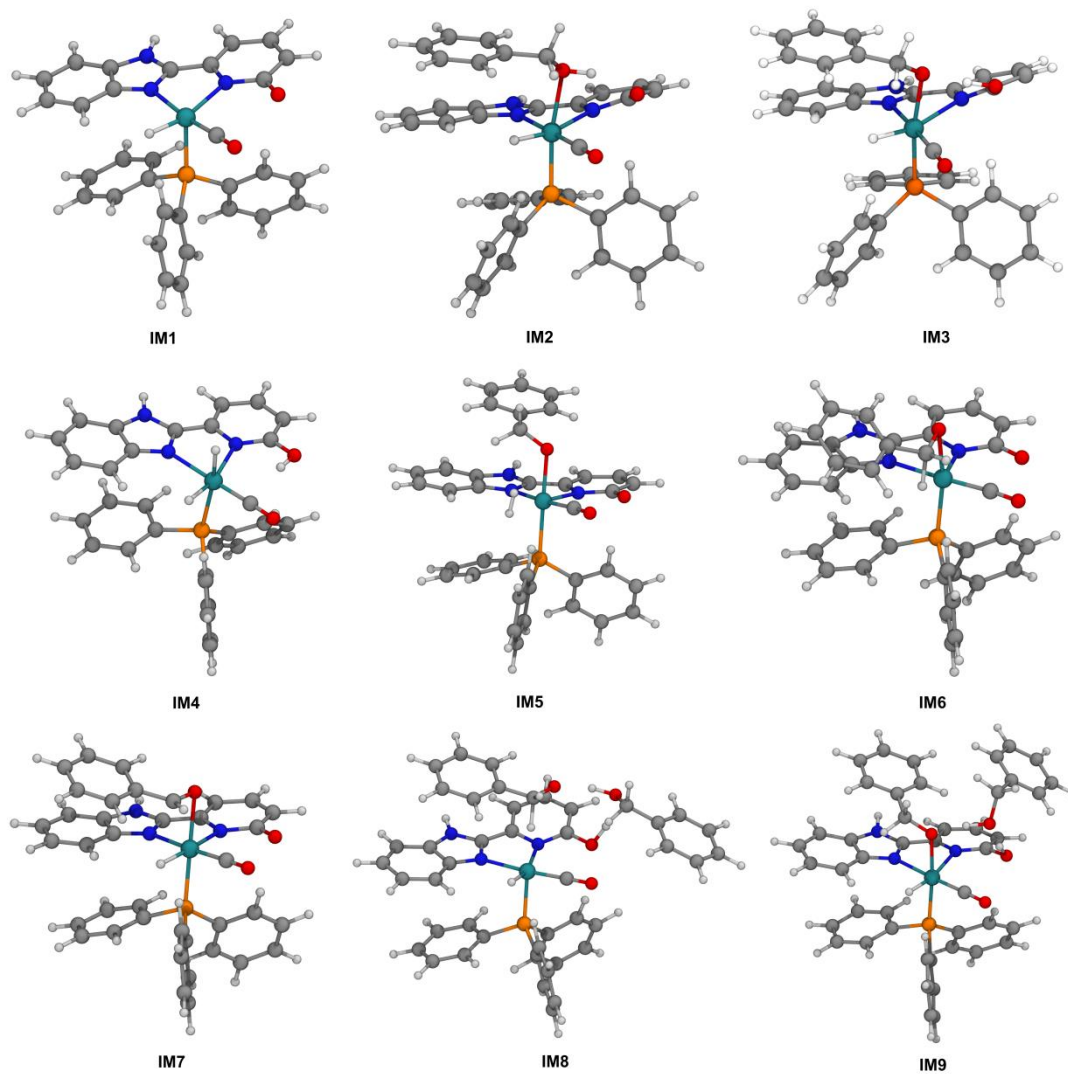


Figure S9. Geometric Structure Diagrams of Intermediates

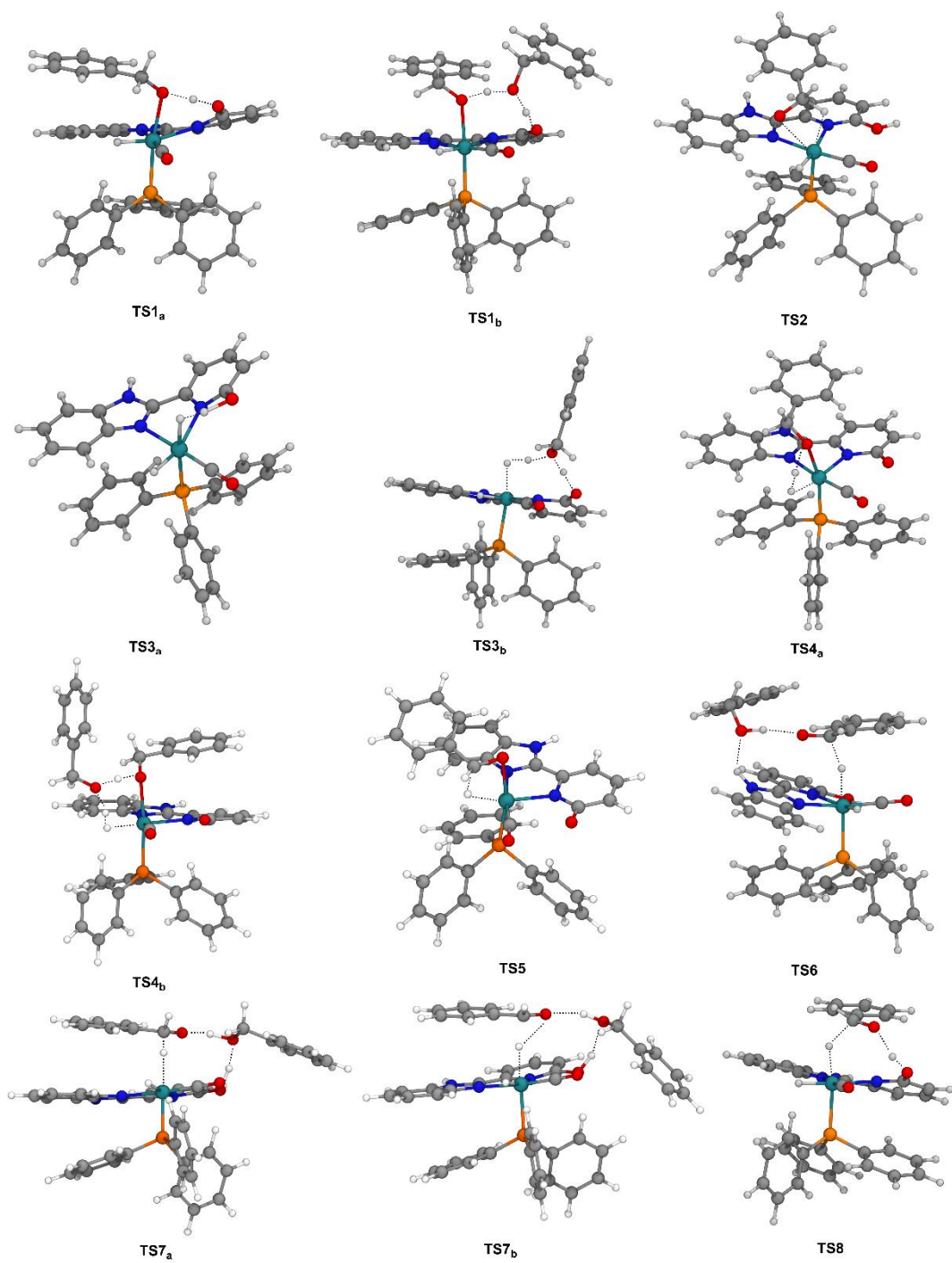


Figure S10. Geometric Structure Diagrams of Transition States

9 The DFT calculated energies of all optimized structures

Table S2. The DFT calculated energies of all optimized structures

Species	G _C hartree	G(gas) hartree	E _{SP} + G _{SOL} hartree	Final G hartree	<i>i</i> (cm ⁻¹)
PhOH	0.087871	-346.374033	-346.854769763	-346.7600463	
PhCHO	0.066621	-345.200148	-345.657401783	-345.5839283	
H ₂	-0.006357	-1.168683	-1.17068990259	-1.170194422	
IM1	0.374643	-1945.129347	-1947.30806299	-1946.926568	
IM2	0.494703	-2291.523907	-2294.19354714	-2293.691992	
IM3	0.493337	-2291.512973	-2294.18018168	-2293.679992	
IM4	0.392114	-1946.305225	-1948.49760961	-1948.098643	
IM5	0.493842	-2291.496636	-2294.16464403	-2293.66395	
IM6	0.473248	-2290.32514	-2292.97463577	-2292.494535	
IM7	0.472516	-2290.338334	-2292.98689778	-2292.507529	
IM8	0.607571	-2637.869194	-2641.02784268	-2640.413419	
IM9	0.614666	-2637.900903	-2641.06225805	-2640.44074	
TS1 _a	0.490452	-2291.515431	-2294.17924599	-2293.681942	-569.27
TS1 _b	0.609301	-2637.902853	-2641.05862923	-2640.442476	-868.95
TS2	0.490745	-2291.441932	-2294.11030643	-2293.612709	-409.53
TS3 _a	0.389219	-1946.282363	-1948.47113013	-1948.075059	-1448.01
TS3 _b	0.502272	-2292.670364	-2295.35084115	-2294.841717	-1352.84
TS4 _a	0.492462	-2291.489501	-2294.15406366	-2293.654749	-880.88
TS4 _b	0.60638	-2637.86829	-2641.0263193	-2640.413087	-938.67
TS5	0.471335	-2290.325877	-2292.97361061	-2292.495423	-497.19
TS6	0.604025	-2637.876474	-2641.03112788	-2640.42025	-415.20
TS7 _a	0.604363	-2637.870832	-2641.02656161	-2640.415346	-878.17
TS7 _b	0.605765	-2637.867778	-2641.02293548	-2640.410318	-428.06
TS8	0.489789	-2291.489221	-2294.15368153	-2293.65704	-559.07

- The G_C designate the Gibbs Free Energy at the M06-L/def2-SVP level.
- The $G(\text{gas})$ designate Gibbs Free Energy in the gas phase at the M06-L/def2-SVP level.
- The $E_{SP} + G_{SOL}$ designates the sum of single point energy at the M06-L/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.
- The **Final G** designates the sum of $E_{SP} + G_{SOL}$ and G_C .
- The *i* designates the imaginary frequency of transition states

10. The cartesian coordinates for all structures

H ₂				C	-1.73319300	1.05973000	0.00002400	C	-3.28700900	-2.26101800	0.67811600
H	0.00000000	0.00000000	0.37724500	C	-0.36010400	1.29073400	-0.00003400	H	-3.16996400	-1.91242600	1.70759900
H	0.00000000	0.00000000	-0.37724500	C	0.53573000	0.21470100	-0.00002500	C	-2.44583500	-1.77030700	-0.33230000
				C	0.04622300	-1.09977000	-0.00000500	C	2.46388100	1.29363000	-0.17484000
Benzyl alcohol				C	-1.32364400	-1.32987600	-0.00001100	C	-1.85264700	0.48025400	1.37901400
C	1.87581600	1.00047500	0.00000100	C	-2.21293600	-0.25049600	0.00002200	C	-4.28065800	-3.18960700	0.38090200
C	0.51632900	1.29858700	-0.00002900	H	-2.43245800	1.89863200	0.00004600	H	-4.92840600	-3.56242900	1.17761600
C	-0.44039600	0.27564300	-0.00002000	H	0.03186400	2.31270800	-0.00008000	C	2.89021000	-2.06463200	-1.23678400
C	-0.00936500	-1.05282800	-0.00000200	H	0.76786300	-1.92041500	-0.00000500	H	2.03097100	-2.41996200	-1.80946100
C	1.35377400	-1.35152200	0.00000300	H	-1.70839500	-2.35221600	-0.00004600	C	1.00827400	-0.97979200	1.88663300
C	2.30026900	-0.32937600	0.00001100	H	-3.29000000	-0.43439400	0.00002800	H	0.92210200	0.09713200	2.06866200
H	2.60961700	1.81016400	0.00001400	C	1.99010600	0.46506100	0.00000600	C	-1.70754500	0.85575000	-2.26711900
H	0.18875100	2.34328000	-0.00005100	O	2.83887800	-0.39500500	0.00001700	C	0.09821800	-1.61305500	1.02626500
H	-0.75529800	-1.84869500	0.00001800	H	2.26701900	1.55522600	0.00005500	C	2.02510700	-1.70806100	2.49673300
H	1.67790400	-2.39527100	0.00000700					H	2.73414400	-1.20251800	3.15753400
H	3.36693900	-0.56539100	0.00002800	IM1				C	0.22170400	-2.98848300	0.79722400
C	-1.90095300	0.62176700	0.00003900	P	-1.10066500	-0.59337000	0.09277400	H	-0.47747300	-3.49325600	0.12396800
O	-2.67819800	-0.54401500	-0.00005100	O	-2.74375900	1.02779900	-2.76378900	C	3.99433400	-2.86689900	-0.97115400
H	-2.11542900	1.25897000	0.88345900	O	-1.40149100	3.57118600	-1.33223000	H	4.01481000	-3.89232800	-1.34634600
H	-2.11549500	1.25917500	-0.88322100	N	1.97117300	0.24704000	-0.82954800	C	0.17949900	4.78354400	-0.06569400
H	-3.60424600	-0.28659000	0.00013500	N	3.69062100	1.00948300	0.34895900	C	-2.41137700	1.70039800	0.97811600
				H	4.26931200	1.65581400	0.86812900	H	-2.36497800	2.02012800	-0.06690300
Benzaldehyde				N	0.50470500	2.46776500	-0.69113600	C	2.21395000	3.66241300	0.55163600

