

Supplementary Information

Mechanistic insight into the borrowing-hydrogen N-alkylation catalyzed by an MLC catalyst with dual proton-responsive sites

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1. The comparison of free energy barriers using different functionals

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

Functionals	3	α -TS4 _a	γ -5	γ -TS4 _a
M06-L	0.0	31.4	0.0	20.7
BP86	0.0	36.4	0.0	22.4
BMK	0.0	43.3	0.0	34.1
M06	0.0	31.6	0.0	22.4

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 catalytic hydrogenation and 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 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 catalytic cycle proposed by Beller et al.

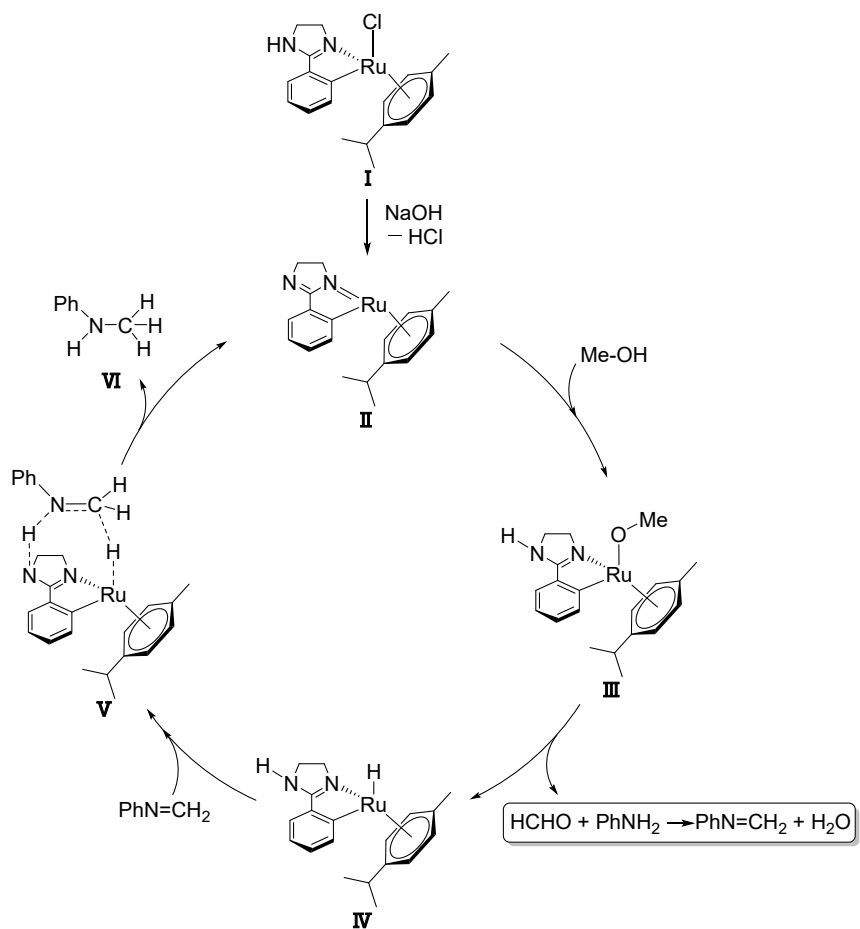


Figure S1. The catalytic cycle proposed by Beller et al.

3. The newly proposed catalytic cycle according to the DFT calculation

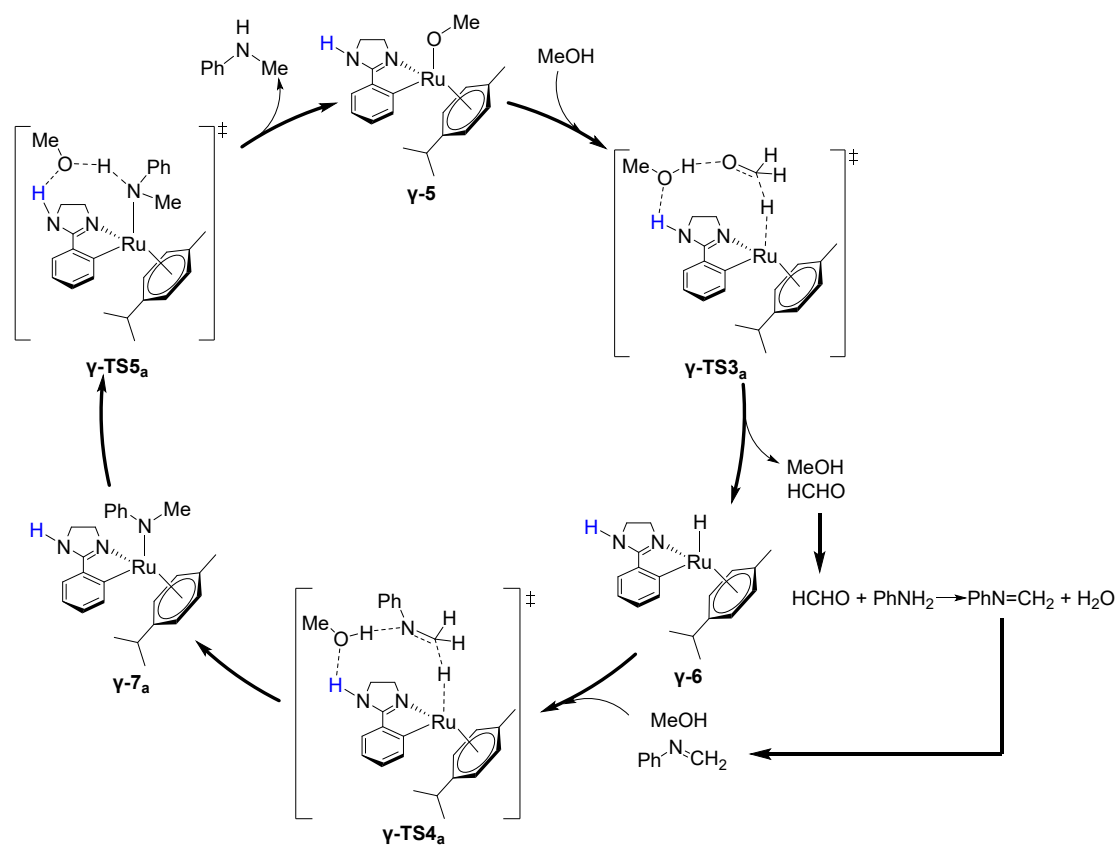


Figure S2. The newly proposed catalytic cycle according to the DFT calculation.

4. The potential energy surface involving the condensation reaction

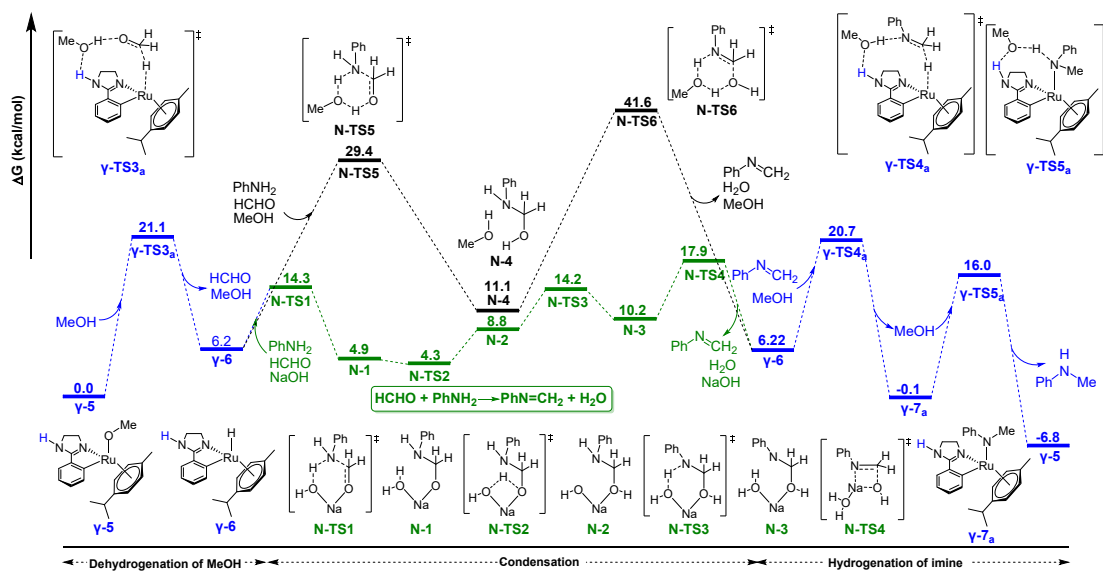


Figure S3. The potential energy surface involving the condensation reaction.

We tried to search for transition states of the condensation reaction. The proton shuttle transition states were successfully located, which possesses a high activation free energy barrier ($\Delta G^\ddagger = 41.6$ kcal/mol) and seems less plausible. Considering the use of NaOH as the base in Beller's system, inspired by the work of Lei et al. (*Asian J. Org. Chem.*, **2021**, 10, 634-641), we perform further calculation including NaOH. The results show that the activation energy barrier for the condensation reaction assisted by NaOH is 13.6 kcal/mol, which does not surpass the activation free energy barrier of hydride transfer and is consistent with the experimental results. Although **N-TS2** is lower compared with **N-1** and **N-2** in solvated free energy, the electronic energy in gas phase **N-TS2** is higher than **N-1** and **N-2** as the transition states were located on the potential electronic surface. Similar results have been obtained in Lei's work..

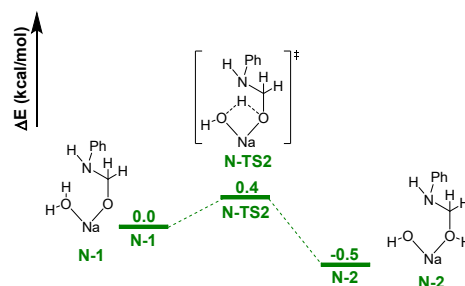


Figure S4. The electronic potential energy surface.

5. The comparison of the condensation reaction using different functionals

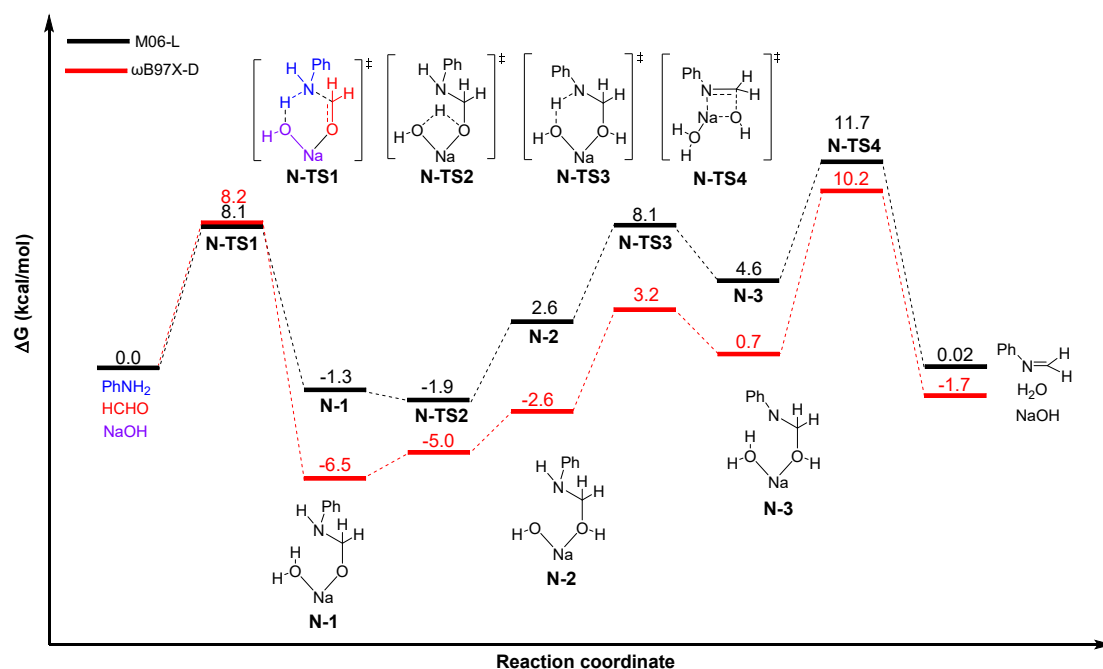


Figure S5. The comparison of the condensation reaction using different functionals.

Given the successful simulation of the condensation reaction process under alkaline conditions using the ω B97X-D functional by Lei et al. (*Asian Journal of Organic Chemistry*, 2021, 10, 634-641.), we performed a comparative calculation using ω b97x-d functional. The results show that the trends of M06-L and ω B97X-D are basically the same, and the rate-determining steps are both located in the C-O bond cleavage step. With regard to the reliability of M06-L, the effect of CsCO₃ on C-H activation reaction was investigated by Musaev et al using M06-L (*J. Am. Chem. Soc.*, 2014, **136**, 14834-14844) and the mechanistic selectivity of [4 + 1] annulation in the presence or absence of a catalyst was investigated by Lan et al using M06-L (*Chin. Chem. Lett.*, **2022**, 33, 2031-2035.). These works also demonstrate the reliability of M06-L. The main objective of this paper is to compare the energy barrier differences and the mechanistic selectivity of ruthenium catalysts mediated by different ligand sites. Considering that the condensation reaction is not a rate determining step and the efficiency and reliability of M06-L in dealing with transition metal systems, we have continued to use the M06-L calculated data to analyze the

mechanism.

6. The mechanistic preference analysis using energetic span model

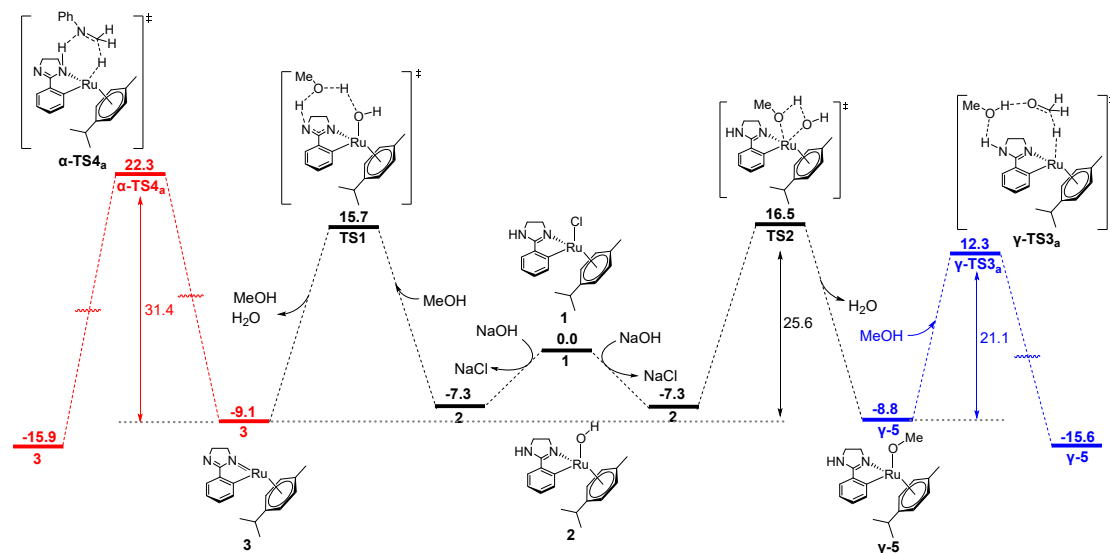


Figure S6. The mechanistic preference analysis using energetic span model.

We used the energetic span model to analyze the calculated potential energy surface. For the calculated data without the entropy correction, the pre-catalyst **1** undergoes the activation process and the **TS1** was found to have lower activation energy barrier. However, the subsequent α -NH pathway way requires to overcome the barrier of 31.4 kcal/mol. Therefore, intermediate **3** returns to **TS2** with the activation energy barrier of 25.6 kcal/mol and give γ -**5**. The rate-determining step of the followed γ -NH pathway requires to overcome 21.1 kcal/mol. Therefore, the generation of γ -**5** is an irreversible process with the activation energy barrier of 25.3 kcal/mol (γ -**5**→**TS2**).

7. The catalytic activity of the catalyst without the γ -NH site

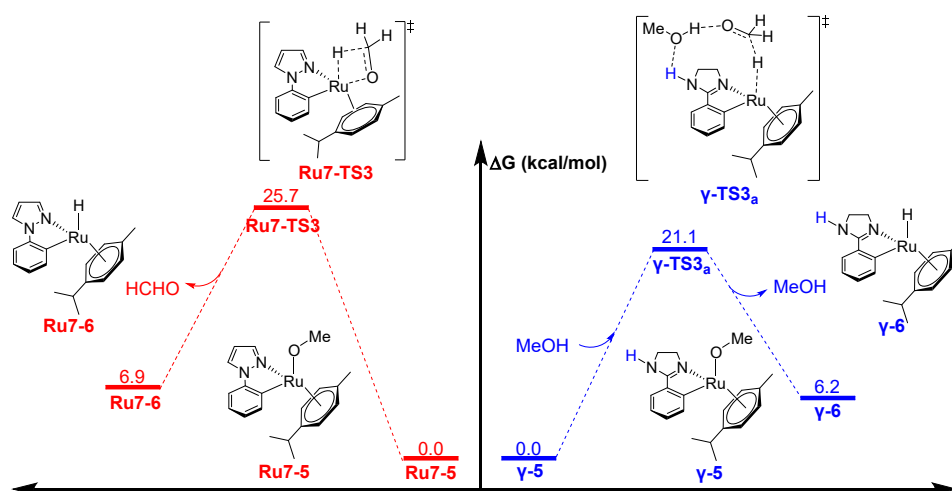


Figure S7. The comparison of the catalytic activity with and without the γ -NH site.

We have selected an example of a catalyst from the Beller's article that showed good activity without the γ -NH site and performed calculations on the absolute speed step of the reaction. The results show that the outer-sphere hydride transfer transition state cannot be located without the assistance of the γ -NH site and MeOH. However, the β -H elimination TS is located with an accessible activation free energy barrier of 25.7 kcal/mol, which can be overcome under reaction conditions at 70 °C. It is worth pointing out that the energy barrier of γ -NH site assisted transition state is only 21.1 kcal/mol, and thus the catalyst with γ -NH site exhibits superior catalytic activity.

8. The DFT calculated energies of all optimized structures

Table S2. The DFT calculated energies of all optimized structures

Species	Hc hartree	Gc hartree	H(gas) hartree	G(gas) hartree	Esp + G _{SOL} hartree	Final G hartree	<i>i</i> (cm ⁻¹)
MeOH	0.055685	0.028759	-115.557604	-115.584530	-115.755600	-115.726841	
PhNH ₂	0.124106	0.088281	-287.238504	-287.274330	-287.676957	-287.588676	
HCHO	0.030316	0.004843	-114.369858	-114.395331	-114.534762	-114.529919	
PhNCH ₂	0.128702	0.090786	-325.275121	-325.313037	-325.757639	-325.666853	
PhNCH ₃	0.153530	0.114002	-326.479922	-326.519450	-326.988703	-326.874701	
H ₂ O	0.025469	0.004038	-76.324566	-76.345997	-76.455741	-76.451703	
NaCl	0.004504	-0.021490	-622.353963	-622.379957	-622.602752	-622.624242	
NaOH	0.015404	-0.010830	-237.969147	-237.995381	-238.181331	-238.192161	
α-site							
1	0.404645	0.329559	-1401.382458	-1401.457544	-1402.884321	-1402.554762	
2	0.416459	0.342591	-1017.018284	-1017.092152	-1018.476954	-1018.134363	
TS1	0.466794	0.388052	-1132.577152	-1132.655894	-1134.212498	-1133.824446	-1322.34
3	0.387952	0.317420	-940.665402	-940.735934	-942.002958	-941.685538	
4	0.446707	0.368780	-1056.224645	-1056.302572	-1057.755439	-1057.386659	
α -TS2 _a	0.441554	0.367525	-1056.225203	-1056.299231	-1057.747974	-1057.380449	-1084.53
α -TS2 _b	0.438750	0.363110	-1056.214160	-1056.289790	-1057.740780	-1057.377670	-583.18
α -5	0.446394	0.369822	-1056.233646	-1056.310218	-1057.762878	-1057.393056	
α -6	0.441576	0.365222	-1056.210215	-1056.286569	-1057.738993	-1057.373771	
α -TS3 _a	0.440144	0.363278	-1056.211390	-1056.288256	-1057.731438	-1057.368160	-265.86
α -TS3 _b	0.441325	0.365162	-1056.185081	-1056.261244	-1057.710648	-1057.345486	-651.96
α -7	0.408848	0.337547	-941.829739	-941.901039	-943.188703	-942.851156	
α -TS4 _a	0.537999	0.451670	-1267.117419	-1267.203748	-1268.950959	-1268.499289	-481.25
α -TS4 _b	0.539070	0.451630	-1267.088760	-1267.176190	-1268.924850	-1268.473220	-698.89
α -8 _a	0.543143	0.457007	-1267.135733	-1267.221870	-1268.973017	-1268.516010	
α -TS5 _a	0.539287	0.455914	-1267.143571	-1267.226943	-1268.973107	-1268.517193	-1284.43
α -8 _b	0.539780	0.452527	-1267.119682	-1267.206935	-1268.960284	-1268.507757	
α -TS5 _b	0.536296	0.449070	-1267.122729	-1267.209955	-1268.959513	-1268.510443	-719.17
γ-site							
TS2	0.469092	0.387462	-1132.565200	-1132.646800	-1134.210700	-1133.823238	-561.27
γ -5	0.445711	0.368762	-1056.256324	-1056.333273	-1057.780557	-1057.411795	
γ -TS3 _a	0.498662	0.410686	-1171.809746	-1171.897722	-1173.515681	-1173.104995	-304.22
γ -TS3 _b	0.441210	0.364606	-1056.211518	-1056.288122	-1057.733200	-1057.368594	-588.88
γ -6	0.408816	0.336496	-941.852113	-941.924432	-943.208425	-942.871929	
γ -TS4 _a	0.594979	0.495506	-1382.721703	-1382.821175	-1384.738057	-1384.242551	-489.94
γ -7a	0.543557	0.455920	-1267.167267	-1267.254904	-1269.004863	-1268.548943	
γ -TS5 _a	0.598085	0.506836	-1382.731211	-1382.822460	-1384.756871	-1384.250035	-327.20
γ -TS5 _d	0.596387	0.503612	-1382.721114	-1382.813889	-1384.732637	-1384.229025	-861.94
γ -TS4 _b	0.538862	0.454731	-1267.138059	-1267.222190	-1268.967963	-1268.513232	-489.52

γ -7 _b	0.540573	0.452331	-1267.139196	-1267.227437	-1268.975437	-1268.523106	
γ -TS5 _b	0.536228	0.448276	-1267.124748	-1267.212700	-1268.958306	-1268.510030	-1445.29
γ -7 _c	0.598507	0.499160	-1382.725554	-1382.824901	-1384.750104	-1384.250944	
γ -TS5 _c	0.594196	0.499203	-1382.721214	-1382.816207	-1384.746136	-1384.246933	-1290.56
α-γ							
TSa	0.487504	0.404059	-1133.722663	-1133.806108	-1135.380269	-1134.976210	-694.64
TSb	0.406891	0.334060	-941.793451	-941.866281	-943.155855	-942.821795	-153.46
TS _c	0.461273	0.382340	-1057.346271	-1057.425204	-1058.895826	-1058.513486	-814.22
TSd	0.519465	0.432678	-1172.954350	-1173.041137	-1174.683772	-1174.251094	-176.68
N-TS1	0.173494	0.122540	-639.642441	-639.693395	-640.420372	-640.297832	-139.04
N-1	0.176906	0.124752	-639.652595	-639.704749	-640.437612	-640.312860	
N-TS2	0.173592	0.124431	-639.655316	-639.704478	-640.438264	-640.313833	-510.54
N-2	0.177485	0.127330	-639.652830	-639.702985	-640.433908	-640.306578	
N-TS3	0.172558	0.123324	-639.647661	-639.696895	-640.421269	-640.297945	-676.96
N-3	0.176288	0.124047	-639.649668	-639.701910	-640.428489	-640.304442	
N-TS4	0.174577	0.123142	-639.640449	-639.691884	-640.415213	-640.292071	-155.54
N-TS5	0.210350	0.161161	-517.162890	-517.212079	-517.959752	-517.798591	-1226.90
N-4	0.218565	0.165884	-517.197661	-517.250342	-517.993571	-517.827687	
N-TS6	0.208466	0.157659	-517.148190	-517.198996	-517.936828	-517.779169	-1517.04
Ru7-5	0.421044	0.344555	-1055.057402	-1055.133892	-1056.553223	-1056.208668	
Ru7-TS3	0.416616	0.341558	-1055.015649	-1055.090708	-1056.509339	-1056.167781	-638.44
Ru7-6	0.384246	0.313856	-940.655050	-940.725440	-941.981551	-941.667695	

- The H_C and G_C designate the thermal correction of Enthalpy and Gibbs Free Energy at M06-L/def2-SVP level.
- The $H(\text{gas})$ and $G(\text{gas})$ designate Enthalpy and 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 M06-L/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.
- The i designates the imaginary frequency of transition states.

9. The Cartesian coordinates (xyz) for all optimized structures

NaCl				O	-0.00000000	0.00000000	0.11920400	C	-0.04022300	1.09575100	-0.15463100
				H	-0.00000000	0.75607600	-0.47681600	C	1.70267200	-1.06473200	0.11265100
Na	0.00000000	0.00000000	-1.42508700	H	-0.00000000	-0.75607600	-0.47681600	H	-0.06965700	-2.30472400	-0.04343100
Cl	0.00000000	0.00000000	0.92211500					C	1.32993300	1.31404300	-0.03769600
								H	-0.72419500	1.93755500	-0.29107100
				MeOH				C	2.20552800	0.23791300	0.10638500
NaOH								H	2.38386800	-1.91275200	0.21513900
				C	0.64930300	-0.01952100	-0.00000000	H	1.71808000	2.33515900	-0.06476700
O	0.00750900	1.00834000	0.00000000	H	1.08655600	0.98731900	0.00008800	H	3.27958700	0.41286600	0.19843500
H	-0.14266800	1.95202100	0.00000000	H	1.04051800	-0.54308500	0.89213500	C	-2.78313000	0.23300100	0.28915600
Na	0.00750900	-0.91079400	0.00000000	H	1.04053200	-0.54293500	-0.89221800				
				O	-0.74189000	0.12189800	-0.00000000				
HCHO				H	-1.12830200	-0.75935400	-0.00000200	PhNCH ₃			
								H	-2.80171700	1.11198400	-0.74105500
C	-0.52196800	0.00000000	0.00000600					H	-3.79837700	-0.13233000	0.01855800
O	0.67421500	0.00000000	-0.00000800	PhNCH ₂				N	-1.78327200	-0.61068200	-0.09884400
H	-1.13095700	0.94249500	-0.00000800					C	-0.44625200	-0.28385800	-0.03829000
H	-1.13095700	-0.94249500	0.00003100	H	-2.53704000	1.07483200	0.96840200	C	0.52939100	-1.30120200	-0.00335900
				H	-3.85026200	0.02810400	0.12641900	C	-0.01098900	1.05512600	-0.03309100
				N	-1.91520000	-0.49138500	-0.28353600	C	1.88158800	-0.98781500	0.02726700
H ₂ O				C	-0.55192200	-0.21253100	-0.14125600	C	1.88158800	-0.98781500	0.02726700
				C	0.33814500	-1.29200200	-0.02867000	H	0.20761000	-2.34692000	-0.00501300

C	1.34990400	1.35296300	-0.00718000	H	-2.78265500	0.83953100	0.25890100	C	1.59120400	-1.50801800	1.14836000
H	-0.74076000	1.86683600	-0.05041300					C	0.77831700	-2.44400800	0.46353400
C	2.30878500	0.34253000	0.02345500					C	0.64210200	-2.38880300	-0.94660200
H	2.61507500	-1.79778300	0.05445500	3				H	1.27710500	-1.28785300	-2.71796400
H	1.66181000	2.40065800	-0.00568300					H	2.92265300	0.16598400	-1.54449600
H	3.37279200	0.58477000	0.04696900	N	-0.22352400	1.47247400	-0.49157800	H	1.58945900	-1.50298700	2.24127200
C	-2.82152300	0.36222600	0.06606300	C	-1.55383800	1.84125000	-0.30201100	H	0.13148000	-3.11000800	1.03904400
H	-2.76695500	0.91306900	1.02485800	C	-2.41073100	0.76215500	0.17577000	C	-0.31260200	-3.27113100	-1.67827600
H	-2.01199700	-1.56532900	0.14004200	C	-3.77016900	0.91942100	0.44981600	H	-0.69589400	-2.78219400	-2.58303500
				H	-4.23216600	1.90031900	0.30755200	H	0.17546900	-4.20791300	-1.98933000
				C	-0.67094600	3.71803300	-1.02777900	H	-1.17430100	-3.53843300	-1.05319900
PhNH ₂				C	-4.50609900	-0.17596900	0.89606500	C	3.28992100	0.38771200	1.23363400
				C	0.44509900	2.65434800	-1.01344000	H	3.95835100	-0.25159000	1.84289100
N	-2.32598300	0.00000700	-0.07351200	C	-2.51085400	-1.55485900	0.78749900	C	4.16921400	1.27181000	0.36617100
C	-0.94323800	0.00001200	-0.00791200	H	-0.44686500	4.57653200	-0.37101800	H	3.56943700	1.95232500	-0.25756000
C	-0.22149500	1.20701900	-0.00335600	H	1.29981000	2.93953700	-0.37514100	H	4.81977100	1.89893500	0.99052500
C	-0.22151700	-1.20700400	-0.00335900	N	-1.87969400	3.05834100	-0.57453600	H	4.81823300	0.68934500	-0.30242000
C	1.16954700	1.20084600	0.00304700	H	0.86403400	2.45751100	-2.01630500	C	2.45797300	1.22771500	2.19791000
H	-0.76649300	2.15534800	-0.00867500	H	-0.83447900	4.15436200	-2.02786900	H	1.86049900	0.61541700	2.88627400
C	1.16952600	-1.20085800	0.00305800	C	-3.87285500	-1.41047100	1.06413000	H	3.10338700	1.87415300	2.80898900
H	-0.76653100	-2.15532400	-0.00870600	H	-4.44887400	-2.27041200	1.41857900	H	1.75332800	1.86971600	1.64778100
C	1.88000000	-0.00001300	0.00613700	H	-5.57140500	-0.07175600	1.11545300	C	-1.73975300	-0.47466000	0.33267500
H	1.70587700	2.15321500	0.00787000	H	-2.05142800	-2.53840000	0.94097300	Ru	0.28695300	-0.39273000	-0.14609800
H	1.70583900	-2.15323600	0.00788000	C	1.41433300	-1.39912500	-1.63846100				
H	2.97148800	-0.00002200	0.01275200	C	2.36503700	-0.57382300	-0.96819300				
H	-2.78257300	-0.83957900	0.25887000	C	2.42948200	-0.57627000	0.44087900	γ -7 _a			