H	3.19929500	3.66514700	1.02115400	H	-1.97833200	-1.83999400	-2.43647000	C	0.55348700	-1.20965300	-2.39334200
C	2.14180700	-3.07960400	2.26306400	C	-3.62656500	-3.14776500	-1.94003800	C	1.52764900	1.24628500	1.31244700
H	2.94413500	-3.64936300	2.73769500	H	-3.76086800	-3.48547900	-2.97007400	C	2.27331300	0.80883000	3.58203900
C	1.71563200	2.53407500	-0.08163700	Ru	-0.06917000	0.49378300	-1.52715700	H	2.86646600	0.21004300	4.27781900
C	-1.89264900	0.12154000	2.73606200	H	-0.07565700	-0.95715800	-2.24568100	C	0.76012800	2.31776000	1.79368300
H	-1.45560300	-0.82388600	3.07036400	H	-0.47285200	5.65847300	-0.08602400	H	0.15140500	2.90717100	1.10120200
C	-0.31774000	3.59853100	-0.74702600					C	-3.44001900	2.81505800	1.39976300
C	2.90646800	-0.76068500	-0.73784100	IM2				H	-3.97753900	3.59149900	0.85105100
C	5.08862100	-2.39037300	-0.22783800	P	1.42141500	0.72103800	-0.44766000	C	1.32450400	-4.28418600	1.47387000
H	5.93746100	-3.05220000	-0.04362400	O	1.02882300	-1.47692300	-3.42387300	C	3.28044400	-1.36018200	-0.87905100
C	-2.99619100	2.54730800	1.91803000	O	0.71353000	-3.86109200	-0.79355600	H	2.41315900	-2.02343100	-0.92553400
H	-3.41254600	3.50147100	1.58627900	N	-1.24992900	-0.15608700	1.03174600	C	0.41806500	-2.73874600	3.09524300
C	1.23520500	-3.71755700	1.41890300	N	-1.31002300	-0.16833000	3.25184500	H	0.16474700	-2.48066900	4.12514600
H	1.32166200	-4.79079700	1.23335300	H	-1.07689700	-0.42382100	4.20181800	C	1.52286400	1.88891200	4.04708300
C	5.11971300	-1.09218100	0.27626200	N	0.32538900	-2.23440000	0.74110300	H	1.53132400	2.14724000	5.10914100
H	5.97158100	-0.72436900	0.85131600	C	2.08280100	3.46533500	-0.87742400	C	0.03260500	-1.93982000	2.02593000
C	4.01151700	-0.29167000	0.00865900	H	2.50616500	3.46998500	0.13073500	C	4.24104600	0.84613900	-0.67736500
C	-3.03430100	2.18571300	3.26353600	C	1.47897500	2.30397900	-1.38381400	H	4.12990300	1.92649300	-0.55314500
H	-3.48864800	2.85311100	3.99986100	C	-0.80997000	-0.76044300	2.12886900	C	0.79123000	-3.48702800	0.39640200
C	-2.48316700	0.97024700	3.67052700	C	3.10804600	0.02003100	-0.71333500	C	-2.05221400	0.88030300	1.44233400
H	-2.50694500	0.68157700	4.72415500	C	2.14449300	4.62621700	-1.64636200	C	-3.49499400	2.80972000	2.80650000
C	-4.45302300	-3.63500400	-0.93005900	H	2.61235800	5.52356100	-1.23443100	H	-4.07233800	3.58156600	3.31999400
H	-5.23770800	-4.35839200	-1.16375600	C	-2.72165500	1.85473500	0.69698600	C	4.56115700	-1.90031900	-1.00119100
C	1.39946000	4.81424600	0.55478800	H	-2.66746600	1.83971900	-0.39458000	H	4.67557600	-2.97858400	-1.13348700
H	1.74626200	5.72586900	1.04921100	C	2.27802600	0.48970400	2.22456600	C	0.76580400	2.64237800	3.14889600
C	-2.62685700	-2.22128600	-1.64464200	H	2.86538900	-0.36388300	1.87235100	H	0.16619200	3.48475000	3.50316900

C	-2.83062600	1.84620700	3.56186500	H	-6.35024600	1.29466600	-1.32070600	C	2.25405700	0.38242000	2.29263600
H	-2.86801600	1.85251400	4.65302100	H	-5.49817000	-0.10132700	0.55939900	H	2.84122300	-0.46565100	1.92643400
C	-2.10785500	0.88661100	2.85552000	C	-2.57499100	-2.45918400	-2.21431500	C	0.66051000	-1.18228600	-2.44945300
C	5.68047800	-1.07254400	-0.96142700	H	-2.04488000	-2.26179800	-3.16330300	C	1.53405100	1.17570500	1.38581500
H	6.68230200	-1.49736200	-1.06059900	O	-1.67769200	-2.48005800	-1.11762500	C	2.23055400	0.66161000	3.65857400
C	5.51733400	0.30425700	-0.80132800	H	-0.96258000	-3.15984100	-1.22235600	H	2.80445100	0.03559700	4.34693900
H	6.38965100	0.96161500	-0.77511700	H	-3.04541700	-3.45601900	-2.30871300	C	0.78002600	2.24846200	1.88680900
C	1.61216400	4.64179800	-2.93483700	H	1.81803200	-5.22161300	1.21117500	H	0.19673200	2.87137300	1.20180500
H	1.66100100	5.55205600	-3.53710200					C	-3.35618300	2.87114600	1.26352900
C	1.12682100	-3.91572000	2.78574300	IM3				H	-3.86573100	3.65771800	0.70304400
H	1.48728500	-4.55906600	3.59320500	P	1.44788800	0.69949600	-0.39359200	C	0.96483700	-4.47324600	1.37728100
C	0.94095000	2.33395500	-2.67748000	O	1.21400300	-1.41914500	-3.44849900	C	3.32071900	-1.37774700	-0.74738700
H	0.45314300	1.44148000	-3.07687900	O	0.39904300	-3.96947100	-0.88261600	H	2.44515600	-2.03151700	-0.76037400
C	1.01395600	3.49223600	-3.44869500	N	-1.27304100	-0.17553500	0.94169800	C	0.27600500	-2.83639600	3.01740700
H	0.59284600	3.49666400	-4.45658500	N	-1.35134900	-0.16504500	3.16583700	H	0.09203400	-2.55176800	4.05483300
Ru	-0.25445900	-0.74056900	-0.82823200	H	-1.12619600	-0.40750300	4.12113900	C	1.49398000	1.74388900	4.14180800
H	-1.03315500	0.36552000	-1.70466100	N	0.15631600	-2.34245600	0.67639200	H	1.49154100	1.97494000	5.21015900
C	-4.13725000	-1.21775500	-0.68419900	C	2.15420200	3.45613500	-0.71243800	C	-0.08985100	-2.00784900	1.96009900
C	-3.61890000	-1.41102000	-1.97070500	H	2.56101200	3.42146800	0.30199400	C	4.28383700	0.82951200	-0.64233200
C	-4.09222600	-0.61318800	-3.01643300	C	1.55086000	2.31747700	-1.26931300	H	4.17695000	1.91430200	-0.56396500
C	-5.07377000	0.35032700	-2.78708100	C	-0.86436300	-0.78112600	2.04819700	C	0.51050400	-3.59650300	0.36780200
C	-5.58701500	0.53425900	-1.50380500	C	3.14796700	0.00792700	-0.63388600	C	-2.03810300	0.89150500	1.33864500
C	-5.11306700	-0.25156600	-0.45278500	C	2.24015700	4.64259800	-1.43876400	C	-3.42269100	2.88163900	2.67110600
H	-3.75330400	-1.82304400	0.14073700	H	2.70790500	5.52075200	-0.98708800	H	-3.97809600	3.67825600	3.17087900
H	-3.67690200	-0.74072100	-4.02037800	C	-2.66800100	1.88050100	0.57628200	C	4.59695200	-1.92884600	-0.85953000
H	-5.43113800	0.96828900	-3.61431300	H	-2.61243400	1.84827800	-0.51453000	H	4.71009800	-3.01139500	-0.95262600

C	0.77096800	2.53729900	3.25048800	H	-3.76530200	-0.36930800	-3.98158100	C	3.16465700	-1.59564200	-1.32080800
H	0.18664400	3.38549100	3.61630500	H	-5.55276100	1.24159600	-3.35913100	H	2.39227700	-2.03570500	-1.95485900
C	-2.80110300	1.90448800	3.44303100	H	-6.38457700	1.33876400	-1.01082200	C	1.19007900	-0.81806600	1.97114100
H	-2.84852400	1.92322400	4.53361100	H	-5.40633200	-0.18073800	0.70557900	H	0.95357600	0.22994200	2.18444200
C	-2.10559300	0.91341200	2.75152600	C	-2.51283500	-2.20159300	-2.36294600	C	-1.68423700	0.43380500	-2.64245900
C	5.71849100	-1.10248700	-0.86442500	H	-2.06050300	-1.89579900	-3.33340600	C	0.35815200	-1.55932300	1.11640300
H	6.71820800	-1.53308500	-0.95880000	O	-1.58378100	-2.37188300	-1.35499400	C	2.31751800	-1.39870700	2.54600700
C	5.55809000	0.27920400	-0.75779100	H	-0.36224800	-3.39390300	-1.28432000	H	2.95803600	-0.80420900	3.20350300
H	6.43176100	0.93522800	-0.76845500	H	-3.00878800	-3.17626000	-2.57171400	C	0.68416500	-2.89781500	0.86003500
C	1.73309700	4.70788500	-2.73601800	H	1.32738100	-5.46311500	1.09907900	H	0.05267600	-3.49166300	0.19255100
H	1.80041600	5.63820000	-3.30495000					C	4.36823200	-2.23263500	-1.04925700
C	0.86426000	-4.06757100	2.69860300	IM4				H	4.56664700	-3.21429700	-1.48443300
H	1.18839400	-4.73821400	3.49740100	P	-0.96716700	-0.71496700	0.17133600	C	-0.67418200	4.61793700	0.02915200
C	1.04048500	2.39773100	-2.57220600	O	-2.68874700	0.36532700	-3.24071000	H	-1.45658400	5.37362300	-0.03825000
H	0.55601900	1.52336900	-3.01352100	O	-1.83444400	3.31970400	-1.54996500	C	-2.62843900	1.33727600	1.01627800
C	1.13740400	3.58160000	-3.30125200	N	1.87607100	0.50645000	-0.82079500	H	-2.69203600	1.54065800	-0.05654100
H	0.73670000	3.62389400	-4.31657200	N	3.40140200	1.43973200	0.50862900	C	1.41985900	3.77707400	0.84855400
Ru	-0.23636700	-0.76765000	-0.92414000	H	3.85579600	2.13198200	1.08755600	H	2.31946900	3.88335300	1.45716300
H	-0.92847200	0.36258200	-1.81825300	N	0.10769500	2.46052500	-0.70143600	C	2.63666000	-2.73026400	2.27723000
C	-4.05870100	-1.13335400	-0.68477300	C	-2.96080700	-2.60705900	0.87126600	H	3.52747400	-3.18189200	2.72007000
C	-3.58823900	-1.20460700	-2.00215200	H	-2.91218800	-2.18368800	1.87844400	C	1.22475200	2.64505200	0.05724000
C	-4.13761100	-0.33772200	-2.95245800	C	-2.15819100	-2.08049700	-0.15139600	C	-1.77115200	0.01760600	2.84238700
C	-5.13904200	0.56908000	-2.60281300	C	2.16353100	1.55734100	-0.06617800	H	-1.17256800	-0.81728400	3.21772800
C	-5.60454800	0.62525900	-1.28933400	C	-1.84082200	0.26786100	1.46380100	C	-0.79319400	3.45372700	-0.74268800
C	-5.05843300	-0.23067000	-0.33090100	C	-3.82803800	-3.66601100	0.61508400	C	2.95501300	-0.34096000	-0.74117500
H	-3.60873100	-1.79431000	0.06153700	H	-4.44993400	-4.06428400	1.42039500	C	5.34434300	-1.64215700	-0.22394400