				H	-1.82412400	0.87249900	-2.45602400	C	3.63311100	0.11243500	1.24390000
N	-0.81808000	-1.24640500	1.20412800	H	-3.16851600	0.95269400	1.66244700	C	3.95441900	1.32849700	-1.23380700
C	-0.15545300	-2.26050900	0.71041200	H	-1.48529000	2.70883800	2.19614700	H	1.85327500	1.77686400	-1.12360800
C	0.48521000	-2.08414700	-0.56733300	C	0.41111500	3.74851100	0.52794700	C	4.88230300	0.13948300	0.62657300
C	1.14822400	-3.09952500	-1.27185000	H	1.04044500	3.29472500	1.30775100	H	3.53713200	-0.38734800	2.20968800
H	1.24283000	-4.10314300	-0.84434300	H	1.05812500	3.97986600	-0.32640000	C	5.06510700	0.74231500	-0.61615000
C	-0.77795000	-3.00716700	2.77489100	H	0.00464600	4.69238500	0.91940600	H	4.06552700	1.81350300	-2.20865100
C	1.66975900	-2.82844600	-2.52968600	C	-3.73874200	-0.23733600	-0.73643500	H	5.73075300	-0.33249500	1.13173600
C	-1.44569200	-1.66304100	2.44626200	H	-3.83044800	-0.82250200	0.19759500	H	6.04646400	0.75749700	-1.09474700
C	0.86893800	-0.53941700	-2.35481600	C	-5.09336300	0.40955800	-1.01304300	H	0.23516300	0.60296300	3.04415600
H	0.01849100	-2.89133900	3.53179500	H	-5.05806600	1.01699800	-1.93034200				
H	-1.31198700	-0.91364400	3.24125700	H	-5.87821900	-0.34840200	-1.14867100				
N	-0.22434200	-3.38774800	1.47969700	H	-5.40669400	1.07268500	-0.19401100	2			
H	-2.53624900	-1.77677200	2.29913100	C	-3.34129800	-1.20013500	-1.84327100				
H	-1.48657700	-3.75821700	3.15220700	H	-2.33888200	-1.62096600	-1.67506100	N	0.71191600	1.52114700	0.40891200
C	1.51505300	-1.54727800	-3.07011100	H	-4.05525600	-2.03263500	-1.91033100	C	1.95873500	1.21844500	0.17994000
H	1.91536400	-1.33064300	-4.06456300	H	-3.33604500	-0.71077900	-2.82914900	C	2.22451300	-0.03680900	-0.48359600
H	2.18792600	-3.60687400	-3.09324200	C	0.33858400	-0.76778600	-1.07684400	C	3.50385300	-0.53803800	-0.76328000
H	0.79694900	0.45475400	-2.80859500	Ru	-0.61642500	0.58816300	0.17214100	H	4.39785100	0.01541000	-0.45642200
C	-0.82644600	2.30765800	-1.15949900	H	0.52482300	-4.06656500	1.42957200	C	2.08291400	3.35698200	0.96227100
C	-1.80857600	1.31295700	-1.45553200	C	1.20349000	0.32391800	2.59828000	C	3.63307800	-1.75229600	-1.42646100
C	-2.69814100	0.82315500	-0.46265900	H	1.33655800	-0.77013500	2.77442300	C	0.65168300	2.80564500	1.07597700
C	-2.55150000	1.36751100	0.85732500	H	1.98541400	0.81978600	3.20493900	C	1.21019300	-1.93871900	-1.53205400
C	-1.60097200	2.35960000	1.16762400	N	1.25612800	0.74118900	1.22927000	H	2.16412900	4.10541000	0.15385800
C	-0.68927100	2.81155200	0.16004900	C	2.49310300	0.70174700	0.63543300	H	-0.10258700	3.45637400	0.60828100
H	-0.13201400	2.63699900	-1.93639400	C	2.70819400	1.31104900	-0.62832700	N	2.84767500	2.15285400	0.64413900

H	0.34610900	2.66934200	2.13046300	C	0.50301000	-0.84783700	2.91642300	H	0.26347300	4.66662100	-0.42339800
H	2.43907900	3.83164100	1.88776500	H	0.19917200	0.17283200	3.18781700	C	-4.16224700	-0.94739500	-0.69386800
C	2.48002700	-2.44465100	-1.81404900	H	0.99475800	-1.28748100	3.79614000	H	-4.88955000	-1.75302700	-0.83243300
H	2.57774500	-3.39520900	-2.34677500	H	1.25198300	-0.76423500	2.11379200	H	-5.61399000	0.62289400	-1.02555300
H	4.62220400	-2.15915800	-1.64693600	C	1.03363500	-0.72991400	-0.83985800	H	-2.56089700	-2.32076100	-0.33646800
H	0.33453800	-2.50420700	-1.86922700	Ru	-0.75160700	0.19429400	-0.33587500	C	0.30337700	-1.85108200	-1.46861200
C	-2.41756100	-1.02563200	-0.96786000	O	-0.55242400	1.23742000	-2.07721500	C	1.24383300	-0.79076500	-1.63176700
C	-1.69079600	-1.67110100	0.07539400	H	3.74506900	2.24475000	0.18451300	C	2.32770400	-0.61614800	-0.69722800
C	-1.45974800	-1.05682900	1.34253200	H	0.35404600	1.16774600	-2.39819500	C	2.28573700	-1.37444200	0.48207900
C	-1.92554400	0.28362600	1.46467500					C	1.23957100	-2.32318500	0.70327300
C	-2.73013700	0.92580700	0.46743500					C	0.31422700	-2.68212600	-0.31177500
C	-2.95346300	0.28812500	-0.77038400	4				H	-0.48709600	-1.98164300	-2.21274000
H	-2.52208100	-1.51295100	-1.93941200					H	1.17357000	-0.16107900	-2.51966200
H	-1.24857400	-2.64756300	-0.13509200	N	-0.09435000	1.55006000	0.41579400	H	3.02338500	-1.20665000	1.26932500
H	-1.67607000	0.84827300	2.36841900	C	-1.28984200	2.07637900	-0.05555700	H	1.18938300	-2.84774400	1.66269200
H	-3.06235100	1.95520400	0.61661600	C	-2.31369000	1.07277700	-0.31040600	C	-0.59743600	-3.85180800	-0.13463800
C	-3.55325000	1.01861400	-1.92162000	C	-3.64157400	1.39800500	-0.60169900	H	-1.35980900	-3.90538300	-0.92051700
H	-4.25511800	0.38583800	-2.48128700	H	-3.91792400	2.45425900	-0.66388100	H	-0.02304600	-4.78986200	-0.18002700
H	-4.07571200	1.92842500	-1.60194600	C	-0.11358200	3.88726500	0.25847600	H	-1.10861400	-3.83282600	0.83812600
H	-2.73482900	1.31225600	-2.60068300	C	-4.57233200	0.38348800	-0.79829400	C	3.50207300	0.29887000	-0.99326900
C	-0.66623200	-1.71266700	2.45739600	C	0.83066300	2.67544000	0.37717400	H	4.30199100	-0.41058700	-1.28630300
H	-1.36437000	-1.81677900	3.31145300	C	-2.83062500	-1.26530600	-0.41339000	C	3.29160800	1.21346300	-2.19140200
C	-0.17124500	-3.10375500	2.09708900	H	-0.24666000	4.38744400	1.23766800	H	2.43440700	1.88908000	-2.05868200
H	0.53291100	-3.06619000	1.25047700	H	1.47663800	2.71250000	1.27124800	H	4.17892400	1.83989600	-2.35410400
H	0.36334800	-3.55497500	2.94432200	N	-1.38988800	3.35705400	-0.19019000	H	3.12481100	0.64821800	-3.11812400
H	-0.99029200	-3.78502500	1.82708500	H	1.50780100	2.61349200	-0.49586900	C	4.02420000	1.05574200	0.22113800

H	4.35299500	0.38685800	1.02731000	N	-2.87339200	1.82849200	0.81150700	H	-0.99093300	1.59027000	-2.23822000
H	4.89468200	1.66663100	-0.05443400	H	0.02497400	2.82477600	1.28424600	C	1.62899000	3.63039200	-1.18499600
H	3.26438400	1.73052900	0.63739000	H	-2.15516300	3.78011400	1.12161200	H	2.72720900	3.61199500	-1.22501800
C	-1.86896900	-0.26393800	-0.22085500	C	-2.69098500	-2.87052600	-1.31825700	H	1.29774900	4.54489700	-1.69577500
Ru	0.16279100	-0.52285100	0.17165400	H	-2.82192900	-3.84714400	-1.79383100	H	1.33725600	3.73343200	-0.12837300
C	0.47325200	-0.19374000	3.38202700	H	-4.80336500	-2.39700500	-1.37802300	C	-1.20238600	-1.20929100	-0.33182700
H	0.71429800	-1.24205000	3.59991500	H	-0.56597500	-3.11732000	-1.14270000	Ru	0.64210100	-0.36696400	0.14710800
H	0.09908300	0.26391100	4.31166200	C	1.63367400	-1.37429200	-1.45634100	C	1.22631000	-1.13598700	2.98772700
H	1.40338000	0.32278600	3.08467000	C	1.17491600	-0.11524600	-1.93886600	H	1.49419500	-0.06595100	3.17422400
O	-0.50713300	-0.15964000	2.37017800	C	1.50889000	1.08677000	-1.26593600	H	2.19306000	-1.65970400	2.81602500
H	-0.58736500	0.77026300	2.04032700	C	2.39772500	1.00287000	-0.13542400	H	0.84520200	-1.53060300	3.95095600
				C	2.86559400	-0.23357700	0.32760800	O	0.29140400	-1.31878000	1.99490000
				C	2.44620900	-1.46233600	-0.29614500	H	-0.71672500	0.11042000	1.96704800
α -5				H	1.28032000	-2.29329100	-1.93042400				
				H	0.48618000	-0.08333600	-2.78731200				
N	-0.81737000	0.88292900	1.26670500	H	2.65758600	1.90807800	0.41888900	α -6			
C	-2.11916900	0.81017900	0.65530400	H	3.46023300	-0.27511300	1.24368700				
C	-2.35265300	-0.43091700	-0.06112400	C	2.84892600	-2.79275300	0.24550000	N	-0.55680900	-0.32687800	1.61618300
C	-3.63776800	-0.83951300	-0.44342800	H	2.07490000	-3.54684600	0.05246200	C	-1.90988300	-0.05804200	1.16486100
H	-4.48744700	-0.18762800	-0.22268800	H	3.78366900	-3.14162400	-0.22030400	C	-2.17203800	-0.49645200	-0.19485400
C	-2.15823900	2.79659600	1.61988900	H	3.01290000	-2.75616800	1.32916300	C	-3.46478200	-0.63448200	-0.71442800
C	-3.80705200	-2.06243000	-1.07995500	C	1.00601900	2.40532000	-1.83242400	H	-4.32257600	-0.43512700	-0.06660300
C	-0.73374300	2.23952100	1.82650300	H	1.33865500	2.39859800	-2.88762000	C	-1.91467800	0.77016000	3.20938200
C	-1.41172000	-2.44847200	-0.95240600	C	-0.51407500	2.49811100	-1.84202700	C	-3.63062000	-1.01687800	-2.04056400
H	-2.69447600	2.95107600	2.57246500	H	-0.90915700	2.64717400	-0.82762100	C	-0.45273800	0.43599700	2.87380300
H	-0.41985300	2.20347900	2.87835900	H	-0.85417000	3.34763600	-2.45092500	C	-1.21834400	-1.09857900	-2.31479400

H	-2.32352000	0.12032800	4.00287400	H	-1.64639400	2.08855600	-0.84177000	C	0.21955500	-0.01722000	-2.95550000
H	0.06251000	-0.16594800	3.63366800	H	-1.55627900	3.62597300	-1.72299400	C	-0.37271300	-0.78483300	2.42255200
N	-2.66783700	0.55637100	1.98637000	H	-0.91092500	2.14831500	-2.44762900	H	-1.60161700	-0.72710200	-3.98399700
H	0.14141700	1.34806500	2.71177700	C	0.08617200	3.74096300	0.47602300	H	0.09621200	0.94315400	-3.47395900
H	-2.04484800	1.80255500	3.56931500	H	1.01447400	4.10222200	0.93998400	N	-1.18927200	-1.80542900	-2.23805800
C	-2.50451300	-1.25698200	-2.83422500	H	-0.55828600	4.61580100	0.31743500	H	1.27344100	-0.31960200	-3.05471700
H	-2.63269000	-1.56871100	-3.87509000	H	-0.43030300	3.09193200	1.20231600	H	-0.24249700	-1.83669900	-4.12083700
H	-4.63269600	-1.13425000	-2.45926600	C	-1.01866600	-0.70771600	-0.98342400	C	-1.34251300	-1.65907600	2.91691600
H	-0.35928300	-1.28452100	-2.96934500	Ru	0.79221500	-0.27240800	-0.06558200	H	-1.46301400	-1.77815500	3.99775700
C	2.25951900	-0.25621100	-1.65572100	C	0.42586500	-3.10874000	0.90306600	H	-2.91589900	-3.06792600	2.44261100
C	1.41091700	0.87426800	-1.76502600	H	0.71366800	-2.04474300	0.25320000	H	0.25423300	-0.23547900	3.13431100
C	1.21805300	1.79428300	-0.68740400	H	-0.06168300	-3.62431700	0.03539100	C	2.59771700	1.25293700	1.64351800
C	1.93552800	1.49963500	0.51473700	H	1.48423500	-3.46492200	1.01346600	C	2.73027200	-0.14428600	1.44427400
C	2.82362500	0.40349300	0.63960500	O	-0.26064400	-2.87513300	1.95265700	C	2.99621900	-0.71049100	0.15623400
C	2.94013700	-0.53030900	-0.42647300	H	-0.51399100	-1.38238900	1.85231400	C	3.12123100	0.22409800	-0.91915000
H	2.33196800	-0.96349900	-2.48502100					C	3.04345800	1.62872700	-0.73577000
H	0.82949800	0.99682700	-2.68318900					C	2.71862800	2.15787700	0.53989900
H	1.76360200	2.12141100	1.39664500	α -8 _b				H	2.33177700	1.63619900	2.63151100
H	3.32102900	0.20880100	1.59196000					H	2.52847500	-0.80568400	2.28947600
C	3.75876500	-1.76914200	-0.27575700	N	-0.12236100	0.12908300	-1.52844000	H	3.25516600	-0.15408300	-1.93598000
H	3.34876700	-2.59720700	-0.86868300	C	-0.85589200	-1.09359400	-1.23333400	H	3.11791300	2.29514600	-1.59787800
H	4.78900700	-1.59606400	-0.62295500	C	-1.05587600	-1.32955500	0.18450100	C	2.50788000	3.62254200	0.73955400
H	3.81215900	-2.09324300	0.77125400	C	-2.01570600	-2.22377100	0.67309200	H	1.73201400	3.82000500	1.49127900
C	0.32323600	3.01109200	-0.83648300	H	-2.64648600	-2.76609700	-0.03616900	H	3.43304100	4.10079500	1.09617800
H	0.87760700	3.70098400	-1.50398600	C	-0.72973500	-1.12601700	-3.43536400	H	2.21765000	4.12403200	-0.19224300
C	-1.01159600	2.69759900	-1.50209000	C	-2.16068000	-2.38572500	2.04587600	C	3.12940600	-2.20445700	-0.06956300

H	4.21619700	-2.39599400	-0.17740200	H	-4.52360100	0.47941800	2.55146300	C	1.35921700	-0.56029800	1.33089800
C	2.63119800	-3.02945500	1.10787300	H	-6.09159700	-0.56426700	0.91526100	C	2.01118900	-1.21322000	0.24588600
H	1.56729400	-2.82940500	1.31309400					C	2.76740200	-0.52942800	-0.74267600
H	2.72886500	-4.10163000	0.89155000					C	2.77909900	0.89358500	-0.74966600
H	3.19665800	-2.83723900	2.02982800	α -7				H	2.10861200	2.68092400	0.32323700
C	2.45410500	-2.66708400	-1.35501100					H	0.82700900	1.42917900	2.04599300
H	2.83847600	-2.16294900	-2.25269000	N	-0.78329400	-1.07436900	-1.55256500	H	1.92233200	-2.30341400	0.17153300
H	2.61455400	-3.74297200	-1.50757900	C	-2.04608400	-0.93867300	-0.82468100	H	3.25480400	-1.08528100	-1.54595200
H	1.36577100	-2.50348400	-1.31103000	C	-2.27812500	0.39251300	-0.30371500	C	3.49028700	1.65313600	-1.82132600
C	-0.20659700	-0.59315300	1.04318300	C	-3.54388400	0.80809600	0.13656100	H	3.51641000	1.09019100	-2.76268700
Ru	1.22875400	0.58062300	0.10976100	H	-4.38404100	0.11134500	0.06944500	H	3.00194300	2.61568300	-2.01741000
C	-0.95084500	2.67133500	-0.04011600	C	-2.05397700	-3.06070200	-1.44706400	H	4.53043700	1.86091400	-1.52632800
H	-0.14879200	1.85656800	0.38602600	C	-3.70359700	2.08794300	0.64979600	C	0.62134600	-1.36031300	2.37974600
H	-1.28955000	3.08794100	0.92843000	C	-0.63903800	-2.53202200	-1.71796900	H	0.16649600	-2.21970800	1.84930500
H	-0.29382600	3.39774700	-0.54493400	C	-1.33550100	2.51455100	0.29421600	C	1.59573300	-1.92061700	3.41329000
H	-0.84843200	0.92741600	-1.44154900	H	-2.60970800	-3.28818800	-2.37529300	H	2.08902100	-1.10758200	3.96785500
N	-1.86506900	2.09839100	-0.87698800	H	-0.23003700	-2.77846900	-2.70555100	H	1.07920400	-2.55572500	4.14767100
C	-2.95465400	1.44677200	-0.33699700	N	-2.73892100	-2.00547800	-0.72364500	H	2.38725400	-2.52416800	2.94641900
C	-3.85537300	0.83749600	-1.24399100	H	0.07291000	-2.89959100	-0.96394700	C	-0.50525300	-0.58655000	3.04593400
C	-3.23305600	1.30006300	1.04351600	H	-2.04949500	-3.99484200	-0.86581000	H	-1.19064200	-0.13971200	2.31057000
C	-4.96335200	0.12846900	-0.80189200	C	-2.59363100	2.93969300	0.71843300	H	-1.09501800	-1.24436600	3.69894100
H	-3.64724600	0.94397400	-2.31266200	H	-2.71587400	3.95268800	1.11374000	H	-0.11959600	0.22580900	3.68099800
C	-4.34624200	0.58896300	1.47750100	H	-4.68303900	2.42930200	0.99196500	C	-1.13039900	1.22276700	-0.22080200
H	-2.55084800	1.71757400	1.78783000	H	-0.49022100	3.20655100	0.37299200	Ru	0.67799800	0.31823600	-0.64881600
C	-5.22256300	-0.00264200	0.56548300	C	2.11596800	1.58883000	0.31174000	H	0.43689900	1.13882300	-2.04011700
H	-5.63582600	-0.33045000	-1.53177700	C	1.40334300	0.86136700	1.30967300	H	-0.88664800	-0.60778200	-2.45582700

				C	2.75952100	-0.74243900	0.74524400	O	0.51211500	-1.82427400	-1.48021400
				C	2.95811000	-0.52835300	-0.63455800	H	-3.77398000	-1.84108900	0.94292200
γ -5				H	2.53099000	0.83170900	-2.29664000				
				H	1.34048700	2.51062200	-0.90489900				
N	-0.71759900	-1.20219600	0.96016700	H	1.77398500	-0.04497800	2.55271800	γ -6			
C	-1.95862000	-0.91387700	0.68417700	H	3.07751900	-1.68284500	1.20024800				
C	-2.20051700	0.12583500	-0.28779200	C	3.50283600	-1.60116200	-1.51068600	N	-1.01424500	-1.45541700	0.50162700
C	-3.46867400	0.59677200	-0.65326900	H	4.14859200	-1.19431200	-2.29996700	C	-2.20557700	-0.91771300	0.43788200
H	-4.36717800	0.22023700	-0.15263800	H	4.06703700	-2.34968100	-0.94114000	C	-2.33832000	0.31510800	-0.29067500
C	-2.14308900	-2.80249800	1.94986400	H	2.64559200	-2.10647000	-1.98940700	C	-3.53159400	1.04135600	-0.42310400
C	-3.58022900	1.55466900	-1.65404000	C	0.83479300	2.45176700	1.86459700	H	-4.45125300	0.68883300	0.05668500
C	-0.68337800	-2.31746000	1.88453200	H	1.58015500	2.80392400	2.60513100	C	-2.59832800	-2.93079600	1.43338400
C	-1.16143000	1.54987300	-1.91089500	C	0.34070000	3.66706400	1.09711500	C	-3.53931700	2.22161300	-1.15375100
H	-2.29151700	-3.72020900	1.35380500	H	-0.40200700	3.37906700	0.33575200	C	-1.09235500	-2.65750700	1.31198100
H	0.01247700	-3.09378400	1.52962300	H	-0.14822200	4.37941500	1.77581900	C	-1.16971100	1.92873900	-1.62538800
N	-2.86889100	-1.67627900	1.36591300	H	1.15458000	4.20472900	0.59076900	H	-2.92927100	-3.69370000	0.70501000
H	-0.31384000	-1.98502800	2.87244300	C	-0.31947500	1.81841300	2.63374500	H	-0.53678600	-3.48863700	0.85287800
H	-2.48175200	-3.01655100	2.97389500	H	-0.02006200	0.92533500	3.19964500	N	-3.16540900	-1.62190200	1.12437400
C	-2.42097000	2.02075100	-2.28459100	H	-0.74858400	2.53171500	3.35191700	H	-0.63014600	-2.47585600	2.30057600
H	-2.50542800	2.76318000	-3.08370400	H	-1.11775700	1.51408600	1.93973900	H	-2.89515300	-3.27974800	2.43286600
H	-4.56047100	1.93532500	-1.94857200	C	-1.00305600	0.59815800	-0.89109700	C	-2.35079500	2.65649700	-1.75607300
H	-0.28288100	1.92912300	-2.44435900	Ru	0.76257900	-0.22981200	-0.19231200	H	-2.35257000	3.58338000	-2.33778000
C	2.43996200	0.67079500	-1.22035700	C	-0.68057500	-2.24111600	-2.00071500	H	-4.45817400	2.80211800	-1.25996800
C	1.76683600	1.63368200	-0.41276500	H	-0.51445900	-3.12667900	-2.64786500	H	-0.26849700	2.30077100	-2.12530800
C	1.56095800	1.44924300	0.98744600	H	-1.20048700	-1.48692200	-2.63476300	C	2.22993600	0.49207200	-1.44853900
C	2.00489500	0.20118100	1.51197700	H	-1.43932600	-2.57247300	-1.24716400	C	1.85535200	1.24274400	-0.29697800

C	1.84989700	0.67826700	1.01564600					C	0.99325200	-2.37224600	-1.00665500
C	2.09442600	-0.71437000	1.09185200					C	0.69666700	-1.55818300	-2.13308700
C	2.47037300	-1.50063000	-0.03701800	α -8 _a				H	1.17074600	0.35023200	-3.09053000
C	2.51623700	-0.90465900	-1.32511500					H	2.96119600	0.95587900	-1.48187300
H	2.24066500	0.96626900	-2.43228900	N	0.62304600	1.56471400	0.81137000	H	2.36558100	-2.76599000	0.64381400
H	1.56573500	2.29064800	-0.43017400	C	-0.17001600	2.52845600	0.08262300	H	0.39053300	-3.26460700	-0.81645400
H	1.98274000	-1.20983800	2.06225600	C	-1.24468400	1.93784800	-0.69015000	C	-0.32396700	-1.96949000	-3.13975500
H	2.66021900	-2.56979400	0.07671000	C	-2.34841300	2.68950600	-1.11913100	H	-0.84438800	-1.11117300	-3.58181300
C	2.85871400	-1.71361600	-2.53383800	H	-2.35771500	3.76676600	-0.93228400	H	0.17861900	-2.50765000	-3.95892100
H	2.58116300	-2.76732200	-2.40494400	C	1.28652200	3.80701900	1.13844200	H	-1.07236500	-2.65124300	-2.71661200
H	2.34353900	-1.33567600	-3.42568300	C	-3.41115900	2.05109800	-1.74391400	C	4.14001800	-0.70592100	0.48653200
H	3.94079100	-1.67505900	-2.73380300	C	1.73884700	2.35233300	1.35440300	H	4.76167300	-1.60508400	0.31486600
C	1.51628900	1.50284900	2.23758200	C	-2.25635300	-0.07348500	-1.50876800	C	4.97595000	0.48332300	0.04147300
H	1.46250200	0.79731000	3.08664700	H	0.95414200	4.28956300	2.07512300	H	4.46814900	1.44343100	0.21750200
C	2.63324000	2.49980700	2.53360400	H	1.92611300	2.09108800	2.40431800	H	5.92034500	0.51827500	0.60129500
H	2.73013300	3.23792200	1.72229700	N	0.17694000	3.75125000	0.20734500	H	5.22981100	0.43531300	-1.02658800
H	2.43591300	3.05832400	3.46017300	H	2.65617900	2.12730200	0.78909500	C	3.84334500	-0.65602700	1.97994000
H	3.60772700	2.00303000	2.64148400	H	2.09309700	4.44479800	0.74599900	H	3.37406400	-1.58145600	2.33972500
C	0.16488600	2.19754400	2.12885000	C	-3.36713200	0.66340000	-1.91761600	H	4.76595800	-0.51393000	2.56042400
H	-0.64921400	1.47312600	1.98594200	H	-4.22088200	0.14539500	-2.36429800	H	3.16048700	0.17076900	2.22478300
H	-0.05123300	2.78586000	3.03274500	H	-4.28272500	2.62115400	-2.07344000	C	-1.15153000	0.54408400	-0.90622300
H	0.12837800	2.89001600	1.27358600	H	-2.28360500	-1.16031000	-1.61870300	Ru	0.60946500	-0.36941200	-0.29800000
C	-1.10842400	0.74058000	-0.87388400	C	1.44515800	-0.35045700	-2.29877100	C	0.17379600	-1.95042400	2.24199300
Ru	0.53403500	-0.43697800	-0.48782300	C	2.46079800	-0.00970100	-1.37457600	H	0.17784400	-2.92141400	1.69956900
H	-0.10338400	-1.11239200	-1.81646600	C	2.89673500	-0.93303900	-0.35831600	H	-0.32696000	-2.14579300	3.20797800
H	-4.12334400	-1.56862900	0.80023700	C	2.12545600	-2.08635300	-0.17817700	H	1.22523400	-1.71316700	2.46424200

H	0.07399100	1.05074100	1.53356500	H	1.69800300	-0.67989600	3.54719100	H	-5.48295300	-1.51597600	-1.30894800
N	-0.44737600	-0.84315900	1.55058500	H	-0.58178200	-0.02449800	3.34990400	H	-5.56997800	-2.87163100	-0.16810800
C	-4.03242800	0.13932900	1.64283800	N	1.54334400	-1.98717500	1.90115800	H	-5.76666500	-1.20531400	0.41288400
C	-2.64541000	0.19834100	1.69482800	H	-1.14473700	-1.68355400	3.07865000	C	-2.94338100	-2.67383200	-1.01405500
C	-1.84803900	-0.95182800	1.52522900	H	1.02677800	-2.29807000	3.94461800	H	-1.85566200	-2.57550200	-0.88496800
C	-2.52341900	-2.17715900	1.35384600	C	1.47159700	-0.85092800	-3.17783300	H	-3.21699700	-3.72192300	-0.83048300
C	-3.91525500	-2.23767300	1.30981800	H	1.61495800	-0.70039100	-4.25191600	H	-3.17402200	-2.46910200	-2.07055300
C	-4.68221500	-1.08093800	1.44420900	H	3.20043300	-2.14125600	-2.98570200	C	0.19364800	-0.38646600	-1.15199900
H	-4.61374100	1.05713900	1.76663000	H	-0.25370000	0.42542300	-3.11489500	Ru	-1.25094600	0.49605200	0.04626600
H	-2.15101600	1.15863900	1.86825800	C	-2.36240500	1.63900700	-1.42032500	H	2.55145700	-1.98687500	1.76224800
H	-1.94432500	-3.09655100	1.23061700	C	-2.83251400	0.29579800	-1.38208800	C	1.21260400	1.94968800	1.22115000
H	-4.40703100	-3.20413200	1.16558000	C	-3.25204900	-0.30960000	-0.16021400	H	0.59996800	2.29221100	2.07214900
H	-5.77285600	-1.13039300	1.40883400	C	-3.23619500	0.51024300	1.01725200	H	1.47728000	2.81853800	0.58194600
				C	-2.77668600	1.84006700	0.99559400	N	2.19241000	1.07604900	1.58439300
				C	-2.26697500	2.40258100	-0.22166600	C	3.22554200	0.83514700	0.72677500
γ -7 _b				H	-1.97194900	2.05306100	-2.35278700	C	3.33542200	1.31555900	-0.60629600
				H	-2.77764100	-0.30803700	-2.29175900	C	4.27869700	0.00071800	1.19111100
N	-0.27409000	-0.76310200	1.38918300	H	-3.50219800	0.05344200	1.97607100	C	4.42512900	0.98493800	-1.40155000
C	0.82410400	-1.33410500	0.94529300	H	-2.70003800	2.40672000	1.92682100	H	2.53185300	1.92325100	-1.03100300
C	1.10255600	-1.23513600	-0.46563600	C	-1.67103600	3.77232500	-0.23307600	C	5.36601000	-0.31952600	0.38772800
C	2.17658600	-1.86188300	-1.10889000	H	-1.16759600	4.00148100	0.71548000	H	4.22388100	-0.35013600	2.22720000
H	2.87125500	-2.49208100	-0.54497600	H	-0.93830400	3.88578000	-1.04239200	C	5.45340200	0.17015000	-0.91855900
C	1.05174600	-1.49873300	3.19047700	H	-2.44970000	4.53650300	-0.38171500	H	4.46814100	1.35906200	-2.42909000
C	2.36138900	-1.66717100	-2.47203200	C	-3.70311100	-1.74912600	-0.07632000	H	6.16350800	-0.95334000	0.78667800
C	-0.34173800	-0.96454600	2.82794200	H	-3.48830600	-2.07439000	0.95848200	H	6.30634900	-0.08291900	-1.55205600
C	0.40996000	-0.21950400	-2.52810300	C	-5.21140300	-1.83988300	-0.29244800	H	0.37291400	1.43801000	0.50878600

				C	2.81170500	-0.47122900	2.14186600	N	-2.39245800	0.28122500	1.26266200
				C	2.11716600	-1.69101700	1.84984700	C	-4.53484900	2.96857500	1.12327200
$\gamma-7_c$				H	1.62069000	-3.12851200	0.28706900	H	-4.12861000	3.33570500	2.08706900
				H	2.67483700	-1.80490000	-1.54930800	H	-5.27548600	2.18291400	1.36428900
N	0.65654700	1.76477200	0.24503900	H	3.81967500	1.25560200	1.31452500	H	-5.08527300	3.80331100	0.66425600
C	-0.40327200	1.92443300	-0.52123800	H	2.78218000	-0.06180700	3.15422700	O	-3.55225200	2.52333500	0.24251700
C	-0.81703800	0.79355900	-1.31758600	C	1.39427200	-2.42180000	2.93345900	H	-3.11358900	1.70868300	0.64493500
C	-1.85877500	0.81976600	-2.25433100	H	0.92363400	-1.73002000	3.64501200	C	-2.86099400	-0.87947800	0.71543500
H	-2.44376200	1.73203300	-2.40161300	H	0.61575900	-3.08207700	2.53087300	C	-2.27009600	-2.15796300	0.90690400
C	-0.35353500	3.83748900	0.68170600	H	2.09293600	-3.05033900	3.50723600	C	-3.99611800	-0.81353300	-0.13579500
C	-2.15189900	-0.33108600	-2.97369600	C	3.98744200	0.66072700	-1.35445700	C	-2.78910600	-3.28685200	0.28451800
C	0.92210400	3.02001300	0.92695200	H	3.93835900	1.70490700	-0.99386000	H	-1.37662800	-2.25675900	1.52751800
C	-0.37087100	-1.51226700	-1.82065000	C	5.45891400	0.29560900	-1.53268700	C	-4.50831100	-1.94927000	-0.74307600
H	-1.04392000	3.78481300	1.54443900	H	5.56665500	-0.74274800	-1.88204700	H	-4.44373400	0.16813200	-0.31300100
H	1.13687500	2.86169100	1.99610000	H	5.94242200	0.94528200	-2.27596800	C	-3.90920600	-3.19808700	-0.54449100
N	-0.94891400	3.16899200	-0.47236700	H	6.02200100	0.38531900	-0.59280000	H	-2.30697500	-4.25654500	0.44272000
H	1.81507400	3.51118000	0.49569800	C	3.22669300	0.59331500	-2.66900900	H	-5.38293100	-1.86228400	-1.39389900
H	-0.15549900	4.90038800	0.48363900	H	2.16015600	0.82350300	-2.53197300	H	-4.31303200	-4.09059200	-1.02794200
C	-1.40172500	-1.49339100	-2.75886400	H	3.64180400	1.30785400	-3.39296100	H	-0.32111900	-0.14401400	1.50243900
H	-1.64056600	-2.40218400	-3.31849800	H	3.29490600	-0.40156400	-3.13461500				
H	-2.96954700	-0.33269400	-3.69794500	C	-0.05392200	-0.37654900	-1.06149300				
H	0.16867900	-2.45202800	-1.65764900	Ru	1.34349600	-0.19806100	0.45492700	I			
C	2.15704700	-2.20602200	0.52232900	H	-1.97694200	3.19735500	-0.51369800				
C	2.76494400	-1.45060900	-0.51898200	C	-1.30428400	0.18880200	2.09201600	N	0.66331200	1.30040900	0.89909000
C	3.37533100	-0.18469700	-0.26204100	H	-1.02697900	1.15097600	2.55223000	C	1.91533200	1.15310400	0.56661900
C	3.40398000	0.26567900	1.09991800	H	-1.32767900	-0.60220800	2.87027600	C	2.23676100	0.09047700	-0.35432900