H	6.27896600	-2.17624200	-0.03936400	P	1.93137400	0.31005600	0.02604700	C	-0.55891000	-4.12803900	1.13575000
C	-3.32553300	2.13990800	1.91645400	O	2.02809100	-2.19206600	-2.95499600	C	2.90178600	-2.15727400	0.85624100
H	-3.93275000	2.96850700	1.54331400	O	0.76103900	-3.66666200	-0.76514500	H	2.52225700	-2.52098600	-0.10209700
C	1.81228700	-3.47804800	1.43886900	N	-1.27114200	0.58937500	-0.10506900	C	-1.88681000	-2.34198300	2.03923200
H	2.05251300	-4.52234100	1.22465500	N	-2.73852300	0.53194100	1.55783700	H	-2.63755900	-1.96882200	2.73720800
C	5.15114100	-0.39546200	0.36299100	H	-3.38122500	0.12161000	2.22298800	C	0.09046300	3.81635300	2.41973100
H	5.90976700	0.05632900	1.00497400	N	-0.42444900	-1.93035100	0.15535700	H	-0.40576800	4.63237600	2.95000600
C	3.94006100	0.24017200	0.09311200	C	4.41645900	1.61961400	-0.10077300	C	-1.35989000	-1.52274800	1.05464200
C	-3.23918800	1.88924800	3.28555400	H	4.33888000	1.67647300	0.98911900	C	3.19302000	-0.39208300	2.48342800
H	-3.77743100	2.52163200	3.99560800	C	3.39109100	1.01383000	-0.84383000	H	3.06190300	0.64684100	2.79839800
C	-2.46312100	0.82505100	3.74467800	C	-1.79568100	-0.15752800	0.85693000	C	-0.01992900	-3.26734900	0.10076800
H	-2.39751900	0.61789200	4.81576700	C	2.71628700	-0.82230400	1.23524200	C	-1.89524000	1.81242200	-0.04998700
C	-3.90531400	-4.21355700	-0.66620700	C	5.53187900	2.15353500	-0.73769300	C	-3.49661000	4.01071900	0.48976400
H	-4.58951000	-5.04141600	-0.86739700	H	6.32027800	2.62484500	-0.14646100	H	-4.11872800	4.88823800	0.67766300
C	0.44047900	4.76917700	0.84161700	C	-1.74592100	2.95458500	-0.84121600	C	3.53913800	-3.05008600	1.71599800
H	0.55516100	5.66389600	1.45585300	H	-1.01583900	2.97735300	-1.65336100	H	3.65992200	-4.09137300	1.40876700
C	-2.24421500	-2.63429600	-1.43456400	C	0.59478200	1.46235100	2.20277900	C	0.83855400	4.07793900	1.27463700
H	-1.62251900	-2.22526200	-2.23523400	H	0.48613900	0.43513100	2.56629900	H	0.93360900	5.10137100	0.90427300
C	-3.11206900	-3.69652400	-1.68825700	C	1.28784800	-1.62682100	-2.27118800	C	-3.65763000	2.88125400	1.28703900
H	-3.17150500	-4.11599500	-2.69518200	C	1.34311500	1.71515100	1.04184400	H	-4.39678000	2.84991800	2.08973100
Ru	-0.10328500	0.47355800	-1.73640700	C	-0.02759200	2.50470800	2.88332400	C	-2.84342200	1.78844600	0.99912300
H	0.15840000	-0.94647000	-2.44634100	H	-0.61476200	2.29079100	3.78010600	C	4.00437900	-2.61927500	2.95694500
H	-1.71135000	2.47418000	-2.03659200	C	1.45706200	3.03420800	0.58580800	H	4.49982800	-3.32102500	3.63209400
H	0.59195900	1.01423900	-3.12082900	H	2.02958300	3.25058000	-0.32147700	C	3.83280700	-1.28804900	3.33736800
				C	-2.55668500	4.04709500	-0.55670200	H	4.19689300	-0.94293800	4.30799500
IM5				H	-2.46681000	4.95376400	-1.15852700	C	5.64487300	2.08230500	-2.12772400

H	6.52328200	2.49701400	-2.62742800	IM6				H	-4.56647700	1.56139700	2.14058300
C	-1.45498900	-3.68158700	2.07058900	P	1.38658700	0.82430700	0.28450300	C	2.36034000	-4.10023900	-1.26226900
H	-1.84509400	-4.36380400	2.83064700	O	2.01271500	0.65936500	-3.41206000	C	3.84413700	-0.35664000	-0.30083100
C	3.51491200	0.94623600	-2.23547500	O	2.56211400	-2.09266600	-2.48369000	H	3.44744700	-0.46290600	-1.31312800
H	2.73669700	0.46807700	-2.83389900	N	-1.22262900	-1.05393800	0.25414000	C	0.53765100	-4.29339900	0.28796300
C	4.63741000	1.47686000	-2.87360600	N	-1.77232300	-2.77805300	1.53849300	H	-0.06039100	-4.87430600	0.99170100
H	4.72189500	1.41011400	-3.96037300	H	-1.75162600	-3.70871500	1.93218000	C	-0.95157600	0.85160600	4.28495200
Ru	0.14651100	-0.51669200	-1.30577000	N	0.90775500	-2.20910900	-0.89344400	H	-1.54585400	0.82801700	5.20133400
H	0.08276600	0.49096200	-2.70437100	C	2.62334700	3.33377000	0.68571300	C	0.20504900	-2.98144500	-0.01883100
C	-3.86287000	-1.85637200	-0.86168300	H	3.16738000	2.84664000	1.49988000	C	3.58699700	0.27748000	2.01687000
C	-3.72372200	-0.65017300	-1.55933200	C	1.71860100	2.59585600	-0.09191700	H	2.99268300	0.70485500	2.82911500
C	-4.64274000	0.37613700	-1.30727400	C	-0.92538400	-2.30409000	0.57803800	C	1.98186400	-2.74797700	-1.61654400
C	-5.67014800	0.20837900	-0.37862700	C	3.05754200	0.19198200	0.71923700	C	-2.28410600	-0.67433500	1.04415400
C	-5.79442700	-0.99560200	0.31727800	C	2.83958200	4.68475300	0.42891300	C	-4.39296700	-0.47809900	2.83411900
C	-4.88676300	-2.02834200	0.06864400	H	3.54820200	5.24595000	1.04235800	H	-5.23277400	-0.37734900	3.52490400
H	-3.12820000	-2.64548700	-1.04812500	C	-2.95900500	0.54454300	1.14728700	C	5.13075400	-0.81815200	-0.02771900
H	-4.53691900	1.33160800	-1.83422700	H	-2.66410200	1.39601000	0.53034600	H	5.72198800	-1.25601300	-0.83518600
H	-6.37126100	1.02666900	-0.18980700	C	0.48759300	-0.26256600	2.69586000	C	-0.88049100	2.01662900	3.52609100
H	-6.60193000	-1.13233900	1.04186100	H	1.02556800	-1.16085500	2.37327200	H	-1.41613200	2.91304800	3.84753800
H	-4.97653600	-2.97748200	0.60541500	C	1.32596800	0.20658700	-2.59617300	C	-3.72154600	-1.69551200	2.75682800
C	-2.60051200	-0.48283200	-2.56573000	C	0.55003700	0.90269500	1.91462800	H	-4.01199200	-2.54697300	3.37519200
H	-2.37499400	0.61082500	-2.63333400	C	-0.26072100	-0.28844700	3.86823300	C	-2.66014800	-1.76922100	1.85653800
O	-1.50572300	-1.27639300	-2.34521900	H	-0.30909300	-1.20589200	4.46073500	C	5.64920000	-0.73328800	1.26298600
H	0.62987100	0.91120300	-2.16286800	C	-0.13819400	2.04255300	2.34443200	H	6.65600500	-1.10010700	1.47684800
H	-3.03107800	-0.72135200	-3.56778700	H	-0.10214700	2.95973700	1.74933800	C	4.87507100	-0.18244400	2.28425800
H	-0.21811900	-5.16442000	1.11717500	C	-4.01363400	0.62407700	2.04715500	H	5.27415300	-0.11161200	3.29903500

C	2.15897600	5.31828800	-0.61187400	IM7				H	4.25118700	-2.82652900	1.42271500
H	2.33379600	6.37707200	-0.81642800	P	-1.49272200	-0.80710700	0.12370700	C	-1.55542100	4.59868300	-0.23174400
C	1.66010700	-4.84852200	-0.35215200	O	-2.02044200	0.28280100	-3.45309900	C	-3.55037900	1.04999500	0.01067600
H	1.96537100	-5.87425300	-0.12916100	O	-2.11444200	2.97691800	-1.85789400	H	-3.14357100	1.29892600	-0.97339400
C	1.04501900	3.24029000	-1.13513500	N	1.34966900	0.66418800	0.44815100	C	0.21813500	4.07362800	1.30464000
H	0.34756800	2.67243200	-1.75811000	N	2.18672900	1.89619200	2.09134900	H	0.89902700	4.35785500	2.10887000
C	1.26292800	4.59347600	-1.39411400	H	2.32189200	2.68802700	2.70487600	C	0.85937700	-2.45124600	3.75543400
H	0.73385700	5.07944000	-2.21693000	N	-0.52505500	2.42065300	-0.30253500	H	1.45724900	-2.81702700	4.59340000
Ru	0.11811100	-0.29938900	-1.29474500	C	-3.30870200	-2.94020000	0.01027200	C	0.28726800	2.82459800	0.70243000
C	-3.99100400	-0.45295000	-1.81637300	H	-3.66917900	-2.56230800	0.97095900	C	-3.45880700	-0.17728200	2.09290000
C	-3.14918700	0.60524400	-2.16431900	C	-2.26765600	-2.27852600	-0.65968400	H	-2.99477700	-0.92734700	2.73917800
C	-3.62995300	1.91714800	-2.10076100	C	1.26748600	1.82578900	1.08382500	C	-1.44065100	3.30259300	-0.87696500
C	-4.93136800	2.17043200	-1.67381300	C	-2.93105500	0.09032200	0.81983600	C	2.34078800	-0.06550900	1.06333500
C	-5.76687800	1.10914200	-1.31837900	C	-3.89472700	-4.07662800	-0.53910100	C	4.40553100	-1.04284900	2.63106700
C	-5.29581800	-0.20121200	-1.39643300	H	-4.70424500	-4.57952400	-0.00526900	H	5.22257900	-1.44937500	3.23095000
H	-3.59125900	-1.46816700	-1.87718200	C	2.81482300	-1.35338800	0.80734400	C	-4.66875700	1.74172200	0.47157600
H	-2.97253200	2.74794100	-2.38108300	H	2.38055300	-1.94803200	0.00022800	H	-5.12313700	2.50145900	-0.16865500
H	-5.29924400	3.19818800	-1.62178900	C	-0.34790500	-0.66108200	2.67216200	C	0.55153300	-3.29761200	2.69280500
H	-6.78869400	1.30622200	-0.98501900	H	-0.69664300	0.37710100	2.66592400	H	0.90325100	-4.33198500	2.69642100
H	-5.94962000	-1.03315800	-1.12203600	C	-1.27917100	0.38663900	-2.56864400	C	3.93764400	0.24062000	2.90436200
C	-1.73434600	0.31413500	-2.61161400	C	-0.65368900	-1.50414900	1.59292000	H	4.36743900	0.84500000	3.70552100
H	-1.07646000	0.98316100	-1.76732600	C	0.40568300	-1.13119400	3.74338400	C	2.89614500	0.70994600	2.10650900
O	-1.36334400	-0.95206500	-2.64406900	H	0.64530100	-0.46147500	4.57328300	C	-5.18606800	1.47684700	1.73818700
H	-1.46677700	0.92913200	-3.50705100	C	-0.19696700	-2.82698400	1.61392900	H	-6.05993500	2.02331700	2.10109500
H	3.22734400	-4.50267700	-1.78846900	H	-0.42259600	-3.49534200	0.77784600	C	-4.58112000	0.51362400	2.54605400
				C	3.85152700	-1.82593900	1.60279100	H	-4.98208800	0.29914600	3.53959100

C	-3.45478600	-4.56578300	-1.76975500	IM8				H	-5.67047200	0.14299400	-2.62526300
H	-3.91999300	-5.45353600	-2.20444200	P	-0.53822300	2.10757700	0.06162100	C	1.80896300	-2.49990700	2.63025600
C	-0.75179800	4.96998300	0.81437700	O	2.61034900	0.90984000	-1.62277300	C	1.50129900	2.07113300	1.95760800
H	-0.85315800	5.96235000	1.26261400	O	2.59404300	-0.83654700	1.11725000	H	1.99917000	1.40419400	1.24962400
C	-1.83330800	-2.77697400	-1.89272100	N	-1.96911400	-0.80271200	0.00753800	C	-0.55236200	-2.88229200	2.70307000
H	-1.02469400	-2.27222600	-2.42473000	N	-3.18092700	-2.09326400	1.34855200	H	-1.41837000	-3.44693800	3.05305000
C	-2.42561400	-3.91343700	-2.44375800	H	-3.39132200	-2.79025300	2.04977900	C	-5.10470700	2.53518000	0.71802300
H	-2.07997000	-4.28573800	-3.41063000	N	0.35562700	-1.17202100	1.25399500	H	-6.18739400	2.58689300	0.85447800
Ru	-0.05875000	0.44513200	-1.19145500	C	-0.00169300	4.81532100	-0.53180900	C	-0.69088600	-1.88826600	1.73997800
C	3.89548900	0.84357900	-1.53047400	H	-0.17363600	5.00371200	0.53136900	C	-0.40293100	3.40912700	2.60552200
C	3.01848900	0.05589500	-2.28960500	C	-0.07737800	3.50853700	-1.03633400	H	-1.39901800	3.81214900	2.40138800
C	3.42591500	-1.22040500	-2.70038800	C	-1.94177800	-1.59587200	1.06897700	C	1.59088600	-1.50261900	1.65672300
C	4.67701300	-1.71128000	-2.33907200	C	0.22497400	2.57246200	1.67025100	C	-3.26664700	-0.78974100	-0.44568100
C	5.54039500	-0.92383700	-1.57424400	C	0.29739300	5.88220900	-1.37502100	C	-5.96737500	-1.15838600	-0.92687700
C	5.14832500	0.35537500	-1.17518200	H	0.35565500	6.89425900	-0.96772500	H	-7.03013000	-1.28911000	-1.14163600
H	3.56703100	1.84213000	-1.22922900	C	-3.83439700	-0.14811400	-1.54877400	C	2.13590500	2.39725600	3.15438300
H	2.74245800	-1.83054800	-3.29950900	H	-3.21361400	0.47256400	-2.19878800	H	3.12923400	1.99229000	3.36182100
H	4.98537200	-2.71000200	-2.65762300	C	-2.93709400	1.77058100	1.46077700	C	-4.50581000	3.15700800	-0.37537300
H	6.52352500	-1.30778600	-1.29123700	H	-2.32279300	1.22089400	2.18248300	H	-5.11734100	3.70318500	-1.09761200
H	5.82625900	0.97229600	-0.57974800	C	1.57571500	0.54666500	-1.22738600	C	-5.41392200	-1.80932600	0.17184000
C	1.70635900	0.59716300	-2.70315300	C	-2.32559400	2.38408600	0.35610200	H	-6.01581500	-2.45170300	0.81725800
H	0.40818600	-1.08107600	-1.50869900	C	-4.31513600	1.84410700	1.63913700	C	-4.05300800	-1.61054700	0.39418000
O	1.30252200	1.73418200	-2.32625600	H	-4.77828600	1.35508900	2.50005300	C	1.50360400	3.22570500	4.08079300
H	1.26387400	0.12112300	-3.60573800	C	-3.12492900	3.08051300	-0.55857100	H	1.99868200	3.47625300	5.02206900
H	-2.30394100	5.27731100	-0.64485700	H	-2.66577800	3.56435300	-1.42563400	C	0.23394900	3.73172300	3.80308800
				C	-5.19139600	-0.34330700	-1.77280400	H	-0.26744300	4.38205100	4.52403400

C	0.52801600	5.65843600	-2.73273800	C	7.59601600	-0.72788500	0.40231900	C	4.84991500	-2.00496900	-0.26471800
H	0.76815100	6.49541800	-3.39266200	C	6.47120800	-1.51751600	0.16721900	H	4.82230300	-2.11067100	0.82370200
C	0.73171000	-3.18160000	3.16106200	C	5.64028100	-1.26314700	-0.92967600	C	3.76197000	-1.43324800	-0.94149900
H	0.88499700	-3.96144800	3.90942500	C	5.95467900	-0.19715700	-1.78036700	C	-0.56918000	1.52004200	1.07599800
C	0.15842000	3.29287400	-2.39925800	H	7.30929700	1.42036100	-2.22051900	C	2.11337500	-2.10253200	1.29768700
H	0.10560800	2.27599400	-2.79599800	H	8.78859000	0.94460100	-0.27151100	C	5.96861400	-2.44461400	-0.96669800
C	0.45852400	4.36328900	-3.24152500	H	8.23542600	-0.93752700	1.26381200	H	6.80808800	-2.88869500	-0.42647800
H	0.64475400	4.17961500	-4.30211200	H	6.22082700	-2.34258100	0.83795200	C	1.50030800	3.51927100	-0.98181300
Ru	-0.06614700	-0.00499100	-0.64508300	H	5.29511300	0.02837700	-2.62296500	H	1.93183300	2.93905100	-1.80074800
H	3.03874200	-3.08966300	-0.24695600	C	4.44890900	-2.13139000	-1.20806100	C	2.41049400	1.06583900	2.09904000
C	-1.76579000	-3.22043100	-2.09513800	O	3.94920300	-2.70312000	-0.02263000	H	1.61812800	0.46977400	2.56352200
C	-3.01685300	-3.82762600	-2.02242200	H	3.67208600	-1.53656500	-1.72619500	C	0.55180900	-1.74698200	-2.14775100
C	-3.24724700	-4.84591500	-1.09297200	H	4.73819900	-2.93214400	-1.91899300	C	3.00750400	0.62428100	0.90739800
C	-2.21653600	-5.25040200	-0.24382200	H	3.30668200	-1.49531200	0.83184000	C	2.80108000	2.26512200	2.68816000
C	-0.96398000	-4.63875800	-0.32064800	H	0.37644900	-1.76735600	-1.25514400	H	2.31768100	2.59873800	3.61038800
C	-0.72772900	-3.61768200	-1.24495200	H	-0.65413700	0.42707900	-2.07778200	C	4.01303900	1.40969100	0.33015500
H	-1.59292200	-2.40004900	-2.80198800	H	2.83415300	-2.71956500	2.93099500	H	4.48518400	1.08722900	-0.60272200
H	-3.82389200	-3.49582700	-2.68179900					C	1.74720900	4.87544200	-0.81106700
H	-4.22966300	-5.32291000	-1.03653500	IM9				H	2.39654800	5.39699400	-1.51730200
H	-2.38713500	-6.05702200	0.47592000	P	2.30594000	-0.80881200	-0.00211400	C	-2.27342100	-2.17672800	2.01471900
H	-0.13348400	-4.93167900	0.32731800	O	0.65507800	-2.73219800	-2.76191600	C	1.27876600	-3.18743700	0.99683300
C	0.64916400	-2.97840800	-1.30327100	O	-1.64404300	-2.83463000	-0.14953900	H	0.77004200	-3.23167700	0.03102700
O	1.49516700	-3.36821200	-0.40754400	N	0.21596200	1.59988300	0.01458100	C	-1.83763100	0.08427100	2.68335500
H	1.00263900	-2.94822800	-2.36983800	N	-0.65689900	2.71917500	1.72342000	H	-1.90880300	0.89776600	3.40760500
C	7.08160100	0.58828800	-1.54971300	H	-1.32377500	2.94111000	2.45091700	C	3.79960700	3.04329300	2.10010500
C	7.90776200	0.32509300	-0.45690200	N	-1.06312400	-0.71703800	0.54001100	H	4.09944700	3.98914500	2.55734700

C	-1.19399100	0.26937400	1.46281200	Ru	0.43122300	-0.21043100	-1.16846600	H	-4.06271200	-3.92116000	-1.14468300
C	2.75325000	-2.07181800	2.54572400	H	1.40979600	0.47203900	-2.23469500	H	-5.23133600	-4.51099400	0.96178400
H	3.42510500	-1.24732000	2.79948400	C	-3.18881400	1.73437900	-0.61293000	H	-6.53530900	-2.78137100	2.19631800
C	-1.65375300	-1.89941500	0.77920800	C	-2.36808000	2.49250400	-1.45520600	H	-6.68079700	-0.46479300	1.28586500
C	0.66016200	2.89734900	-0.05381900	C	-2.36520800	3.88479400	-1.29917500	C	-3.97467700	-1.51725400	-2.40345900
C	1.17753300	5.59854200	0.25507500	C	-3.15544500	4.50045700	-0.32917300	H	-4.21356800	-0.47874900	-2.69544900
H	1.39479100	6.66461900	0.35029700	C	-3.96692600	3.73173500	0.50853900	H	-4.34781900	-2.16299300	-3.22065500
C	1.07451500	-4.20786400	1.92294500	C	-3.98059700	2.34334600	0.36089200	O	-2.57831200	-1.67958900	-2.29423100
H	0.41213000	-5.03883900	1.66764100	H	-3.16770100	0.64565100	-0.71720400	H	-2.12559300	-0.77430700	-2.38650500
C	4.40829100	2.60802400	0.92523100	H	-1.71291000	4.49311100	-1.93578900				
H	5.19105900	3.21065100	0.45832000	H	-3.12945800	5.58826100	-0.21846600	TS1a			
C	0.34468700	4.99185800	1.19017700	H	-4.58942100	4.21400000	1.26706000	P	1.43768600	0.68270800	-0.41348000
H	-0.09989800	5.55779300	2.01096800	H	-4.60764900	1.72531700	1.01201700	O	1.15374700	-1.51070500	-3.39167600
C	0.10007200	3.63079500	1.01714100	C	-1.50742300	1.81056800	-2.50228000	O	0.15442900	-4.00586500	-0.81965500
C	1.70060200	-4.15900400	3.16787600	H	-0.57191900	2.40551000	-2.61076900	N	-1.24203600	-0.14526300	1.01115500
H	1.53509500	-4.95392400	3.89905000	O	-1.26265600	0.48326000	-2.27153200	N	-1.24302800	-0.10244700	3.23548200
C	2.54392600	-3.09140500	3.47407900	H	-1.86176300	-2.42256200	-1.04741800	H	-0.99455000	-0.34122600	4.18596700
H	3.04686700	-3.05079600	4.44346800	H	-2.02265600	1.94738900	-3.48269100	N	0.11005700	-2.35427500	0.72577300
C	6.01441600	-2.32303700	-2.35641900	H	-2.70355200	-3.16703100	2.16511000	C	2.16655600	3.42530600	-0.74690200
H	6.89018200	-2.67327000	-2.90801100	C	-5.44769700	-0.90275800	-0.43122500	H	2.64983100	3.36200600	0.23202500
C	-2.36400400	-1.17812900	2.96673400	C	-4.70391300	-1.86042400	-1.12919500	C	1.49942600	2.30893300	-1.27604500
H	-2.86059000	-1.36856400	3.92030200	C	-4.63989700	-3.16119300	-0.61105700	C	-0.81251600	-0.74845300	2.11215100
C	3.81672100	-1.31531700	-2.33484200	C	-5.29035800	-3.49005400	0.57514700	C	3.11712900	-0.01574600	-0.75103000
H	2.97414700	-0.86975100	-2.86889300	C	-6.02149000	-2.52221900	1.26717900	C	2.22415000	4.62216900	-1.45836800
C	4.93789800	-1.75902900	-3.03700600	C	-6.10164000	-1.22760700	0.75848100	H	2.74272000	5.48277400	-1.02895600
H	4.96466300	-1.66526200	-4.12504000	H	-5.52060400	0.11317000	-0.83096300	C	-2.58841900	1.94596500	0.66278600