C	3.53315300	-0.26941300	-0.74510500	H	-4.68560900	0.77115300	-1.69505600	C	-2.78088300	-0.62439600	2.45694000
H	4.40346800	0.23400700	-0.31130100	H	-3.97958100	2.15097000	-0.81687700	C	-1.69291700	3.58393000	-1.36168400
C	1.91549300	3.13440700	1.69372200	H	-3.15604400	1.50005200	-2.24452000	C	-1.39269200	-1.22416000	2.17634300
C	3.70800900	-1.27811800	-1.68493300	C	-0.49084000	-2.47234000	1.91773400	C	0.18537400	2.10540400	-1.80200700
C	0.52977000	2.46751700	1.74833200	H	-1.17311900	-2.86036800	2.70003300	H	-3.60036600	-1.35339700	2.36564300
C	1.29410300	-1.53419400	-1.84331400	C	0.05549200	-3.66574200	1.15147100	H	-1.44596800	-2.15561700	1.57412900
H	1.91219000	4.01372500	1.02674400	H	0.73634600	-3.34275300	0.34787100	N	-2.92891600	0.46330000	1.48523200
H	-0.27430500	3.12285000	1.37971500	H	0.62931800	-4.32195300	1.81997800	H	-0.83529300	-1.47781800	3.09307300
N	2.75162400	2.06740500	1.14551100	H	-0.73911900	-4.27614500	0.69994000	H	-2.83706500	-0.22080800	3.48290600
H	0.25573200	2.16542700	2.77631100	C	0.64504800	-1.73439500	2.61738900	C	-0.55658400	3.25019200	-2.10427500
H	2.27452300	3.46525800	2.67886200	H	0.30327000	-0.85900300	3.18675600	H	-0.25026500	3.88766300	-2.93907500
C	2.58269900	-1.89929800	-2.23697300	H	1.16528400	-2.39903400	3.32151700	H	-2.26948000	4.47714400	-1.61325500
H	2.71543200	-2.68074500	-2.99083200	H	1.38019800	-1.37850900	1.87981700	H	1.04645400	1.86114400	-2.43416300
H	4.71142600	-1.57575000	-1.99623800	C	1.07907600	-0.54534700	-0.87338300	C	2.13405000	-1.11277100	-1.64444100
H	0.44167100	-2.02899900	-2.32051900	H	3.60381700	2.31462800	0.65763300	C	2.55450000	0.01727000	-0.89618000
C	-2.39163300	-0.89580600	-1.10200400	Cl	-0.44884100	1.91929200	-1.82881700	C	2.58424700	0.02144100	0.53256400
C	-1.61317400	-1.79025700	-0.32195400	Ru	-0.73996300	0.15148300	-0.16578900	C	2.15810600	-1.18526600	1.17095000
C	-1.33561100	-1.54937000	1.05966100					C	1.81259600	-2.36181300	0.44871200
C	-1.85818800	-0.33102400	1.59069200					C	1.73031500	-2.30639200	-0.96586200
C	-2.73182900	0.52729500	0.85473400	TS1				H	2.04776200	-1.04910500	-2.73110500
C	-2.97716000	0.27187100	-0.50780000					H	2.76971300	0.94227200	-1.43509000
H	-2.51600900	-1.07532400	-2.17186200	N	-0.73518300	-0.18113500	1.40364800	H	2.06583100	-1.19730200	2.26085000
H	-1.14862100	-2.64319100	-0.82113100	C	-1.68037900	0.67779400	1.03646100	H	1.47878700	-3.25407900	0.98355200
H	-1.58857200	-0.04473200	2.61152900	C	-1.32943900	1.63164900	-0.00221200	C	1.18491900	-3.45443600	-1.74922600
H	-3.10892400	1.44420700	1.31226900	C	-2.09075700	2.76417600	-0.31095100	H	2.00197200	-4.05744600	-2.17315600
C	-3.74294700	1.22669000	-1.35693100	H	-2.98801900	2.98296800	0.27445200	H	0.57809500	-4.12363100	-1.12452700

H	0.56848700	-3.10693000	-2.58878900	N	-0.69006000	-0.85343500	0.75409000	H	2.99038600	0.83019300	-2.06222000
C	2.99732000	1.23080100	1.35029200	C	-1.90417600	-0.23485500	0.86598400	H	2.13024400	2.84533500	-0.87894100
H	3.91492400	0.92328600	1.89033500	C	-2.02041500	1.01113400	0.12636300	C	1.41263100	3.09125100	1.76195700
C	3.34822500	2.43669700	0.49465100	C	-3.22045300	1.72914600	0.02478900	H	0.69943600	3.62224800	1.11425000
H	2.47523400	2.77821000	-0.08401900	H	-4.11319300	1.34962100	0.53169100	H	0.89175600	2.83316700	2.69299600
H	3.66550400	3.27630200	1.12786500	C	-2.22459600	-2.12248100	1.96568000	H	2.21644300	3.80080500	2.01348000
H	4.16754600	2.23359700	-0.20936000	C	-3.25898400	2.91064900	-0.70455500	C	3.46148100	-1.69263300	-1.04828100
C	1.95042700	1.61373600	2.38995100	C	-0.71537600	-1.91449900	1.75389000	H	3.25640000	-1.50504300	-2.11748600
H	1.65061700	0.77265900	3.02966900	C	-0.89957100	2.64394700	-1.22819800	C	4.97242200	-1.81969000	-0.87715000
H	2.32986400	2.40960900	3.04641200	H	-2.59329800	-2.99086800	1.37793700	H	5.23412200	-2.00581900	0.17607200
H	1.03708300	1.97908300	1.89698300	H	-0.18066500	-2.81658900	1.41480200	H	5.37535300	-2.65286200	-1.47135800
C	-0.17714200	1.27479300	-0.73473700	N	-2.86167200	-0.89075400	1.49068700	H	5.49667400	-0.90424600	-1.18631900
Ru	0.62892600	-0.55516300	-0.18258100	H	-0.21700800	-1.58323000	2.68650400	C	2.74425700	-2.97746500	-0.66711000
O	-1.20511500	-1.32764800	-1.11180200	H	-2.48967500	-2.34026500	3.01179200	H	1.65482000	-2.86535200	-0.77223700
H	-3.43493700	0.02627600	0.44101400	C	-2.09159800	3.36077800	-1.33260900	H	3.06785300	-3.81298400	-1.30403700
H	-1.25404000	-2.27505600	-0.94531900	H	-2.11548900	4.28696800	-1.91556500	H	2.95238900	-3.27338300	0.37282300
C	-4.41527000	-1.62821800	-0.77009200	H	-4.18666800	3.48185200	-0.78752800	C	-0.81294600	1.45322500	-0.48257600
H	-5.41818800	-1.31822400	-0.42645700	H	-0.01292900	3.02456000	-1.74716700	Ru	0.87509700	0.31373000	-0.11444600
H	-4.13873600	-2.52328000	-0.16800900	C	2.09347000	0.64282400	1.74135400	H	0.40029900	-0.34205900	-1.54478200
H	-4.53437600	-1.97489500	-1.81350000	C	2.57569800	-0.52197000	1.05366000	H	-1.14443300	-1.54384200	-0.63823600
O	-3.50463700	-0.58839000	-0.67951700	C	2.94846500	-0.48097000	-0.30556100	O	-1.67077900	-1.84324400	-1.49797800
H	-2.28127700	-0.94487800	-0.93028500	C	2.77594000	0.77223500	-0.99181200	H	-1.38362800	-1.15299600	-2.12098000
				C	2.28648400	1.91951900	-0.31807700	H	-2.77081300	-1.71381500	-1.23206100
				C	1.95368200	1.87947200	1.08032800	C	-4.87147900	-2.64957100	-0.80846100
TSa				H	1.77151000	0.55404700	2.78245000	H	-5.07406500	-2.89199800	-1.85942800
				H	2.60785900	-1.47251100	1.59326600	H	-4.46727300	-3.54834300	-0.31428100

H	-5.82578200	-2.38958800	-0.33043600	C	2.27552200	0.83130000	-1.21211200	C	-0.45486000	-1.77501500	-2.57415800
O	-3.98471700	-1.55414300	-0.75651900	C	2.34418200	1.19504200	0.16802200	H	0.54311500	-2.21821200	-2.69047900
H	-3.79840500	-1.23900600	0.21546600	C	2.61754200	0.07769400	1.02447600	H	-1.18242200	-2.44229600	-3.06929500
				C	3.46528300	-1.02040500	0.56791600	N	-0.74119500	-1.62686200	-1.16301000
				C	3.40156200	-1.35587400	-0.74549500	C	-2.08645100	-1.43467000	-0.82991800
γ -TS5 _d				H	2.35822100	-0.81250000	-2.61176000	C	-3.01211600	-0.84813700	-1.71292200
				H	1.98947400	1.57051700	-1.96440800	C	-2.55100100	-1.82367000	0.44224400
N	-0.41789900	-0.03481200	1.57908900	H	2.53459200	0.24939500	2.10422500	C	-4.32950600	-0.62214200	-1.32183900
C	-1.34949800	0.87571200	1.48924800	H	4.04689500	-1.60159400	1.28785000	H	-2.68878600	-0.53571400	-2.70806800
C	-1.47180100	1.57247300	0.23408200	C	4.07507700	-2.53134800	-1.35242700	C	-3.86839000	-1.59850800	0.82491700
C	-2.49125700	2.48397800	-0.07107200	H	4.71827500	-3.05559300	-0.63405200	H	-1.84940700	-2.31084700	1.12609800
H	-3.21919900	2.77473900	0.69323000	H	3.32178200	-3.25080800	-1.71306800	C	-4.76962900	-0.98603500	-0.04993500
C	-1.76433500	-0.07111800	3.51322500	H	4.68738300	-2.25530300	-2.22564800	H	-5.02140800	-0.15027800	-2.02480600
C	-2.58914300	3.00340400	-1.35551100	C	2.18465700	2.59100600	0.73309600	H	-4.20417600	-1.92623800	1.81383500
C	-0.43004900	-0.56243900	2.93448800	H	1.37490800	2.53677400	1.48699200	H	-5.80620900	-0.81533000	0.24962100
C	-0.64533800	1.69953900	-2.01428300	C	3.46724000	3.00039700	1.45618300	H	-0.46158800	-0.81883400	-3.12869600
H	-2.54131400	-0.85439700	3.45183600	H	4.31554800	3.04503000	0.75576100	C	0.97787300	-3.34345400	1.36376700
H	-0.33474900	-1.65702200	2.94574500	H	3.36340100	3.99586000	1.91148500	H	1.30612600	-4.38786000	1.18314900
N	-2.08132500	1.05070100	2.63441400	H	3.74012400	2.29536200	2.25343600	H	1.67424700	-2.93111800	2.12421200
H	0.43355600	-0.16517500	3.49969600	C	1.80874500	3.64418500	-0.29466100	H	-0.01711500	-3.42345100	1.85912700
H	-1.69068500	0.24199100	4.56433200	H	0.85760500	3.42831400	-0.79678400	O	0.97578100	-2.59110100	0.21347400
C	-1.67264900	2.59052200	-2.32762600	H	1.71177600	4.62972500	0.18258700	H	-0.04483300	-2.38865400	-0.44153500
H	-1.75587400	2.97865700	-3.34714200	H	2.58596000	3.73954000	-1.06954200				
H	-3.38101100	3.71192900	-1.60710600	C	-0.49177500	1.18082000	-0.71846700				
H	0.05252000	1.41212400	-2.80771000	Ru	0.81109200	-0.28105100	-0.13428200	TSc			
C	2.49734300	-0.53390100	-1.56146800	H	-3.05145700	1.32701400	2.53542100				

N	0.64302500	1.12251100	0.76774400	H	-2.34802400	-1.47296300	-2.07541800					
C	2.00953700	1.05762000	0.75314000	H	-0.87863300	-3.21081500	-1.06730900					
C	2.53062300	-0.10953500	0.06527000	C	-0.03407800	-3.41282900	1.54063300	TSb				
C	3.90334000	-0.35053800	-0.08012800	H	0.79577200	-3.63599100	0.85442000					
H	4.61252900	0.35761600	0.35900600	H	0.39936400	-3.07970000	2.49207400	N	1.26493500	2.29700300	-1.07879600	
C	1.65329100	2.99006000	1.77245000	H	-0.56918500	-4.35708300	1.72642700	C	1.85125500	1.51411300	-0.09021300	
C	4.33455300	-1.47676500	-0.76932900	C	-3.59258500	0.66123500	-0.84152200	C	2.45848700	0.20861800	-0.46192700	
C	0.29202000	2.26309700	1.60114200	H	-3.43784800	0.58873400	-1.93302000	C	3.84080300	0.01887700	-0.52118000	
C	2.01752700	-2.09480100	-1.17714700	C	-5.04835600	0.30804700	-0.55099700	H	4.51095700	0.85138100	-0.28805200	
H	1.65272300	4.01307900	1.34824000	H	-5.25894800	0.36919700	0.52803700	C	1.10973900	3.27794300	0.99350500	
H	-0.49814000	2.87982200	1.13276800	H	-5.74027100	0.99243800	-1.06347800	C	4.35027600	-1.22824800	-0.88320100	
N	2.66028100	2.15008300	1.11425000	H	-5.28997600	-0.71498900	-0.87203200	C	0.46623700	3.30660500	-0.40258900	
H	-0.12775900	1.93181500	2.56870300	C	-3.27641500	2.09150800	-0.43360600	C	2.09047600	-2.09005800	-1.07336400	
H	1.90680100	3.13234400	2.83629900	H	-2.22560400	2.33622500	-0.64922000	H	1.85201200	4.08937800	1.10605900	
C	3.38284600	-2.34541700	-1.31684700	H	-3.91650700	2.80622300	-0.97107000	H	0.53247000	4.28733700	-0.89583500	
H	3.71458100	-3.23101900	-1.86810700	H	-3.44293400	2.26226600	0.64127600	N	1.79337700	1.99367600	1.10861300	
H	5.40138500	-1.68216500	-0.88591700	C	1.53755800	-0.97723800	-0.47020000	H	-0.60497600	3.01866800	-0.37484400	
H	1.30887500	-2.78961000	-1.64132900	Ru	-0.44151000	-0.46892700	-0.09649300	H	0.38299500	3.42001800	1.80851100	
C	-1.44730900	-1.31263200	1.73071500	H	-0.18381800	0.36723200	-1.49058300	C	3.47238900	-2.27508700	-1.16760800	
C	-2.28153100	-0.30763000	1.13956600	H	0.82295400	1.79701300	-0.69195600	H	3.87000900	-3.25162200	-1.45901200	
C	-2.67132900	-0.36033800	-0.21595300	O	1.42454500	2.48977200	-1.27190800	H	5.43000100	-1.38161400	-0.94539800	
C	-2.12966400	-1.43397600	-1.00489500	H	2.17137400	2.62747800	-0.57952900	H	1.42253400	-2.93200000	-1.28622800	
C	-1.29359200	-2.42394600	-0.43185400	C	0.73758400	3.66935300	-1.69385800	C	-1.08373600	0.15153600	1.89635500	
C	-0.94465700	-2.38272000	0.96124800	H	0.31208700	4.21497800	-0.84126800	C	-2.15322600	0.43212200	0.98820200	
H	-1.13921600	-1.21108800	2.77452900	H	1.44502300	4.30641900	-2.23446000	C	-2.49203800	-0.49072600	-0.02209500	
H	-2.59534300	0.54041400	1.75583500	H	-0.06048900	3.35325800	-2.37286800	C	-1.74183000	-1.72008200	-0.07370600	