H	-2.56900300	1.89820300	-0.42889200	H	4.65727700	-3.06174300	-0.86986400	H	-3.66620900	-1.68485200	0.09073500
C	2.34347700	0.33104200	2.23676700	C	0.96183600	2.52005500	3.26520200	H	-3.71903600	-0.46408700	-4.02302100
H	2.89114900	-0.53078700	1.84320300	H	0.41646700	3.38172900	3.65868500	H	-5.44357200	1.24812900	-3.50553200
C	0.60987100	-1.24391600	-2.39554200	C	-2.61970700	2.01456100	3.53150300	H	-6.29620500	1.49919600	-1.17668600
C	1.60516000	1.14606400	1.36510600	H	-2.62739000	2.05078700	4.62267300	H	-5.40204300	0.02905200	0.62716600
C	2.38852900	0.60585600	3.60290200	C	-1.97969500	0.99250700	2.83189400	C	-2.56060600	-2.25638700	-2.29633500
H	2.97558900	-0.03780800	4.26313500	C	5.65013600	-1.16307900	-1.15375800	H	-2.07452500	-2.01851200	-3.26768500
C	0.90231800	2.23612000	1.90164000	H	6.63457700	-1.60823300	-1.31608000	O	-1.65523200	-2.39063500	-1.25423100
H	0.30511600	2.87699700	1.24602100	C	5.48954700	0.22077600	-1.20827400	H	-0.66228500	-3.34800300	-1.18957700
C	-3.22331000	2.96643600	1.35847400	H	6.34774000	0.86458500	-1.41505300	H	-3.07996300	-3.22615700	-2.45744900
H	-3.72700500	3.76122400	0.80427500	C	1.62513500	4.71960300	-2.71403000	H	1.11554600	-5.53502400	1.13598700
C	0.81517100	-4.52460300	1.41538000	H	1.67004300	5.65818600	-3.27151100				
C	3.28866900	-1.40669900	-0.70847900	C	0.77897200	-4.10709000	2.73456200	TS1 _b			
H	2.42203700	-2.04931700	-0.53197100	H	1.09264600	-4.79017200	3.52738100	P	2.27800900	-0.93139300	0.00852700
C	0.26408900	-2.84441300	3.06627200	C	0.90084100	2.41994700	-2.53797800	O	0.41218000	-2.89825500	-2.55946600
H	0.11776100	-2.54959500	4.10685900	H	0.37193100	1.56032400	-2.95695000	O	-1.93965100	-2.55273300	-0.04643300
C	1.70311200	1.70533900	4.12124500	C	0.96870900	3.61464300	-3.25306900	N	0.38700300	1.62842400	-0.06729500
H	1.75461600	1.93262800	5.18915500	H	0.49841300	3.68188400	-4.23671500	N	-0.28720200	2.87134100	1.64621400
C	-0.08487300	-2.00403900	2.01375400	Ru	-0.26447700	-0.78000100	-0.86969500	H	-0.87952300	3.16312800	2.41250100
C	4.23380500	0.79099500	-1.00690900	H	-0.95984900	0.34362400	-1.77032600	N	-1.05847600	-0.53903700	0.60389000
H	4.12752400	1.87685700	-1.06295300	C	-4.07957900	-1.04643300	-0.69492200	C	4.69366700	-2.37345200	-0.23435200
C	0.36552900	-3.63746000	0.40405200	C	-3.59947200	-1.20384600	-2.00125300	H	4.69163800	-2.40492500	0.85871900
C	-1.96238000	0.94905400	1.41805900	C	-4.10104100	-0.36549500	-3.00191800	C	3.64142700	-1.74957400	-0.92121100
C	-3.23922000	2.99918100	2.76703400	C	-5.06680900	0.59864500	-2.71093600	C	-0.32803200	1.64602400	1.04692800
H	-3.75205000	3.81955100	3.27380600	C	-5.54334300	0.74116600	-1.40804400	C	1.99951400	-2.09719100	1.40741800
C	4.54586500	-1.97559700	-0.90321800	C	-5.04441500	-0.08631700	-0.40034500	C	5.74491800	-2.96147200	-0.93210800

H	6.55645400	-3.44505100	-0.38325000	H	1.92992300	6.60736800	-0.02442700	C	-3.75695900	3.63785600	0.77241600
C	1.72943000	3.41395300	-1.22556000	C	0.73171700	-3.98565000	2.25867200	C	-3.87030100	2.26733600	0.53127500
H	2.06321500	2.77539100	-2.04673200	H	-0.05813500	-4.72684500	2.11297600	H	-3.22714000	0.60180900	-0.68559100
C	2.64932400	1.04692700	1.98494200	C	4.65525800	2.37538100	0.58338600	H	-1.56513100	4.42867200	-1.71805500
H	1.85729400	0.53343600	2.53947400	H	5.44033500	2.89383900	0.02778600	H	-2.83178300	5.48606500	0.13369200
C	0.40541600	-1.87008500	-2.01364900	C	0.82891500	5.04515800	0.95294400	H	-4.31469800	4.10277900	1.58981000
C	3.12925200	0.49770200	0.78589300	H	0.48297400	5.67122300	1.77767000	H	-4.50993700	1.64384500	1.16378600
C	3.15988100	2.24833700	2.46953400	C	0.48182000	3.69900400	0.85525300	C	-1.57476400	1.79773400	-2.48277900
H	2.76787600	2.66757900	3.40015600	C	1.45599400	-3.94815000	3.44924200	H	-0.65898900	2.39191500	-2.67945900
C	4.13961300	1.17596800	0.09268600	H	1.24073000	-4.66304500	4.24704600	O	-1.25218300	0.46638200	-2.30497700
H	4.51931500	0.76737400	-0.84878100	C	2.45980400	-2.99440200	3.61715100	H	-2.21166400	-2.09585100	-1.02301600
C	2.07922800	4.75499100	-1.12921000	H	3.03689100	-2.96321300	4.54463500	H	-2.18646700	1.91711400	-3.40420600
H	2.71214600	5.20210400	-1.89860000	C	5.75821400	-2.93787500	-2.32744200	H	-2.99806600	-2.70718300	2.30254100
C	-2.43076100	-1.79260700	2.12580100	H	6.58038900	-3.40449300	-2.87529400	C	-5.69446400	-0.66424800	-0.65174100
C	0.99977200	-3.06615300	1.24660800	C	-2.34598900	-0.78661900	3.06690400	C	-4.89920500	-1.67404500	-1.20449500
H	0.41311700	-3.09830400	0.32460600	H	-2.83542800	-0.89632300	4.03714700	C	-4.91059200	-2.93728300	-0.59697100
C	-1.65441900	0.38905400	2.75421800	C	3.66384100	-1.72989700	-2.32044200	C	-5.68563200	-3.17902300	0.53401600
H	-1.59683100	1.21555600	3.46488700	H	2.84945600	-1.24424400	-2.86299200	C	-6.46765700	-2.15949600	1.08062000
C	4.16272400	2.91891300	1.76787700	C	4.71717800	-2.32194000	-3.01800800	C	-6.47320800	-0.90119300	0.48207300
H	4.55679900	3.86591100	2.14407900	H	4.71811500	-2.30349800	-4.11023100	H	-5.70339800	0.32572500	-1.11855700
C	-1.04025200	0.46933700	1.50926300	Ru	0.43614300	-0.26288100	-1.14332000	H	-4.29242900	-3.73624700	-1.01494700
C	2.73311400	-2.07705700	2.60350200	H	1.44302000	0.26995900	-2.27076800	H	-5.68347800	-4.17170300	0.99188400
H	3.52617600	-1.33843700	2.75009200	C	-3.16270400	1.67969300	-0.51654100	H	-7.07820400	-2.35001000	1.96679600
C	-1.80314800	-1.63785400	0.86302400	C	-2.33066000	2.44368300	-1.34238400	H	-7.08906200	-0.09828100	0.89608400
C	0.91487300	2.88754900	-0.21893300	C	-2.22646200	3.81830800	-1.09301000	C	-4.02309300	-1.41800700	-2.40597500
C	1.63499600	5.55643600	-0.05985300	C	-2.93283400	4.41202200	-0.04714100	H	-4.28255400	-0.43256500	-2.83885800

H	-4.25463300	-2.16616100	-3.18957300	H	1.50278800	-2.54780100	4.11029800	C	5.77947700	-2.25263500	-0.70099500
O	-2.65295600	-1.45656500	-2.10504200	C	0.78151000	0.87833900	2.44907300	H	6.68686300	-2.83986800	-0.85968700
H	-2.06968400	-0.45105400	-2.26617000	H	0.56658800	1.84640900	1.98655200	C	5.85384400	-0.86693700	-0.58182800
				C	-2.08843000	4.40977700	-0.68939800	H	6.81987400	-0.36140700	-0.64963900
TS2				H	-1.91435400	5.25683000	-1.35628200	C	3.30473300	4.61955600	0.04733200
P	1.88148600	0.19459800	-0.05230200	C	-1.16183800	-3.85316000	1.42467100	H	3.63665700	5.66018900	0.07171700
O	1.71905200	-2.17559300	-3.09825500	C	3.38044900	-2.13440500	-0.44709100	C	-1.91517600	-3.21263500	2.40320500
O	0.08733800	-3.62148100	-0.61693500	H	2.40695300	-2.63302100	-0.43615100	H	-2.31866400	-3.78132000	3.24305900
N	-1.19932200	0.86950100	-0.03085000	C	-2.14555000	-1.84595300	2.29919800	C	2.15385300	2.81288500	-1.07177000
N	-2.68361100	1.06845900	1.62030000	H	-2.71940200	-1.31397000	3.05943700	H	1.58513400	2.43606200	-1.92580600
H	-3.42602000	0.75777000	2.23331100	C	0.60367400	-0.59812200	4.35451500	C	2.58455800	4.13962100	-1.04387000
N	-0.86593000	-1.77901600	0.25239800	H	0.26722800	-0.79091500	5.37609500	H	2.34950000	4.80088500	-1.88106900
C	3.17059800	2.44247600	1.08519600	C	-1.61647900	-1.16601300	1.19957000	Ru	0.12948900	-0.34279900	-1.36466400
H	3.41044200	1.78161600	1.92357500	C	4.69697800	-0.11362300	-0.38314200	H	0.64106900	0.78357400	-2.33658300
C	2.43689500	1.95098300	-0.00766500	H	4.77662900	0.97229100	-0.30185800	C	-4.15698300	0.26013200	-1.26172900
C	-1.83646700	0.23718900	0.94087200	C	-0.65279300	-3.08459500	0.36780800	C	-3.34827200	-0.75817900	-1.77349700
C	3.44572300	-0.73940400	-0.30404600	C	-1.68306200	2.15595000	-0.04385400	C	-3.60982200	-2.08020400	-1.39317600
C	3.60035100	3.76624900	1.11189500	C	-3.02280300	4.54793700	0.35625200	C	-4.63580000	-2.37815800	-0.49889100
H	4.16813300	4.13464500	1.96962300	H	-3.54078700	5.50063100	0.48607000	C	-5.43180600	-1.35108000	0.01909900
C	-1.41496100	3.21747100	-0.91332600	C	4.53806100	-2.88438700	-0.63404600	C	-5.19417000	-0.03295000	-0.37533600
H	-0.74487500	3.06630900	-1.75911500	H	4.46755500	-3.96863800	-0.74699700	H	-3.92274100	1.28317700	-1.57512100
C	1.72910900	-1.33479100	2.34434300	C	0.35021000	0.63332000	3.75126100	H	-2.97584400	-2.88317000	-1.79045200
H	2.27443200	-2.11600800	1.80858800	H	-0.18957600	1.41328200	4.29458100	H	-4.81725000	-3.41429400	-0.19701800
C	1.11765400	-1.46141600	-2.40163900	C	-3.31769200	3.49406200	1.21523900	H	-6.24121200	-1.58297700	0.71703900
C	1.48022100	-0.10175700	1.72686700	H	-4.05889000	3.59497200	2.01047000	H	-5.82152200	0.77565200	0.01538900
C	1.29510600	-1.58036900	3.64624700	C	-2.62947200	2.30085800	0.99651300	C	-2.20662100	-0.37478000	-2.71378400