C	-0.72429000	-2.00421100	0.89395100	α -TS2 _a				H	-0.09703600	-1.03860400	-2.74690300
C	-0.40216400	-1.08880300	1.94065900					H	1.88147300	0.33610600	-2.15659600
H	-0.74748900	0.94854800	2.56661300	N	-0.18613800	1.65901800	0.05322800	H	2.41642100	-1.92879800	1.47406300
H	-2.62580700	1.41618300	1.01451200	C	-1.49541600	1.94642900	-0.40799000	H	0.42790100	-3.32456000	0.90898800
H	-1.93953400	-2.43647200	-0.87603600	C	-2.44607500	0.87299900	-0.15443700	C	-1.09997300	-3.19753100	-1.40005400
H	-0.13703500	-2.92198200	0.78875900	C	-3.83336200	1.05664400	-0.19129400	H	-1.91405100	-2.59828400	-1.82765400
C	0.71343300	-1.34566900	2.89761800	H	-4.22888500	2.03156200	-0.48958900	H	-0.78097700	-3.91945700	-2.16760400
H	1.46852200	-2.00952200	2.45483300	C	-0.41488100	3.79165800	-0.90304100	H	-1.50306700	-3.77156300	-0.55794500
H	1.21759400	-0.40961100	3.17214800	C	-4.67327500	0.00923600	0.16971000	C	3.76251300	-0.10353000	-0.10502400
H	0.35668400	-1.82191700	3.82416200	C	0.63526700	2.74535900	-0.48186600	H	4.51599500	-0.91312800	-0.05235300
C	-3.56696600	-0.23528200	-1.05124100	C	-2.73444100	-1.38891900	0.59594700	C	4.19373600	0.83485100	-1.21985600
H	-3.24069300	-0.76143000	-1.96590300	H	-0.48536100	4.62045800	-0.17480700	H	3.51634900	1.69822500	-1.30896100
C	-4.87974400	-0.86351500	-0.59048300	H	1.35559700	3.11238800	0.26543600	H	5.19639500	1.23613300	-1.01884500
H	-5.24858300	-0.37947700	0.32670700	N	-1.68647100	3.09038200	-0.95431100	H	4.23029900	0.33479300	-2.19797000
H	-5.66001900	-0.75868000	-1.35751900	H	1.22231700	2.39672400	-1.35117200	C	3.77935100	0.61593900	1.23516300
H	-4.76761800	-1.93519200	-0.37334300	H	-0.18507300	4.26419200	-1.87085800	H	3.51871800	-0.04615900	2.07164400
C	-3.73951300	1.23207800	-1.40122000	C	-4.11881000	-1.20542800	0.58388800	H	4.77255700	1.03733800	1.44645900
H	-2.78276100	1.68766700	-1.69496100	H	-4.77480300	-2.01959900	0.90628400	H	3.05436800	1.44439800	1.23325500
H	-4.44086300	1.35190400	-2.23829500	H	-5.75782700	0.14023900	0.15208900	C	-1.86816100	-0.36456600	0.19939800
H	-4.14945000	1.81208800	-0.56028600	H	-2.33254900	-2.34749200	0.93837700	Ru	0.21358700	-0.46065800	0.10650000
C	1.55757800	-0.84864500	-0.70971100	C	0.48570400	-1.28692200	-1.85733500	C	0.84590500	0.42918500	3.11505200
Ru	-0.30414500	-0.21627900	-0.14210900	C	1.62850500	-0.51034300	-1.51259600	H	1.33008300	-0.55233100	3.27240400
H	-0.40174600	0.05120200	-1.75948200	C	2.44523500	-0.80195800	-0.38158700	H	0.35193900	0.69212500	4.06819100
H	0.91400800	1.83727800	-1.91355800	C	1.92085700	-1.77319200	0.50975000	H	1.65502500	1.16874200	2.95541900
				C	0.77705900	-2.56973400	0.20134700	O	-0.08211000	0.39159600	2.08391100
				C	0.06600700	-2.35261000	-1.01005300	H	-0.15293600	1.35152500	1.26823500

				C	2.33518200	1.91261900	-0.21249100	C	-5.09355700	-2.46675600	-0.33713000
				C	1.99791900	1.83075300	1.18338700	H	-4.76009900	-3.37355600	0.19558000
TSd				H	1.82327900	0.45427600	2.84404400	H	-6.00705100	-2.09853500	0.15374600
				H	2.72901400	-1.51701200	1.61509900	H	-5.35952300	-2.75238400	-1.36373900
N	-0.61554100	-0.87954900	0.78697600	H	3.08591500	0.88970900	-1.97829200	O	-4.10947500	-1.46497900	-0.38324900
C	-1.78372400	-0.22207100	1.02462000	H	2.15440600	2.84761000	-0.75066000	H	-3.82278100	-1.15600500	0.55202700
C	-1.90416300	1.03892300	0.30254900	C	1.42232800	3.01051000	1.89266600	C	-1.99466200	-0.64533300	-2.63649900
C	-3.08945000	1.78347600	0.24888300	H	0.70316700	3.54291900	1.25266100	H	-2.47600700	-1.18141000	-3.46164100
H	-3.95940100	1.44175900	0.81852200	H	0.89785600	2.71415500	2.81032900	H	-2.58229000	0.23544200	-2.34733700
C	-2.09831300	-2.12658500	2.08954300	H	2.20643800	3.73114300	2.17327200	H	-0.98045300	-0.33951000	-2.90981700
C	-3.14590000	2.93792500	-0.52492200	C	3.63318900	-1.62741100	-1.03263400				
C	-0.61257900	-2.00903000	1.70464600	H	3.27289000	-1.50479100	-2.06996900				
C	-0.82768100	2.59555100	-1.17459200	C	5.15701200	-1.54160900	-1.05464600	γ -TS5 _a			
H	-2.59124800	-2.94926200	1.52807700	H	5.57182300	-1.65619400	-0.04122400				
H	-0.19555300	-2.91915900	1.24301700	H	5.59434400	-2.33090900	-1.68342800	N	-1.23770100	1.51822400	-0.33288500
N	-2.70753400	-0.84411600	1.72821700	H	5.50633900	-0.57403000	-1.44249700	C	-0.39647600	2.40575000	0.14514800
H	0.02055600	-1.78921200	2.58764100	C	3.16040100	-2.98406800	-0.54016500	C	0.44533900	2.00875700	1.25220800
H	-2.25145600	-2.36476100	3.15400500	H	2.06310200	-3.02740500	-0.48227200	C	1.24801200	2.89382500	1.97996000
C	-2.00981800	3.33499700	-1.23983100	H	3.49789000	-3.78428700	-1.21379800	H	1.27255300	3.95305200	1.71020100
H	-2.04941900	4.23755300	-1.85808000	H	3.56111900	-3.22072500	0.45754400	C	-1.13080900	3.40073500	-1.73234900
H	-4.06411500	3.52814900	-0.57470900	C	-0.72514200	1.42910100	-0.39362400	C	2.00555100	2.41029600	3.04084600
H	0.03563600	2.93613500	-1.75757900	Ru	0.95750300	0.27160300	-0.06112800	C	-1.96453700	2.15001100	-1.42603800
C	2.15529900	0.57898400	1.80953400	H	0.51017500	-0.43348200	-1.47233700	C	1.16266600	0.17179200	2.61476400
C	2.67601900	-0.55556100	1.09816500	H	-1.19083200	-1.27338300	-0.81791600	H	-0.42413000	3.22249600	-2.56012300
C	3.06164000	-0.46586000	-0.25430100	O	-1.89176900	-1.56240600	-1.52700800	H	-2.08040800	1.47380000	-2.28832100
C	2.85838800	0.79765200	-0.91282300	H	-2.83669700	-1.61587500	-1.03693800	N	-0.35584600	3.60144100	-0.50292900

H	-2.98865500	2.41173100	-1.09905000	C	-4.44110600	0.68401000	0.63327500	H	3.85454200	2.46874100	-1.28922800
H	-1.74864800	4.27557600	-1.97811700	H	-3.58516200	1.32189500	0.89594800	O	1.76597900	2.39612900	-1.40809200
C	1.95097800	1.05060300	3.36103000	H	-5.22777100	1.32450400	0.21072400	H	1.28110400	1.05486000	-1.20993000
H	2.54111200	0.66777500	4.19879300	H	-4.84555000	0.26469200	1.56703000				
H	2.63483900	3.08728900	3.62268300	C	0.39099900	0.62558300	1.53701400				
H	1.18619700	-0.89122300	2.87843300	Ru	-0.72925000	-0.48745000	0.18589000	α -TS3 _a			
C	-1.16196500	-1.90685800	1.71914300	H	0.64687200	3.75010200	-0.73157300				
C	-2.36714800	-1.22848000	1.39657300	C	0.46558100	-0.16181600	-2.64753800	N	-0.45974800	-1.46046400	0.94876300
C	-2.81063200	-1.17214500	0.04116400	H	1.27335100	-0.01003300	-3.38302700	C	-1.84224700	-1.01863500	0.81928800
C	-2.07921800	-1.87917600	-0.95733500	H	-0.00325200	-1.13684300	-2.85134000	C	-2.13468100	-0.36331100	-0.44249400
C	-0.86476000	-2.51742600	-0.60644100	N	0.96851600	-0.04046400	-1.28311800	C	-3.44396500	-0.16394100	-0.90032000
C	-0.38413500	-2.58594500	0.73783500	C	2.13358700	-0.81309600	-1.02427600	H	-4.27909500	-0.52424800	-0.29336700
H	-0.78669300	-1.85258500	2.74495900	C	3.01132700	-0.37699000	-0.01724100	C	-1.79720600	-1.88449400	2.84941300
H	-2.89649500	-0.67683000	2.17433800	C	2.46445300	-1.96683100	-1.75128100	C	-3.65491300	0.48263500	-2.11166600
H	-2.39665600	-1.82965800	-2.00224300	C	4.14932000	-1.11081900	0.29175500	C	-0.33700100	-1.78180100	2.38384300
H	-0.23116700	-2.93658200	-1.39611900	H	2.80092000	0.56744800	0.48719800	C	-1.25347900	0.74491800	-2.38038000
C	0.85659600	-3.32893400	1.10197700	C	3.61600400	-2.69213200	-1.44026200	H	-2.13902500	-2.93053200	2.94472700
H	1.54743700	-3.40921200	0.25385800	H	1.83069000	-2.30396100	-2.57483400	H	0.25272600	-2.69741400	2.51881500
H	1.39650800	-2.84116200	1.92499100	C	4.45623500	-2.28030200	-0.40919100	N	-2.58876900	-1.21294900	1.83453900
H	0.61405900	-4.35159600	1.43080500	H	4.81863800	-0.75060800	1.07761100	H	0.19234800	-0.96421600	2.89644500
C	-4.05487800	-0.40838400	-0.35088600	H	3.85720300	-3.58770800	-2.01913300	H	-1.96147900	-1.42327500	3.83549700
H	-3.83487600	0.06512200	-1.32480900	H	5.35587900	-2.85091100	-0.16815300	C	-2.55410400	0.92551700	-2.85356900
C	-5.20647600	-1.38890800	-0.56299500	H	-0.28616600	0.61713900	-2.81825900	H	-2.71533200	1.42297800	-3.81471900
H	-5.44807600	-1.91890100	0.37083200	C	2.99517900	2.35360900	-1.99719000	H	-4.66944900	0.63759900	-2.48578400
H	-6.11457500	-0.86157500	-0.88775300	H	3.20687900	1.39199200	-2.53424800	H	-0.41833300	1.11643300	-2.98560700
H	-4.97080800	-2.14842500	-1.32136800	H	3.14654800	3.14357800	-2.77069500	C	2.31616700	1.02631100	-1.24603300

C	1.35651700	1.89855400	-0.67031700	H	0.88714800	-1.45138100	-1.24473200	H	-2.90496700	-0.08689600	1.43861100
C	1.06260700	1.90023000	0.73177300	H	-0.19397600	-2.53445600	-2.40167500	C	-0.95329700	-0.84524700	0.86915200
C	1.75209800	0.92181600	1.50004700	H	1.55718100	-3.07268600	-2.04686800	Ru	-1.14587500	-0.57258900	-1.06982900
C	2.74897200	0.05914400	0.95886400	O	0.13153600	-3.58356800	-0.66166200	C	-3.20208300	-1.22098300	-1.15545000
C	3.01155800	0.07040500	-0.43170000	H	-0.36770200	-2.34402000	0.39537400	H	-3.54832300	-1.58538900	-0.16470400
H	2.48142900	1.04065600	-2.32575900					H	-3.66154700	-1.80803400	-1.98059700
H	0.78308700	2.54304300	-1.34041500					H	-2.00111200	-1.97423800	-1.29907800
H	1.50497900	0.81474000	2.56012400	α -TS3 _b				O	-3.09147300	0.07660800	-1.33551600
H	3.23473300	-0.68019900	1.59939700					C	-0.45766900	2.46715200	1.15867100
C	3.97677700	-0.88812100	-1.04680600	N	0.70256100	-1.80763400	-0.94281500	C	0.88577000	2.06290400	1.07993500
H	4.98763200	-0.45349900	-1.08232500	C	1.26678600	-1.68266900	0.40340300	C	1.42146700	1.55597400	-0.09528100
H	4.03712200	-1.82344500	-0.47574400	C	0.28294800	-1.31609600	1.39306300	C	0.54156900	1.38745700	-1.19686000
H	3.69267400	-1.13683200	-2.07738100	C	0.52125100	-1.38239600	2.77497300	C	-0.79733200	1.81836100	-1.12857100
C	0.05667700	2.84519000	1.36145500	H	1.49577800	-1.73422800	3.12638600	C	-1.31038900	2.38996100	0.06816900
H	0.65319100	3.59058100	1.92481900	C	3.02022600	-2.24249600	-0.82287900	H	-0.83683600	2.87358600	2.10098200
C	-0.76980900	3.60203500	0.33312000	C	-0.47403100	-1.00422700	3.66378500	H	1.52246800	2.18287800	1.95979400
H	-1.35031800	2.91026100	-0.29818800	C	1.89682700	-1.88008100	-1.80728100	H	0.96042900	1.10410600	-2.16980000
H	-1.48535300	4.26878400	0.83280400	C	-1.94886700	-0.48134900	1.79836800	H	-1.39892800	1.89300100	-2.03987700
H	-0.15329500	4.22751500	-0.32709900	H	3.27607500	-3.31783800	-0.84818700	C	-2.72339200	2.86272900	0.12985900
C	-0.86358100	2.14919200	2.35730900	H	1.74710400	-2.59961600	-2.62174300	H	-2.94914600	3.56930600	-0.68321000
H	-0.32075200	1.61761400	3.15129900	N	2.52397200	-1.89315200	0.49535800	H	-3.41776100	2.01963600	0.00035300
H	-1.51459800	2.87996600	2.85684600	H	2.05938100	-0.89377500	-2.26722200	H	-2.94495300	3.36071500	1.08267500
H	-1.51840900	1.42338600	1.85082600	H	3.95920000	-1.70837100	-1.04045200	C	2.90601900	1.32575700	-0.28072600
C	-1.00445000	0.10538500	-1.15559500	C	-1.70850900	-0.55870400	3.16657800	H	3.02239800	0.39464000	-0.86251400
Ru	0.82343100	-0.11796300	-0.20030700	H	-2.49280200	-0.25429400	3.86645000	C	3.50414200	2.45307900	-1.12342500
C	0.52060000	-2.94512100	-1.64683400	H	-0.30087000	-1.05111600	4.74107100	H	3.41261600	3.41886700	-0.60338800