O	-1.84515900	0.88916600	-2.70457900	C	0.10278000	-1.88493900	0.81002100	C	4.88359500	-1.30716200	0.33235700
H	-0.97480100	-4.92853500	1.46476000	C	2.03315600	-2.49071400	2.15379100	H	5.66536100	-1.09823700	1.06526000
H	0.15703700	-4.57480400	-0.48673200	H	2.79546900	-2.21250400	2.88647000	C	3.79942800	-0.45080600	0.14738500
H	-1.36371000	-1.16248800	-2.44791900	C	0.09555100	-3.18133900	0.27713500	C	-2.31361800	1.94332700	3.80720300
H	-2.46370700	-0.81773500	-3.72563400	H	-0.65945100	-3.46026500	-0.46353400	H	-2.61590900	2.55906100	4.65766600
				C	3.90686900	-2.72829200	-1.40055200	C	-1.90047600	0.62656000	4.00869800
TS3 _a				H	3.97439400	-3.64156100	-1.99547900	H	-1.88355600	0.20498300	5.01670200
P	-1.02333200	-0.60413300	0.13320100	C	0.40985300	4.85453600	-0.13939700	C	-4.77286200	-3.16741400	-0.85669600
O	-3.03621600	1.20139500	-2.38507900	H	-0.03855200	5.81518100	-0.39530800	H	-5.64677500	-3.77829300	-1.09506900
O	-0.60465600	3.72702500	-1.99893800	C	-1.94838300	1.68521200	1.43308600	C	1.35255700	4.73262100	0.86501600
N	1.85835000	0.30282700	-0.77172500	H	-1.96952600	2.10349700	0.42290500	H	1.63807800	5.61147500	1.44814600
N	3.42566900	0.73079200	0.75503700	C	2.01270700	3.51055300	1.08067000	C	-2.76433900	-2.02073400	-1.55809900
H	3.94374000	1.23369600	1.46251200	H	2.85980000	3.44018400	1.76505500	H	-2.06554100	-1.72770900	-2.34636200
N	0.52261600	2.49813800	-0.49881900	C	2.01902700	-3.77656200	1.61477400	C	-3.87352700	-2.80954200	-1.85916600
C	-3.44690500	-1.94976000	0.75558200	H	2.76883400	-4.50901600	1.92280800	H	-4.03910200	-3.13689800	-2.88813300
H	-3.29755600	-1.61237600	1.78420000	C	1.57776800	2.41743800	0.33921400	Ru	-0.20044300	0.71961200	-1.58998600
C	-2.53603100	-1.58604000	-0.24583000	C	-1.50869900	-0.15862100	2.92545500	H	-0.26351500	-0.56864600	-2.56243000
C	2.26237600	1.14879200	0.17145500	H	-1.19074300	-1.19070200	3.09826800	H	-0.21175000	2.61491100	-2.55854000
C	-1.51960000	0.36350200	1.62276000	C	0.06644900	3.70893600	-0.91343300	H	0.25794900	1.78846100	-2.96110200
C	-4.55763500	-2.73377800	0.45106400	C	2.78405400	-0.71324200	-0.80357800				
H	-5.26201900	-3.00312000	1.24160800	C	4.91773900	-2.44971500	-0.46121200	TS3 _b			
C	2.82976700	-1.87119400	-1.58564700	H	5.74995000	-3.14829300	-0.35108000	P	1.53295700	-1.05210200	-0.31562300
H	2.03320900	-2.07412100	-2.30444900	C	-2.34221200	2.46850900	2.51607000	O	-1.80493200	-2.54606300	-1.22538000
C	1.08425100	-1.55225700	1.75488700	H	-2.67040900	3.49677800	2.34709100	O	-2.46562100	-1.17888200	1.93654600
H	1.10993700	-0.54454300	2.18175900	C	1.04431500	-4.11944000	0.67904400	N	0.47923100	1.95914800	-0.07877600
C	-1.92388900	1.02704500	-2.08707600	H	1.02328200	-5.12541300	0.25318000	N	1.29832800	3.34894500	1.45027100

H	1.46527500	3.76587500	2.35572800	H	0.83740100	2.21684700	3.97815800	H	0.48393200	-1.70635400	-2.98430600
N	-0.83700600	0.39538700	1.64308500	C	4.92918400	2.09651800	-0.47221700	C	1.70916300	-3.30908800	-3.76658100
C	3.08594100	-3.17004500	-1.35013600	H	5.68378600	2.88462200	-0.52748600	H	1.16267400	-3.36225400	-4.71097600
H	3.62949000	-3.12758500	-0.40217000	C	-0.04505800	1.34315800	2.20010400	Ru	-0.49368800	0.06783900	-0.61025900
C	2.00740100	-2.30322300	-1.58059700	C	2.91522800	-2.14591400	1.95366900	H	-0.14325300	0.19463200	-2.17272400
C	0.57124500	2.21510300	1.21747300	H	3.83138100	-1.68521300	1.57377500	H	-3.06569600	-0.53788200	0.96916500
C	1.70680600	-1.99379800	1.25624700	C	-1.58349700	-0.41532700	2.44964500	H	-1.89891700	1.01010200	-1.05368500
C	3.47118000	-4.09312400	-2.31806800	C	1.18326000	2.94507000	-0.72867700	C	-7.99637000	-0.13183400	-1.77630400
H	4.31202100	-4.76317300	-2.12407500	C	2.70313000	5.13021600	-1.49578500	C	-8.40268800	0.94785500	-0.99031700
C	1.42681300	3.13722100	-2.09172500	H	3.29793900	5.98466500	-1.82565400	C	-7.50087800	1.52467500	-0.09862900
H	1.02480500	2.43109100	-2.82120000	C	0.60547400	-3.35160600	2.94251900	C	-6.20137000	1.02834300	0.01133700
C	3.34640600	0.79862900	0.81556900	H	-0.30832500	-3.81478700	3.32284600	C	-5.78794700	-0.05146800	-0.77191900
H	2.86545300	0.58067900	1.77450000	C	4.56584000	1.39106100	-1.61771600	C	-6.69948200	-0.62525100	-1.66764000
C	-1.29968300	-1.52018600	-0.98661500	H	5.03522200	1.62403900	-2.57643500	H	-8.69514800	-0.59093600	-2.47995700
C	2.97210500	0.08402100	-0.33281200	C	2.47034400	4.95310700	-0.13521200	H	-9.41986700	1.33748400	-1.07511300
C	4.31897100	1.79355800	0.74504600	H	2.87141000	5.64650300	0.60656900	H	-7.81039000	2.37075600	0.52022600
H	4.59650000	2.34375100	1.64849400	C	1.70676800	3.84528100	0.22936000	H	-5.48968200	1.47500400	0.70802100
C	3.59412300	0.39401800	-1.54969900	C	1.80749100	-3.48505900	3.63503700	H	-6.38477300	-1.47064100	-2.28763100
H	3.30554600	-0.14332200	-2.45815300	H	1.84668000	-4.05924500	4.56380600	C	-4.39907500	-0.61721000	-0.67074600
C	2.19108900	4.23792500	-2.45689700	C	2.96241900	-2.88246100	3.13621000	H	-3.93468300	-0.65285400	-1.67514400
H	2.40150900	4.41945900	-3.51293900	H	3.91027200	-2.98795000	3.66969700	H	-4.43840700	-1.66817700	-0.33264900
C	-1.35073200	-0.38175000	3.85908700	C	2.78194300	-4.16520400	-3.52958500	O	-3.56482200	0.11933500	0.19966600
H	-1.90673200	-1.08884800	4.47640500	H	3.08122400	-4.89336300	-4.28722200	H	-2.60220500	0.58085200	-0.41703200
C	0.55394900	-2.60845800	1.76495600	C	-0.48039600	0.53548200	4.40489300				
H	-0.40150800	-2.49796100	1.24491700	H	-0.31566800	0.56374900	5.48464400	TS4 _a			
C	0.17172500	1.45445400	3.56910200	C	1.32247600	-2.38176500	-2.79827200	P	1.85721400	0.21733100	0.03637600

O	1.87953200	-2.22954600	-2.87013900	C	2.57877400	-2.30331000	0.94576300	C	-1.61119700	-3.47723000	2.22050600
O	0.34242400	-3.65983800	-0.79998100	H	2.19294300	-2.64931600	-0.01705800	H	-1.97536800	-4.11762800	3.02836800
N	-1.29588300	0.73548400	-0.05417100	C	-1.95393200	-2.11334500	2.19452700	C	3.40037400	0.83593500	-2.26176000
N	-2.65356000	0.79965800	1.70244600	H	-2.61432000	-1.67757300	2.94580200	H	2.51020100	0.58511300	-2.84228100
H	-3.25759500	0.44413600	2.43140300	C	0.43674000	4.01261500	2.27463200	C	4.55690800	1.25586600	-2.91990300
N	-0.63136600	-1.83074600	0.18264000	H	0.04354200	4.90420000	2.76848500	H	4.56148800	1.32556600	-4.00982600
C	4.53350900	1.05462300	-0.14256400	C	-1.45371400	-1.34840100	1.15154900	Ru	0.07241300	-0.43734400	-1.27001300
H	4.53643500	0.97263700	0.94801800	C	3.00921000	-0.53720400	2.53942900	C	-3.45010200	-1.90738800	-1.36635400
C	3.37583500	0.73129600	-0.86707900	H	2.98217700	0.51771600	2.82564100	C	-3.58128100	-0.55463300	-1.70016100
C	-1.80636500	0.03872000	0.95477300	C	-0.33039000	-3.19598500	0.12410500	C	-4.56209700	0.20926400	-1.05563900
C	2.51870900	-0.94699000	1.28987100	C	-1.83694800	1.99779900	0.02064400	C	-5.39241000	-0.36303500	-0.09213400
C	5.68483600	1.47739800	-0.79978700	C	-3.26293300	4.30169500	0.61410900	C	-5.24890400	-1.71106700	0.24133400
H	6.57815300	1.72535300	-0.22205400	H	-3.81799900	5.21893600	0.82130600	C	-4.27732400	-2.48043200	-0.40169500
C	-1.65375300	3.12142700	-0.78995100	C	3.10637300	-3.23383600	1.83890500	H	-2.67046500	-2.49560200	-1.85880000
H	-0.96361900	3.08618300	-1.63574900	H	3.13192000	-4.28888600	1.55657200	H	-4.66249200	1.27287800	-1.30213200
C	0.67302900	1.60918000	2.17297300	C	1.18998800	4.13201100	1.10907200	H	-6.15203000	0.24838800	0.40441400
H	0.45949400	0.62058000	2.59227600	H	1.39348800	5.11890900	0.68693600	H	-5.89631400	-2.16331700	0.99741300
C	1.15892800	-1.60437300	-2.21680100	C	-3.45069500	3.19431400	1.43685900	H	-4.15475000	-3.53522600	-0.14132700
C	1.42374700	1.71929900	0.99193700	H	-4.13957900	3.22332500	2.28320200	C	-2.67946300	0.06542900	-2.73646300
C	0.18193600	2.74733200	2.80634600	C	-2.72168300	2.04923200	1.12337200	H	-2.58346000	1.15138100	-2.50651800
H	-0.41017400	2.64557600	3.71957100	C	3.58367300	-2.82179200	3.08184000	O	-1.45608300	-0.56786900	-2.89072700
C	1.67675500	2.99302800	0.46760400	H	3.99209100	-3.55273600	3.78375200	H	-0.36199700	0.36592300	-2.79936400
H	2.25447600	3.09709500	-0.45583500	C	3.53778400	-1.47143900	3.42832000	H	-3.20661100	0.03696200	-3.71489200
C	-2.37747700	4.26667300	-0.47847700	H	3.91520500	-1.14031000	4.39876800	H	0.38024200	0.84051700	-2.43298500
H	-2.26015300	5.15990600	-1.09544500	C	5.69928600	1.57810600	-2.19191200	H	-0.56425000	-5.05748200	1.19637300
C	-0.83431800	-4.00028400	1.21877700	H	6.60516600	1.90421800	-2.70808900				

TS4 _b				H	2.07903000	-2.46446200	4.41445600	C	-4.28123900	-4.71273900	-1.17052900
P	-2.26917600	-0.67414300	-0.06916600	C	-0.93659100	3.86143000	-2.08231000	H	-4.76410600	-5.65959400	-1.42296500
O	-0.91113100	-1.12777100	-3.58529600	C	-3.51469600	1.07896700	-1.82866600	C	-0.78231600	4.56867900	-0.91890100
O	-0.77944600	1.79609400	-3.21631200	H	-2.69164100	0.83139000	-2.50422200	H	-0.96261600	5.64691100	-0.89902900
N	0.48495700	0.43176600	1.14894600	C	-0.36835800	3.90292300	0.24985800	C	-2.36379100	-3.24386800	-1.28114300
N	0.66157600	2.16555100	2.52444400	H	-0.18075900	4.44537300	1.17765900	H	-1.34489400	-3.06036200	-1.62573300
H	0.72840800	3.13372300	2.80866800	C	-2.01618700	-0.72557600	4.55274300	C	-2.98300000	-4.45324300	-1.60093800
N	-0.37750900	1.80274700	-0.95903400	H	-1.88897100	-0.73094600	5.63773600	H	-2.44141100	-5.19307100	-2.19412400
C	-4.35321900	-2.54815800	-0.10401400	C	-0.17103500	2.53372800	0.16877900	Ru	-0.11449000	-0.30555900	-0.80271800
H	-4.90160500	-1.80379700	0.48058900	C	-4.62980100	0.88523400	0.30730000	C	2.60580500	2.65409100	-1.56164500
C	-3.04267600	-2.27876500	-0.52905000	H	-4.69565500	0.46725800	1.31550200	C	3.01098800	1.84682500	-0.49138300
C	0.31690600	1.74213600	1.27580500	C	-0.69356900	2.43458000	-2.16416800	C	3.45287100	2.46046500	0.68618100
C	-3.56657100	0.53476800	-0.53920300	C	0.96987200	-0.02758500	2.35204600	C	3.49099000	3.85103400	0.79684000
C	-4.96623100	-3.75654600	-0.41861100	C	1.94087400	-0.37107900	4.92660700	C	3.08588900	4.64645500	-0.27480700
H	-5.98592000	-3.95172600	-0.07890600	H	2.33137600	-0.53210700	5.93350500	C	2.64404800	4.04196000	-1.45343100
C	1.31322400	-1.31656600	2.76710800	C	-4.49906100	1.96698400	-2.25835000	H	2.23971700	2.17348600	-2.47294700
H	1.19032400	-2.16569800	2.09092700	H	-4.43268000	2.39055900	-3.26316300	H	3.76466000	1.83454000	1.53039000
C	-2.33153900	0.49230300	2.48854900	C	-2.00992300	-1.92282000	3.84071800	H	3.84317800	4.31543900	1.72270200
H	-2.44885400	1.44563900	1.96294900	H	-1.88055800	-2.87200500	4.36596100	H	3.11342200	5.73609000	-0.19270500
C	-0.61058900	-0.74050200	-2.53863200	C	1.59497100	0.91893600	4.53160100	H	2.31706600	4.65880500	-2.29448600
C	-2.31750100	-0.70858600	1.76199700	H	1.70329200	1.76946400	5.20727500	C	3.01114800	0.34979000	-0.62277000
C	-2.18021800	0.48209000	3.87243300	C	1.10642600	1.06916300	3.23554700	H	3.00441800	-0.10702900	0.39207500
H	-2.18402100	1.42579200	4.42420300	C	-5.54750400	2.31759500	-1.40994600	O	1.99219300	-0.13845900	-1.44325900
C	-2.15464600	-1.91560700	2.45356100	H	-6.31590400	3.01789800	-1.74591900	H	2.12293000	-1.33703000	-1.63750800
H	-2.13275800	-2.86043800	1.90185700	C	-5.61274600	1.77199200	-0.12785800	H	3.98558900	0.04539500	-1.06029400
C	1.79998500	-1.46986000	4.06041300	H	-6.43408700	2.03893200	0.54144400	H	0.08562000	-1.95831400	-0.30697500

H	-1.23780500	4.34694300	-3.01232400	C	2.52582800	3.35495600	0.80621200	C	0.28379700	-3.01041300	-0.08024200
C	6.07808200	-2.16973100	-2.35007200	H	3.03991200	2.85129700	1.62958700	C	3.51665400	0.28942500	2.05502100
C	4.74061800	-2.52370300	-2.18436800	C	1.65370200	2.63251100	-0.02221500	H	2.91680300	0.70593600	2.86886900
C	4.22908700	-2.79618100	-0.91023500	C	-0.86308800	-2.37114800	0.53084100	C	2.03928300	-2.70116700	-1.68091800
C	5.08515700	-2.70496400	0.19235600	C	2.99545800	0.21828400	0.75312300	C	-2.27768300	-0.79585100	1.01889800
C	6.42441900	-2.35408600	0.02899400	C	2.74754000	4.71193300	0.58970300	C	-4.37531100	-0.68953400	2.83143000
C	6.92504100	-2.08407000	-1.24446800	H	3.42959200	5.26015500	1.24362900	H	-5.21075600	-0.62406600	3.53172000
H	6.46248200	-1.95389000	-3.35008500	C	-2.99353700	0.39765500	1.14062100	C	5.07280400	-0.78451400	0.00811400
H	4.06659500	-2.57357400	-3.04334700	H	-2.73221200	1.26527800	0.53074000	H	5.66767900	-1.21487200	-0.80078900
H	4.68938200	-2.89376300	1.19618700	C	0.42711900	-0.28327600	2.70227700	C	-0.99720100	1.95793300	3.54177800
H	7.07823300	-2.27888400	0.90156900	H	0.98734900	-1.16648600	2.37623000	H	-1.55495400	2.83937800	3.86699500
H	7.97208200	-1.80020800	-1.37427700	C	1.30986500	0.32257900	-2.56959900	C	-3.66303000	-1.88226300	2.73541200
C	2.77856600	-3.16510800	-0.73976800	C	0.46823200	0.88944900	1.93147100	H	-3.91705300	-2.74909200	3.34846900
H	2.66824500	-4.26295600	-0.84937300	C	-0.32747300	-0.33530900	3.86987600	C	-2.60895000	-1.91034800	1.82419500
H	2.48845400	-2.95176500	0.31530500	H	-0.35916400	-1.25850300	4.45448000	C	5.58346600	-0.71334600	1.30267600
O	1.93635600	-2.53001800	-1.65060300	C	-0.24905200	2.00992000	2.36492300	H	6.58876200	-1.08290300	1.51895700
H	0.74625000	-2.09121300	-0.93723300	H	-0.22995900	2.93202400	1.77667700	C	4.80315500	-0.17319900	2.32509900
				C	-4.04179100	0.43188000	2.05130900	H	5.19588200	-0.11378200	3.34307900
TS5				H	-4.62445200	1.34938100	2.16014400	C	2.10632800	5.36751000	-0.46234900
P	1.32667900	0.85130700	0.31232600	C	2.44988200	-4.05490800	-1.36498600	H	2.28546800	6.43113900	-0.63575000
O	1.99951700	0.80788700	-3.36432800	C	3.78813500	-0.31932300	-0.26781800	C	1.77136100	-4.83898700	-0.46877900
O	2.59910200	-2.01080400	-2.53539500	H	3.39831300	-0.41554200	-1.28403900	H	2.09834200	-5.86388500	-0.27370800
N	-1.20646800	-1.12857300	0.21956100	C	0.64190500	-4.32316500	0.19361700	C	1.01870600	3.29909300	-1.07553900
N	-1.68772000	-2.88330200	1.49108600	H	0.05926000	-4.93583200	0.88339000	H	0.34494700	2.74540600	-1.73482200
H	-1.62890000	-3.81547200	1.87737000	C	-1.04554700	0.78563800	4.29157600	C	1.24391500	4.65824400	-1.29470200
N	0.96264000	-2.20361500	-0.93741200	H	-1.64417600	0.74139200	5.20436200	H	0.74564600	5.16168400	-2.12624300

Ru	0.11107700	-0.26816700	-1.29978400	C	5.45917800	-0.66458300	0.49204000	H	2.59602000	4.97846600	2.62363800
C	-3.95414700	-0.39763200	-1.86291000	H	5.31538500	-0.67422500	1.57717700	C	-1.52387700	0.50862800	0.79304700
C	-3.06300800	0.62643800	-2.19147300	C	4.35280400	-0.50113500	-0.35655900	C	2.45635900	-1.27827300	3.04268700
C	-3.48528500	1.95840500	-2.12087900	C	-0.98449500	1.68066900	0.13353000	H	2.34733100	-0.24980000	3.39425400
C	-4.77807600	2.26485300	-1.70471100	C	2.69455000	-1.54214800	1.68912900	C	-1.15250700	-1.75203600	1.16491400
C	-5.66348900	1.23746100	-1.36980100	C	6.73736700	-0.81446600	-0.03750200	C	0.44781900	2.86659200	-0.97398000
C	-5.25103300	-0.09206000	-1.45554600	H	7.59179400	-0.93966900	0.63182200	C	0.57825800	5.57944200	-1.49451400
H	-3.60146000	-1.42965300	-1.93092200	C	1.53083000	3.34432400	-1.71687300	H	0.65143000	6.64591500	-1.71843800
H	-2.78665100	2.76005000	-2.38507700	H	2.29617800	2.65262000	-2.07682800	C	2.79354800	-3.91582600	2.20183300
H	-5.10097800	3.30707100	-1.64556100	C	1.69542000	1.75335400	2.00448100	H	2.93223900	-4.94594000	1.86587300
H	-6.67947600	1.47637600	-1.04617300	H	0.87606100	1.05454000	2.20148900	C	3.72471400	3.56978500	1.43834700
H	-5.94439400	-0.89618800	-1.19664100	C	1.27110600	-2.04248900	-1.67252600	H	4.51964500	4.28187300	1.20454400
C	-1.67304700	0.27814900	-2.64818400	C	2.77471200	1.34770000	1.20059200	C	-0.50424500	5.11649800	-0.75255800
H	-0.95024500	1.02842900	-1.59590100	C	1.63578600	3.04390600	2.52022600	H	-1.27948300	5.79376300	-0.39026400
O	-1.33432500	-0.96888300	-2.70846900	H	0.78320700	3.34154500	3.13604100	C	-0.54932100	3.74702100	-0.49264800
H	-1.31335400	0.95643800	-3.45919500	C	3.78868700	2.27382200	0.92432000	C	2.53281500	-3.64445900	3.54607600
H	3.32083800	-4.42781300	-1.90650400	H	4.63080500	1.98970100	0.28767400	H	2.46249200	-4.46132500	4.26783300
				C	1.58116300	4.71018900	-1.96493000	C	2.37039200	-2.32549300	3.96213200
TS6				H	2.41249500	5.12227700	-2.54082200	H	2.18119400	-2.10258800	5.01502600
P	2.67606500	-0.27495900	0.35452600	C	-2.24173700	-1.81906700	2.04887600	C	6.92548100	-0.80977900	-1.42135000
O	1.59523100	-3.06433900	-2.14157500	H	-2.47770400	-2.77443600	2.51769200	H	7.92857000	-0.93284000	-1.83674400
O	-0.45087200	-2.84871700	0.92404600	C	2.86956900	-2.87583000	1.28154000	C	-2.98215200	-0.67019900	2.27660600
N	0.13351400	1.59089500	-0.57336500	H	3.06498900	-3.10323700	0.22807400	H	-3.84584000	-0.69546200	2.94439900
N	-1.42738300	2.96577200	0.23157500	C	-2.62455400	0.52164100	1.64424800	C	4.54922000	-0.50107200	-1.74094300
H	-2.41832300	3.17844000	0.38579000	H	-3.19712400	1.43718800	1.79130200	H	3.68459300	-0.38601800	-2.40054400
N	-0.79460200	-0.61516800	0.55574800	C	2.64966300	3.95990100	2.23260800	C	5.83176100	-0.65517300	-2.26986300

H	5.97319900	-0.65938200	-3.35305700	C	-2.69881300	-4.46152600	-1.97193700	H	-3.10963300	0.52782400	-2.26701600
Ru	0.80967100	-0.39306500	-1.02875400	H	-3.88317700	-3.89761700	-0.25415600	C	-2.87241800	1.90701900	1.38048400
H	1.69128100	0.14492900	-2.25464100	H	-3.49744700	-1.44203000	-0.59062900	H	-2.30716200	1.35440700	2.13880800
H	0.23768200	-2.61781500	0.26622700	H	-1.06441100	-2.28166700	-4.02263400	C	1.65981900	0.46927900	-1.14199200
H	-0.50319500	-0.28121100	-2.15965000	H	-1.45305900	-4.72083200	-3.71976600	C	-2.19829400	2.46339500	0.28225900
C	-6.58004100	-1.13360600	1.72275300	H	-2.85567100	-5.53327300	-1.82866400	C	-4.25152900	2.04240800	1.50730100
C	-6.68258300	0.11226400	2.34188600	C	-2.04142100	-0.24725900	-2.49119300	H	-4.76447700	1.59779900	2.36400900
C	-6.31547900	1.26687400	1.65015600	O	-2.66052600	0.58298800	-1.79236100	C	-2.93490000	3.16587300	-0.67907400
C	-5.84932700	1.19620100	0.33236000	H	-1.69687400	0.03796500	-3.51501600	H	-2.42581500	3.60548700	-1.54180700
C	-5.74776300	-0.06067200	-0.27597400					C	-5.12584400	-0.20514000	-1.87173800
C	-6.10811200	-1.21736800	0.41229600	TS7 _a				H	-5.56513900	0.27487200	-2.74886200
H	-6.87259500	-2.03920200	2.25993200	P	-0.41429500	2.11064500	0.05871800	C	1.66580900	-2.44100400	2.82718700
H	-7.05605100	0.18605800	3.36648800	O	2.71468900	0.79819900	-1.51025300	C	1.54171000	1.97752600	2.03348500
H	-6.40166200	2.24375600	2.13675800	O	2.57579900	-0.92100100	1.25052600	H	2.02725200	1.26985600	1.35675600
H	-5.37023800	-0.13095900	-1.30102600	N	-1.96789300	-0.73349800	0.00339900	C	-0.70792900	-2.75261500	2.82314100
H	-6.02445500	-2.18874100	-0.08187800	N	-3.26039100	-1.93656100	1.34878600	H	-1.60513600	-3.26722800	3.17203100
C	-5.41559600	2.43067200	-0.41184800	H	-3.51432600	-2.60315000	2.06503200	C	-4.97856000	2.73955900	0.54060700
H	-5.82945500	2.41201600	-1.43723800	N	0.31066300	-1.15467800	1.32008100	H	-6.06208100	2.84033600	0.63717100
H	-5.82739600	3.32708000	0.07582300	C	0.28781200	4.77746000	-0.53839900	C	-0.77584600	-1.80752300	1.80531200
O	-4.01557200	2.59492200	-0.45037300	H	0.10852100	4.98124900	0.52055800	C	-0.30364200	3.43605300	2.58894100
H	-3.61686000	1.89556800	-1.01220100	C	0.14749800	3.47435100	-1.03841700	H	-1.26460600	3.89530700	2.33990500
C	-3.27612000	-3.54481800	-1.09343900	C	-1.99679400	-1.49519700	1.08789900	C	1.53187700	-1.49134700	1.78565500
C	-3.06700200	-2.17927800	-1.27344500	C	0.31076900	2.55090600	1.68971100	C	-3.25242200	-0.68466600	-0.48406800
C	-2.27226400	-1.71789600	-2.32606200	C	0.66259600	5.82093000	-1.38077700	C	-5.95222000	-0.96813000	-1.02526000
C	-1.70353900	-2.64194300	-3.20979000	H	0.77127000	6.83004500	-0.97663600	H	-7.01329200	-1.06646500	-1.26419600
C	-1.91339800	-4.00567500	-3.03407900	C	-3.76855900	-0.05267700	-1.61743100	C	2.14490000	2.27972800	3.25270300