H	4.57320500	2.28052500	-1.31784800	H	1.52873600	-1.98045500	-3.84468700	H	-1.37366500	-2.51841400	1.34610500
H	3.00071600	2.55841300	-2.09519600	H	2.90606700	-3.24057000	-2.19671500	C	0.24512900	-0.60865300	-0.98032400
C	3.67762900	1.15824700	1.01668000	H	-0.14859700	-0.33957000	-3.09722900	Ru	-1.21008500	0.60558900	-0.13843200
H	3.24529500	0.37555200	1.65457700	C	-2.56954000	1.17981700	-1.70348100	C	1.07757200	2.81829900	0.01885300
H	4.72050000	0.87687600	0.81181300	C	-2.68035600	-0.21459000	-1.45726600	H	-0.00232500	1.75688600	-0.49107700
H	3.70907200	2.09668200	1.59181300	C	-3.00144400	-0.74863100	-0.16813100	H	1.29252400	3.08416400	-1.03213900
H	0.22320200	-2.70868800	-0.96486300	C	-3.13572200	0.21329200	0.87191500	H	0.32680800	3.45996600	0.49853700
				C	-3.06977300	1.61853200	0.65124000	H	0.80705300	0.99522400	1.46686400
				C	-2.73772300	2.11841300	-0.63270600	N	1.93893800	2.21916800	0.79929000
α -TS4 _a				H	-2.29708700	1.53418600	-2.70047000	C	2.99299700	1.48575200	0.25124100
				H	-2.44982900	-0.89672500	-2.27881000	C	3.93238400	0.94815300	1.15175700
N	0.10700200	0.21750300	1.56359200	H	-3.29503800	-0.13332300	1.89656400	C	3.14609900	1.19586700	-1.11940200
C	0.84600400	-1.02044100	1.33109100	H	-3.17737100	2.30765000	1.49194900	C	4.98833000	0.16298800	0.70323500
C	1.06149800	-1.32386700	-0.07011500	C	-2.56423900	3.58141100	-0.87641300	H	3.80247900	1.16412900	2.21586000
C	2.00125700	-2.27311900	-0.49287200	H	-1.76281200	3.77412900	-1.60227400	C	4.20285500	0.40899700	-1.56140700
H	2.59712800	-2.79973500	0.25781500	H	-3.48671200	4.02116000	-1.28600400	H	2.40501500	1.54874000	-1.84053000
C	0.69826700	-0.93849300	3.53129100	H	-2.32479800	4.12211700	0.04824500	C	5.13248200	-0.10971900	-0.65756900
C	2.16793200	-2.51310200	-1.85083600	C	-3.13566100	-2.23654800	0.09619300	H	5.70326200	-0.24455700	1.42253900
C	-0.27762500	0.11120700	2.98315800	H	-4.22169300	-2.43151100	0.20471300	H	4.28994700	0.17782200	-2.62656100
C	0.44379300	-0.87280400	-2.34459200	C	-2.62977900	-3.09276300	-1.05528200	H	5.95541800	-0.73519200	-1.01119200
H	1.56225900	-0.48218800	4.04848300	H	-1.56108200	-2.90844600	-1.25079100				
H	-0.22202000	1.09297700	3.47124600	H	-2.74018900	-4.15917600	-0.81617400				
N	1.16873300	-1.67964800	2.37477600	H	-3.18073500	-2.91582800	-1.98921500	α -TS5 _b			
H	-1.31886300	-0.24044600	3.04969800	C	-2.46425500	-2.66696400	1.39539800				
H	0.23015300	-1.61382600	4.26362500	H	-2.84054900	-2.12922400	2.27710100	N	-0.13742400	-0.18426200	1.49021000
C	1.39198600	-1.80290800	-2.77342100	H	-2.63727600	-3.73582800	1.58259800	C	-0.87720700	1.03051900	1.22960600

C	-1.07076700	1.30425900	-0.18428100	C	2.57431200	-3.58076000	-0.76565300	C	-4.41433200	-0.65997300	-1.45687700
C	-2.04984200	2.18145500	-0.66301900	H	1.81880800	-3.77956100	-1.53747500	H	-2.64917900	-1.82142400	-1.81594100
H	-2.70073800	2.69272100	0.05108000	H	3.51374300	-4.04297400	-1.10574300	C	-5.22930100	-0.01245000	-0.52685400
C	-0.76845100	1.01231500	3.43028200	H	2.26919700	-4.09646300	0.15354300	H	-5.51171800	0.42584400	1.57226100
C	-2.18710700	2.36625300	-2.03436100	C	3.07919300	2.24170000	0.12828300	H	-4.65630700	-0.60630600	-2.52233400
C	0.17028800	-0.09851700	2.92861600	H	4.15956500	2.44627100	0.27142300	H	-6.11388700	0.53911700	-0.85262900
C	-0.35211800	0.82372500	-2.42683200	C	2.60529000	3.07526500	-1.05297300	H	-0.12704700	-1.88021500	-0.48585400
H	-1.63743300	0.61189000	3.98220200	H	1.55072900	2.86418300	-1.29233700				
H	0.00627900	-1.07520300	3.40630500	H	2.68164500	4.14563400	-0.81985400				
N	-1.23321400	1.71394900	2.24831300	H	3.20076400	2.90271800	-1.95987000	α -TS _{5a}			
H	1.22909600	0.16773700	3.07527300	C	2.35829100	2.67678600	1.39844800				
H	-0.27155800	1.71073400	4.12223500	H	2.71450100	2.15834500	2.29958100	N	-0.70024800	0.50305000	-1.75004900
C	-1.34223300	1.68056600	-2.91261800	H	2.50777400	3.75050600	1.57539000	C	-0.67035100	1.87837100	-1.40982500
H	-1.45727300	1.81785400	-3.99184700	H	1.27325400	2.50869800	1.31564600	C	0.02840500	2.15485900	-0.16268500
H	-2.95763500	3.03512800	-2.42442400	C	-0.19582900	0.60934300	-1.05019600	C	0.43808800	3.44008100	0.21294200
H	0.29669400	0.30654200	-3.14319800	Ru	1.24375800	-0.56327900	-0.11959600	H	0.19450800	4.28447000	-0.43801200
C	2.65185400	-1.20020900	-1.64068800	C	-0.91562300	-2.66892400	-0.04256000	C	-1.80177800	1.89194400	-3.29503300
C	2.75683100	0.19537400	-1.42372800	H	-1.30139800	-3.09536500	-0.98617900	C	1.15139500	3.61424100	1.39342600
C	2.97807200	0.74886300	-0.12109900	H	-0.26780400	-3.41008100	0.45258700	C	-1.61829600	0.41486400	-2.88663300
C	3.10392900	-0.19680400	0.94618900	H	-0.90052400	-1.02837000	1.35287100	C	1.02427800	1.22668600	1.81892900
C	3.05586700	-1.59925100	0.74361500	N	-1.80485300	-2.07302600	0.82126100	H	-1.26816200	2.13390600	-4.23205100
C	2.76186100	-2.11591400	-0.54481700	C	-2.92226000	-1.43756900	0.31156300	H	-1.20070300	-0.21916800	-3.68344700
H	2.40986000	-1.57636600	-2.63752100	C	-3.76314700	-0.77615000	1.23813900	N	-1.25841100	2.69022200	-2.20886500
H	2.56088100	0.86418900	-2.26435000	C	-3.28109100	-1.35891100	-1.05425000	H	-2.57287300	-0.04713200	-2.57793700
H	3.20947000	0.17230100	1.96960500	C	-4.88909900	-0.07703100	0.82732200	H	-2.85611900	2.15427800	-3.47870400
H	3.12269500	-2.27559600	1.59861400	H	-3.49366300	-0.82860400	2.29715100	C	1.45514100	2.50210400	2.18625500

H	2.03601300	2.63340000	3.10399000	H	-2.70413300	1.95886200	0.15003900	C	-1.56484400	1.09675100	-0.23935800
H	1.48269000	4.61065800	1.69555900	C	0.29140000	1.02341200	0.64154000	C	-2.59101900	1.94190900	-0.68053200
H	1.28936900	0.37428300	2.45514200	Ru	-0.51555000	-0.77840500	-0.00135100	H	-3.43131100	2.17649700	-0.01977300
C	-0.38086200	-2.20143900	1.64296400	C	1.40123800	-2.13585600	-2.04539800	C	-2.06842400	-0.49598800	3.02571300
C	-1.20597000	-1.10100900	1.99492300	H	1.81242600	-3.00037800	-1.49411500	C	-2.52948700	2.48027400	-1.95995900
C	-2.33988700	-0.71447100	1.21802700	H	2.05603000	-1.99413500	-2.92557000	C	-0.58431600	-0.72612000	2.70911800
C	-2.55617500	-1.47295400	0.02788800	H	0.40426800	-2.42659800	-2.41419000	C	-0.43146800	1.31234600	-2.34339100
C	-1.80723800	-2.63923100	-0.29617500	H	0.38465400	0.02607300	-1.84491200	H	-2.66455700	-1.41018300	2.84704100
C	-0.69193400	-2.99417500	0.49330000	N	1.29705800	-0.91837400	-1.26962100	H	-0.28474100	-1.78403800	2.77685300
H	0.49889100	-2.43830600	2.24646900	C	4.14836400	1.26140300	-0.29028800	N	-2.43690400	0.54447500	2.06830400
H	-0.90640900	-0.48553200	2.84644400	C	2.99036400	0.80298000	-0.91250400	H	0.07701500	-0.16593800	3.39818700
H	-3.34863500	-1.16049500	-0.65839900	C	2.51679000	-0.49921000	-0.68865100	H	-2.24660000	-0.18216400	4.06389300
H	-2.03577000	-3.20354300	-1.20367200	C	3.26735700	-1.33827600	0.15226900	C	-1.44598700	2.16109000	-2.78640000
C	0.12708600	-4.19990000	0.17494200	C	4.43022800	-0.88205500	0.76664400	H	-1.39548300	2.58306200	-3.79471700
H	1.18631100	-4.05723000	0.42673500	C	4.87519000	0.42365700	0.55461000	H	-3.31841200	3.14580600	-2.31764600
H	-0.22910100	-5.05222500	0.77437000	H	4.48393900	2.28655100	-0.46787900	H	0.39187700	1.07776000	-3.02703500
H	0.05478900	-4.48909500	-0.88053100	H	2.42152900	1.46318400	-1.57237800	C	2.47115400	-0.66732900	-1.70860700
C	-3.26097000	0.42942900	1.59716700	H	2.91254600	-2.35542200	0.34558500	C	2.62467200	0.54310600	-0.97160600
H	-4.20983700	-0.05449800	1.90473300	H	4.99137800	-1.55015100	1.42578400	C	2.76202500	0.54911200	0.44593200
C	-2.75703400	1.23871800	2.78170300	H	5.78344400	0.78351100	1.04344000	C	2.70359700	-0.72074500	1.09846600
H	-1.78766600	1.71262600	2.55877200					C	2.56672500	-1.94043000	0.39678400
H	-3.46560800	2.04266900	3.02323500					C	2.38239500	-1.91469800	-1.02236200
H	-2.63768400	0.63038300	3.68918200	γ -TS3 _a				H	2.33334200	-0.63510100	-2.79173600
C	-3.58026600	1.35632400	0.43037600					H	2.57744200	1.49435600	-1.51060800
H	-3.92203200	0.82399000	-0.46874000	N	-0.44302600	-0.21609300	1.35645100	H	2.71311600	-0.74138900	2.19338400
H	-4.38001600	2.05764600	0.70595400	C	-1.51419200	0.48327500	1.06713400	H	2.49616500	-2.88454200	0.94090200

C	2.11688100	-3.17802700	-1.77452800	H	-0.29205300	-1.55078800	-0.77165400	H	-3.14974500	2.40712000	0.96378300
H	1.54352300	-3.89190200	-1.16771100	O	-2.60010400	-1.83657900	-0.39092600	C	2.84971300	1.74326000	-1.11726500
H	1.55119100	-2.98509400	-2.69504800					H	3.05266700	2.18676800	-0.11852600
H	3.05928100	-3.67063800	-2.05935800					H	3.17014600	2.42945400	-1.93218700
C	2.90906100	1.82598200	1.24006000	γ -TS _b				H	1.48270100	2.17675100	-1.34734900
H	2.66619000	1.56632500	2.28714100					O	3.07692100	0.46259000	-1.28876100
C	4.35554400	2.31090700	1.20132100	N	-1.00281600	1.23958900	-0.99031600	C	0.96838200	-2.41369700	1.21621700
H	4.65050500	2.58300900	0.17594600	C	-1.48379800	1.46178200	0.20601300	C	-0.42368000	-2.22914600	1.14018700
H	4.49592000	3.20113900	1.83121100	C	-0.57240900	1.29398200	1.30468000	C	-1.03821200	-1.83485800	-0.03774100
H	5.05687700	1.53948900	1.54976700	C	-0.86986300	1.45929400	2.66454300	C	-0.20793200	-1.59828200	-1.16617300
C	1.93993800	2.91480200	0.80296300	H	-1.88717700	1.71721900	2.98030000	C	1.18480400	-1.78283800	-1.09279700
H	0.89785300	2.56756700	0.84690100	C	-3.19992500	2.10639600	-1.15634100	C	1.79303100	-2.20714700	0.12166300
H	2.03580700	3.80307900	1.44318400	C	0.12966700	1.28026400	3.61280600	H	1.41329500	-2.72211400	2.16688200
H	2.12999300	3.24464200	-0.22996100	C	-2.04806400	1.48302600	-1.96718900	H	-1.02390900	-2.40503800	2.03638800
C	-0.45155200	0.75788000	-1.05468100	C	1.72442300	0.76822200	1.84220500	H	-0.67742700	-1.41317200	-2.13864800
Ru	0.92521300	-0.52782400	-0.19781100	H	-3.27285800	3.19524400	-1.32591100	H	1.79216500	-1.77383300	-2.00361700
H	-3.41366600	0.55407000	1.75558200	H	-1.68917200	2.13854500	-2.77638100	C	3.27142600	-2.39130700	0.18861000
C	-1.56521400	-2.49791700	-0.46345200	N	-2.81248900	1.80861200	0.21960400	H	3.62754200	-3.09852500	-0.57609400
H	-1.07688100	-2.93391700	0.44335400	H	-2.35026800	0.53590300	-2.45305300	H	3.78223500	-1.43789800	-0.01338200
H	-1.27797600	-3.01851800	-1.40832700	H	-4.18086000	1.67244800	-1.40269200	H	3.59351600	-2.76413400	1.16950200
C	-5.48694500	-0.14772700	-0.42030600	C	1.42372300	0.94033900	3.19145500	C	-2.53999900	-1.71923100	-0.18188300
H	-6.04887100	-1.03344100	-0.76839800	H	2.21096100	0.80048900	3.93851500	H	-2.73302800	-0.82276600	-0.79866300
H	-4.91197100	0.24101000	-1.28044500	H	-0.08862700	1.40220500	4.67580300	C	-3.09986700	-2.91688600	-0.94837200
H	-6.22500400	0.61612800	-0.13698800	H	2.73794500	0.47808900	1.54494800	H	-2.93830900	-3.85019500	-0.38753500
O	-4.68273000	-0.42498200	0.69022200	C	0.73366600	0.93313400	0.85554100	H	-4.18227100	-2.81372600	-1.11723600
H	-3.96703600	-1.01894900	0.38824600	Ru	1.01127200	0.62064800	-1.06285400	H	-2.61964300	-3.04040400	-1.92967700