H	3.10154400	1.81581300	3.50469400	H	-1.60149600	-2.39952000	-2.85009500	H	2.67114900	-2.67008800	3.18267100
C	-4.31666000	3.30507700	-0.54710800	H	-3.88840000	-3.37456600	-2.79405200				
H	-4.87920400	3.85578400	-1.30477000	H	-4.46042900	-5.11962500	-1.10969500	TS7 _b			
C	-5.45079300	-1.60693300	0.10524100	H	-2.72534100	-5.89413000	0.50585900	P	-0.15261400	2.05460900	0.03311800
H	-6.09209100	-2.20814500	0.75237800	H	-0.41194500	-4.89828200	0.42021900	O	2.45512300	0.32072900	-2.25086300
C	-4.08965700	-1.45126800	0.35750400	C	0.53529400	-3.03584600	-1.24187800	O	2.40569300	-1.38993700	0.61679700
C	1.52713400	3.15686400	4.14315900	O	1.32974600	-3.48998600	-0.30327400	N	-2.13348800	-0.52964300	-0.06008000
H	1.99729200	3.38897900	5.10181700	H	0.93201800	-3.06860500	-2.28980700	N	-3.43806700	-1.51107300	1.45106500
C	0.30293700	3.73547400	3.80793900	C	7.06789500	0.18659900	-1.73354500	H	-3.71074900	-2.12581700	2.20533900
H	-0.18676700	4.42415300	4.50071100	C	7.80012100	0.01854000	-0.55794000	N	0.17411800	-1.34313100	0.94526400
C	0.90499400	5.57709200	-2.73277600	C	7.35666400	-0.88851600	0.40352200	C	0.32250300	4.78583300	-0.51069000
H	1.20468600	6.39537700	-3.39176300	C	6.19479800	-1.62868000	0.18896500	H	0.28002300	4.92731300	0.57343700
C	0.54902400	-3.06276300	3.34784500	C	5.45759000	-1.47030100	-0.98938000	C	0.16064700	3.50345800	-1.05678200
H	0.64791300	-3.80443700	4.14317900	C	5.90422100	-0.54900700	-1.94347500	C	-2.15914500	-1.28994100	1.02404000
C	0.39578700	3.23814900	-2.39578100	H	7.39872100	0.90620100	-2.48655700	C	1.08026600	2.31988700	1.37750000
H	0.29391400	2.22377200	-2.78918500	H	8.70963600	0.60004300	-0.38855000	C	0.53997500	5.88386500	-1.33789400
C	0.77140900	4.28512100	-3.23695200	H	7.92080300	-1.02137000	1.33038100	H	0.66333600	6.87739900	-0.90025200
H	0.96680700	4.08518900	-4.29291800	H	5.83999700	-2.33754700	0.94068300	C	-3.97732800	0.49621800	-1.42758300
Ru	-0.01984700	-0.01929300	-0.60731000	H	5.31845300	-0.39508800	-2.85455700	H	-3.31068200	0.96788900	-2.15342700
H	2.61406400	-3.13315600	-0.25523600	C	4.22560300	-2.29159300	-1.24312100	C	-2.10760100	1.80904900	2.01669800
C	-1.84669300	-3.18381400	-2.12427200	O	3.61557800	-2.70457800	-0.04986000	H	-1.37005000	1.18124600	2.52887500
C	-3.12960400	-3.72370300	-2.08827900	H	3.53034200	-1.71407000	-1.88394700	C	1.43568500	0.16727900	-1.69840000
C	-3.45275600	-4.69611300	-1.13804500	H	4.50253500	-3.18589800	-1.83744400	C	-1.75052000	2.46755600	0.82775900
C	-2.48205000	-5.12303300	-0.23153500	H	3.17117900	-1.66467000	0.71988100	C	-3.39075800	1.93538000	2.53992500
C	-1.19600900	-4.58113800	-0.27195200	H	0.35624500	-1.84031200	-1.20410600	H	-3.65340000	1.41342700	3.46415800
C	-0.86754800	-3.60586400	-1.21746500	H	-0.55566100	0.43195000	-2.05686100	C	-2.70942000	3.25872200	0.18376700

H	-2.45379900	3.77140300	-0.74840100	C	1.81536800	3.26754400	3.48892700	C	7.18880800	0.08728900	0.38297500
C	-5.36076800	0.59286500	-1.50298100	H	1.60450400	3.87478600	4.37280100	C	6.90922300	-1.16490000	0.93014500
H	-5.81703900	1.16121000	-2.31621700	C	0.60632100	5.71414900	-2.72222000	C	5.98831800	-2.01047500	0.31340600
C	1.49422000	-2.85296400	2.26661700	H	0.78255100	6.57559000	-3.37095300	C	5.33222300	-1.61566000	-0.85891600
C	2.33909100	1.71948400	1.23438900	C	0.36813400	-3.27778000	2.95160100	C	5.61200000	-0.35401800	-1.39613300
H	2.55178600	1.09503700	0.36467300	H	0.45298000	-4.03126700	3.73715900	H	6.73759800	1.47442800	-1.21075600
C	-0.87557300	-2.74626000	2.61274000	C	0.22939700	3.34225400	-2.44454900	H	7.90997800	0.75063000	0.86677200
H	-1.78761700	-3.09519700	3.10030500	H	0.10438800	2.34293200	-2.86975300	H	7.41385000	-1.48713500	1.84467400
C	-4.34203500	2.72105900	1.88478300	C	0.45245500	4.44373500	-3.27214500	H	5.76339200	-2.98959800	0.74367600
H	-5.35261400	2.81205800	2.28998700	H	0.50877500	4.30401400	-4.35422100	H	5.08200000	-0.02378900	-2.29269000
C	-0.92900600	-1.80514100	1.58645600	Ru	-0.18226100	-0.07634400	-0.90788900	C	4.34302600	-2.52893200	-1.52527500
C	0.82987300	3.09974300	2.51655300	H	2.80132700	-3.57060000	-0.91909900	O	3.68603600	-3.32771200	-0.55637100
H	-0.14465000	3.57798900	2.65203600	C	-2.44258500	-3.11448500	-2.02843800	H	3.61674500	-1.92927300	-2.10091100
C	1.36511300	-1.86673200	1.26874300	C	-3.71250900	-3.49486100	-1.60838700	H	4.86432800	-3.17855300	-2.25598700
C	-3.44037300	-0.24274600	-0.36970500	C	-3.85867800	-4.34896100	-0.51007900	H	3.04570900	-2.12723400	0.41009800
C	-6.19445000	-0.02871000	-0.55305600	C	-2.72790500	-4.81789500	0.15881900	H	-0.18695900	-1.61136400	-1.71213300
H	-7.27777600	0.06964100	-0.65074000	C	-1.45557500	-4.42977800	-0.26195300	H	-0.83026300	0.52637600	-2.25000400
C	3.32336200	1.89013500	2.20525100	C	-1.30268200	-3.57240100	-1.35510500	H	2.48570300	-3.25096700	2.48838400
H	4.29405300	1.40464800	2.07373100	H	-2.32202000	-2.41812000	-2.86532000	H	0.16468600	-2.98606600	-2.88533100
C	-3.99506900	3.38582300	0.71130900	H	-4.59656400	-3.11621600	-2.12876500				
H	-4.73386500	4.00113400	0.19202000	H	-4.85779400	-4.65013100	-0.18268300	TS8			
C	-5.67532900	-0.76991200	0.50434600	H	-2.83714000	-5.49623100	1.01044200	P	1.86319400	0.29873300	0.01306800
H	-6.32640300	-1.25591000	1.23356500	H	-0.55219000	-4.77721300	0.24653200	O	1.78479900	-2.23997200	-2.78145300
C	-4.28651100	-0.86418500	0.57843800	C	0.07826500	-3.17783600	-1.78846200	O	-0.29577500	-3.71309200	-0.31427600
C	3.06295100	2.66273200	3.33674100	O	1.07038000	-3.54922000	-1.13262100	N	-1.36793100	0.92955700	-0.19703600
H	3.83096200	2.79216600	4.10320900	C	6.53590000	0.48975100	-0.78203500	N	-2.63269400	1.35838200	1.58304000

H	-3.17404400	1.17585000	2.41700400	C	3.76112400	-3.42038400	2.04569800	C	0.56251900	3.77715300	1.69308800
N	-0.88030000	-1.62027800	0.43355100	H	4.18252300	-4.32326400	2.49322200	H	0.15136300	4.70909600	1.29608300
C	1.62423400	1.39329600	2.68161900	C	-1.48906600	-0.88056800	1.39683200	Ru	0.02227800	-0.35122100	-1.27087200
H	2.06620400	0.47975900	3.08535900	C	3.38738900	1.07473900	-2.23625900	C	-3.87696300	-0.22282800	-1.72272900
C	1.48277500	1.55959200	1.29852000	H	2.59216900	0.61471500	-2.82771100	C	-4.85561200	0.18848000	-0.82369100
C	-1.81484200	0.46044700	0.95833300	C	-0.69710800	-2.93321300	0.65848000	C	-5.26902300	-0.67168200	0.19921900
C	3.28301700	1.09469500	-0.84198800	C	-1.94128000	2.16607800	-0.36429700	C	-4.70440200	-1.94376100	0.30533500
C	1.22229100	2.40214000	3.56002400	C	-3.36551700	4.53563300	-0.20063700	C	-3.72176500	-2.35058200	-0.59682000
H	1.34266100	2.25709300	4.63656900	H	-3.91888200	5.47631300	-0.16345000	C	-3.28665900	-1.48744900	-1.60795400
C	-1.83233400	3.07774000	-1.41857300	C	5.40112000	2.27190500	-0.71892400	H	-3.53122600	0.45485500	-2.51066200
H	-1.20019000	2.84232000	-2.27791300	H	6.18602400	2.74252400	-0.12204100	H	-5.29631200	1.18544600	-0.91706700
C	3.87577700	-1.64030400	0.41249000	C	2.56170600	-2.89360300	2.52397300	H	-6.04409900	-0.35431900	0.90237800
H	4.39712200	-1.16853400	-0.42423500	H	2.03538900	-3.38159200	3.34853700	H	-5.03567800	-2.62589800	1.09327200
C	1.09136100	-1.51112900	-2.19398100	C	-3.47985600	3.64045900	0.85874000	H	-3.27245600	-3.34626300	-0.53683800
C	2.67608700	-1.09280900	0.89178700	H	-4.10931200	3.85902600	1.72332600	C	-2.22968100	-1.94192300	-2.56990700
C	4.41065900	-2.79314700	0.98466500	C	-2.75580500	2.45358300	0.75592800	O	-1.63707700	-3.03095100	-2.43704700
H	5.34342400	-3.20486200	0.59262500	C	5.50128900	2.24248000	-2.11140700	H	-0.68940600	-3.39735500	-1.19282300
C	2.01860400	-1.74921600	1.94564100	H	6.36629600	2.68990400	-2.60688400	H	-1.22371300	-0.68821400	-2.39811900
H	1.06576100	-1.36535200	2.32152700	C	4.49526700	1.64399100	-2.86645100	H	0.41758100	0.77871000	-2.33803000
C	-2.55587600	4.25955600	-1.31991600	H	4.56811300	1.61935700	-3.95613000	H	-0.72518900	-4.55888700	2.06977000
H	-2.50057700	4.99294000	-2.12697800	C	0.68440300	3.59110000	3.07166200	H	-2.36795300	-1.51829400	-3.59426200
C	-0.93909300	-3.49885100	1.93048400	H	0.37107000	4.37764400	3.76233400				
C	4.29991700	1.70063600	-0.08817400	C	-1.47622100	-2.71281900	2.93326500				
H	4.22843100	1.72151300	1.00396800	H	-1.68129000	-3.13879400	3.91772000				
C	-1.79159800	-1.37783000	2.66115800	C	0.95654300	2.77026800	0.81811100				
H	-2.25138300	-0.74116400	3.41904100	H	0.85003900	2.91573600	-0.26201000				