C	-3.27170600	-1.52752900	1.13589400	C	2.22114400	-2.14919100	0.71846000	H	-1.89150500	3.24174000	-0.69219800
H	-2.84759500	-0.69860600	1.72098300	C	2.77394400	-1.49694200	-0.42161100	C	-1.49225200	0.16995000	2.12335100
H	-4.33445400	-1.30556600	0.96201000	C	3.43520000	-0.23845500	-0.32712600	H	-1.09537000	1.10694600	2.53491900
H	-3.23231200	-2.43356600	1.76016300	C	3.47047500	0.36464000	0.96600500	H	-1.35959800	-0.71611400	2.76721800
				C	2.94732500	-0.26281200	2.12248700	N	-2.43210600	0.25051500	1.22646900
				C	2.25947500	-1.50838600	1.99307000	C	-4.44948400	3.02891900	1.05298400
γ -TS4 _a				H	1.69221400	-3.09836000	0.60381200	H	-3.97906300	3.38406000	1.99123800
				H	2.63915900	-1.95911300	-1.40415500	H	-5.19867600	2.26551100	1.33511200
N	0.66447600	1.78923200	0.24865600	H	3.88619000	1.37390700	1.05665100	H	-4.99750800	3.87870000	0.62141700
C	-0.35077100	1.93536100	-0.57012400	H	2.98115400	0.24553600	3.08821500	O	-3.52953500	2.55689400	0.11665300
C	-0.76600900	0.77467300	-1.31983800	C	1.60508700	-2.14086500	3.17848900	H	-3.09519200	1.74733200	0.50132700
C	-1.79033800	0.77350500	-2.27730500	H	1.25030000	-1.38588600	3.89256000	C	-2.98175400	-0.91360400	0.69315600
H	-2.34449100	1.69220100	-2.49157300	H	0.74731000	-2.75874800	2.88198400	C	-2.42639100	-2.19793300	0.86698700
C	-0.31751100	3.89955600	0.55004700	H	2.31151800	-2.79393600	3.71365100	C	-4.13116800	-0.78663200	-0.10996700
C	-2.10431900	-0.40792000	-2.93588100	C	4.02598600	0.46119300	-1.52854700	C	-3.02129700	-3.30921400	0.28044600
C	0.92960400	3.06906800	0.88123400	H	4.13135800	1.52453700	-1.24390600	H	-1.49195700	-2.31664100	1.42155000
C	-0.37683000	-1.56451300	-1.67687100	C	5.42129500	-0.08251600	-1.82529300	C	-4.72283200	-1.90384800	-0.68816900
H	-1.04468800	3.89133700	1.38429400	H	5.37602200	-1.14475300	-2.11158600	H	-4.53388100	0.21495500	-0.28139600
H	1.10528900	2.95625500	1.96298100	H	5.89441300	0.46178500	-2.65534800	C	-4.17478300	-3.17269900	-0.49414000
N	-0.87125300	3.19826800	-0.60531600	H	6.08540800	-0.00697600	-0.95261100	H	-2.57004700	-4.29600400	0.41562800
H	1.84815500	3.52003700	0.45936700	C	3.12927000	0.40310500	-2.75642100	H	-5.61573100	-1.78210200	-1.30659600
H	-0.09030200	4.95106200	0.32389800	H	2.12556600	0.79662500	-2.54151300	H	-4.63647200	-4.04963700	-0.95374900
C	-1.39019100	-1.57369000	-2.63448700	H	3.56044200	0.98649900	-3.58210000	H	-0.08162200	-0.27761000	1.39246300
H	-1.64256500	-2.50775800	-3.14535000	H	3.00357300	-0.62569000	-3.12698500				
H	-2.90646000	-0.43004900	-3.67696000	C	-0.03236500	-0.39467500	-0.98164800				
H	0.13329700	-2.50752300	-1.44844700	Ru	1.37202600	-0.16726900	0.52201300	γ -TS5 _c			

				H	-2.67856700	-1.88055300	1.51998300	H	4.87630000	3.82040000	-0.42480800
N	-0.74776500	1.75586200	-0.19381700	H	-3.86767900	1.18999900	-1.32186600	H	3.81824600	3.76285500	-1.84639900
C	0.35465200	1.92353000	0.52342300	H	-2.76487700	-0.07211300	-3.15985700	O	3.31317500	2.46829500	-0.27230600
C	0.80718700	0.78405200	1.29479000	C	-1.30401200	-2.38688200	-2.94699200	H	2.85205700	1.35369800	-0.84379600
C	1.88162400	0.81749300	2.18975400	H	-0.85376000	-1.66843100	-3.64509900	C	2.95776500	-0.81860200	-0.70168000
H	2.47643000	1.72892400	2.29163700	H	-0.50432100	-3.01920500	-2.54107300	C	2.39999100	-2.10263300	-0.90390000
C	0.22352000	3.84767200	-0.63055600	H	-1.96850000	-3.03689900	-3.53718500	C	4.09607900	-0.70840900	0.13388300
C	2.19618100	-0.33025500	2.90808500	C	-4.02258100	0.55921600	1.34922900	C	2.96556800	-3.22039300	-0.30006100
C	-1.05406000	3.01865300	-0.84651000	H	-4.13525300	1.58409500	0.95071800	H	1.50052800	-2.21705800	-1.51404800
C	0.38984100	-1.52555800	1.81009500	C	-5.41690000	0.01598000	1.64962900	C	4.65017300	-1.83476500	0.72218600
H	0.86051500	3.86828700	-1.53392900	H	-5.36333200	-1.00838800	2.04946500	H	4.50130500	0.29219200	0.30806400
H	-1.30599200	2.87391800	-1.91020900	H	-5.92996500	0.63497500	2.39898200	C	4.09233900	-3.10083300	0.51439400
N	0.92231500	3.13836900	0.43800400	H	-6.04937700	-0.01501600	0.75103000	H	2.51471600	-4.20373800	-0.46348800
H	-1.93720200	3.49294700	-0.37749700	C	-3.16411000	0.64629500	2.60116500	H	5.52921700	-1.72654900	1.36354000
H	0.01681400	4.89328500	-0.36013400	H	-2.17072900	1.06029000	2.37764300	H	4.53409000	-3.98437500	0.98076400
C	1.44253600	-1.49433200	2.72527400	H	-3.64297000	1.28660300	3.35475600	H	0.37840700	-0.11690700	-1.53816700
H	1.69809400	-2.39766000	3.28661500	H	-3.01233800	-0.33784000	3.06997400				
H	3.03863000	-0.32812200	3.60350200	C	0.04784000	-0.39100200	1.06260700				
H	-0.14698300	-2.46967700	1.66345400	Ru	-1.36883700	-0.21073200	-0.43861600	γ -TS4 _b			
C	-2.12511400	-2.24089300	-0.54966900	H	1.99137900	3.08587200	0.32767500				
C	-2.76110000	-1.51519200	0.49266600	C	1.33577800	0.25218200	-2.08966000	N	0.13018100	-0.50618200	1.47518300
C	-3.38707100	-0.25207800	0.24459800	H	1.07521200	1.23992600	-2.49742300	C	-0.89683100	0.30464100	1.51382900
C	-3.43076600	0.20780600	-1.11576900	H	1.42083200	-0.47866700	-2.91629800	C	-1.00595100	1.28448700	0.45939500
C	-2.80314900	-0.49784900	-2.15432900	N	2.44005900	0.32116300	-1.25380200	C	-1.98216800	2.28669200	0.39021300
C	-2.07159200	-1.69940000	-1.86611800	C	4.24592400	3.13306900	-1.02813400	H	-2.71917100	2.39896300	1.19216900
H	-1.56800900	-3.15240000	-0.31935400	H	4.95897300	2.44223000	-1.53273900	C	-1.38399900	-1.20170100	3.14442500

C	-2.01434900	3.13546800	-0.70951600	C	3.58747100	1.72322900	0.98572700	H	-6.14212900	1.27402600	-1.08809200
C	0.02764200	-1.43713500	2.58476400	H	4.63270500	1.60532000	1.33412700	H	-0.09101300	-1.30076500	-0.81959500
C	-0.11105900	1.96202200	-1.66267000	C	3.50520200	3.02420200	0.20415400	H	-2.72048400	0.28363400	2.40892700
H	-2.07740800	-1.97705700	2.77980500	H	2.48289200	3.19852600	-0.16801700				
H	0.18166900	-2.47403600	2.24546500	H	3.76564500	3.87628600	0.84668300				
N	-1.73497300	0.09985200	2.57456500	H	4.18846000	3.04412800	-0.65667300	γ -TS5 _b			
H	0.81548700	-1.22582800	3.33236300	C	2.69160100	1.79879000	2.21781400				
H	-1.41536400	-1.18306200	4.24342400	H	2.74007100	0.89306000	2.83804900	N	-0.76797900	1.78777100	-0.18739800
C	-1.07676100	2.96591400	-1.73462900	H	2.97428400	2.64738400	2.85701600	C	0.47682300	1.92247900	0.26262700
H	-1.10416000	3.62936000	-2.60443800	H	1.64137100	1.92955300	1.91487300	C	0.97001600	0.89263800	1.16348500
H	-2.77001200	3.92124800	-0.77744600	C	-0.03374200	1.09476900	-0.56099500	C	2.12000800	1.02504300	1.94895300
H	0.59285800	1.85127700	-2.49536200	Ru	1.30037400	-0.45557000	-0.25887400	H	2.69090800	1.95708600	1.92078900
C	2.57765800	-0.56699000	-2.00652400	C	-1.22266200	-2.36274700	-0.76139800	C	0.37703000	3.57558500	-1.23809400
C	2.91249100	0.58132100	-1.23795800	H	-0.53238100	-3.15860800	-0.44939400	C	2.53035300	-0.04608500	2.73381500
C	3.27930300	0.50295700	0.13906800	H	-1.34516300	-2.28209500	-1.85936300	C	-0.95978300	2.79513900	-1.22464700
C	3.23269000	-0.79873200	0.72013000	N	-2.16694600	-2.03644700	0.08214200	C	0.64815800	-1.36242100	1.93946900
C	2.94999400	-1.97234100	-0.03236900	C	-3.18052700	-1.17318900	-0.30015600	H	0.83847000	3.62860700	-2.23774000
C	2.56790800	-1.86012700	-1.39578200	C	-3.17022800	-0.36434400	-1.45778100	H	-1.19466300	2.31197000	-2.19266600
H	2.27858200	-0.45468900	-3.05128700	C	-4.29015600	-1.06166900	0.56637200	N	1.25174100	2.85759600	-0.31070000
H	2.82650800	1.55991500	-1.71534400	C	-4.22380300	0.50088800	-1.72957000	H	-1.82040300	3.44549600	-0.99502400
H	3.40958800	-0.90414200	1.79496200	H	-2.30078800	-0.37663800	-2.12083600	H	0.23740400	4.61828400	-0.90885000
H	2.92629900	-2.94569000	0.46316100	C	-5.34377700	-0.19884800	0.28416300	C	1.78694600	-1.23190900	2.73440000
C	2.16311900	-3.06261100	-2.18383900	H	-4.30288100	-1.69416100	1.45936200	H	2.11397600	-2.07193000	3.35396900
H	1.80074600	-3.87120600	-1.53601600	C	-5.31956200	0.58964600	-0.86801300	H	3.43572000	0.03223100	3.33975300
H	1.37138100	-2.82154500	-2.90539400	H	-4.18046200	1.13295200	-2.62114100	H	0.10894300	-2.31640300	1.94333100
H	3.01691500	-3.45729500	-2.75589000	H	-6.19538400	-0.14185100	0.96799800	C	-1.91306800	-2.33488700	-0.26112800

C	-2.60006800	-1.52967700	0.68999900	C	1.37196100	0.29940100	-2.10859500	C	-3.65239900	0.66467900	-2.12929300
C	-3.27068300	-0.32783100	0.29789900	H	0.79148800	1.02923100	-2.69471300	C	-0.49440400	0.85893900	2.95879600
C	-3.29500600	-0.00875800	-1.10178200	H	1.62995800	-0.55462300	-2.76391600	C	-1.40280700	-0.24754200	-2.27566800
C	-2.60445600	-0.78393100	-2.04586000	N	2.44250400	0.89727100	-1.45517000	H	-2.28070300	-0.01081000	3.88177600
C	-1.83759100	-1.92306000	-1.62183000	C	3.39699500	0.11343600	-0.86643300	H	0.05366900	0.01570900	3.40240700
H	-1.33287900	-3.19868600	0.07144700	C	3.30102800	-1.29350100	-0.73316400	N	-2.67049700	1.24789500	2.21844500
H	-2.52875600	-1.78483100	1.75057100	C	4.53917600	0.74172300	-0.31021300	H	0.07409400	1.78284500	3.17434500
H	-3.76023200	0.93065700	-1.41659500	C	4.29870600	-2.01887000	-0.08946300	H	-2.09751800	1.73051100	4.21338100
H	-2.54945300	-0.45549200	-3.08681600	H	2.41397300	-1.81470300	-1.10301700	C	-2.62390700	0.06772900	-2.86880700
C	-1.00627200	-2.67978500	-2.60562100	C	5.53081600	0.00493900	0.32066300	H	-2.78485800	-0.15927200	-3.92687600
H	-0.59152600	-2.01727200	-3.37698800	H	4.62139800	1.82892500	-0.39686400	H	-4.60467100	0.90722300	-2.60592200
H	-0.17184300	-3.19786500	-2.11598200	C	5.42485500	-1.38498000	0.43718500	H	-0.63603500	-0.74749100	-2.87661900
H	-1.61136300	-3.44105900	-3.12194500	H	4.18951400	-3.10286100	0.00979900	C	1.93713600	-1.10829800	-1.40463900
C	-3.94718800	0.58725600	1.29133300	H	6.40298800	0.52147400	0.73122100	C	1.72378900	0.29811500	-1.51827000
H	-3.89976800	1.59897800	0.84890000	H	6.20504800	-1.96271400	0.93730900	C	1.94892800	1.17841400	-0.41235400
C	-5.41724400	0.20222300	1.43494700	H	0.57469100	-0.18500100	-1.38706500	C	2.41556200	0.58513500	0.80729400
H	-5.52084500	-0.80694300	1.86245700					C	2.68206700	-0.79803200	0.91992600
H	-5.94529900	0.89835000	2.10180500					C	2.37173500	-1.66628600	-0.16870500
H	-5.94043600	0.20430700	0.46804600	TS2				H	1.63732300	-1.77649400	-2.21385800
C	-3.24326700	0.64346700	2.63739200					H	1.29239600	0.69548300	-2.44109000
H	-2.17464800	0.87643900	2.52376100	N	-0.62154700	0.67185700	1.52595600	H	2.51007700	1.22277500	1.69278000
H	-3.69464900	1.41516900	3.27566200	C	-1.86258900	0.86712600	1.18275000	H	2.95944200	-1.22248600	1.88703500
H	-3.32643700	-0.30650400	3.18700300	C	-2.21290800	0.63247200	-0.19849000	C	2.40518400	-3.14723700	-0.00622600
C	0.22009200	-0.30632500	1.12212300	C	-3.44931700	0.94119800	-0.78364500	H	1.40450600	-3.55218300	-0.23779000
Ru	-1.22994000	-0.28274700	-0.33737400	H	-4.24202200	1.41125600	-0.19207200	H	3.12172300	-3.60022000	-0.70641400
H	2.05221400	2.13422700	-0.85506000	C	-1.94582400	0.95027400	3.45398600	H	2.69381900	-3.44098800	1.01147000

C	1.71902200	2.66976300	-0.47681600	C	-1.89862100	-0.98615900	0.69389400	H	3.27370500	-0.98433100	1.40471900
H	1.36962300	2.96676000	0.52951900	C	-2.14772600	-0.22351400	-0.51744600	C	3.83343800	-0.99470300	-1.29054400
C	3.04480900	3.37928000	-0.74241800	C	-3.43495000	0.04382700	-0.99881000	H	3.47074400	-1.13618000	-2.31701100
H	3.44812400	3.10124100	-1.72816600	H	-4.29775100	-0.34172600	-0.44906800	H	4.86732400	-0.62249000	-1.35701000
H	2.91979300	4.47145800	-0.73320500	C	-1.93863200	-2.03681600	2.62853500	H	3.86608200	-1.97681200	-0.80198200
H	3.80688300	3.12302900	0.00740800	C	-3.58846000	0.78831100	-2.16246700	C	0.21856800	2.64742600	1.63776200
C	0.65477700	3.08688600	-1.47707500	C	-0.46097200	-1.86833200	2.24202700	H	0.86273000	3.34181100	2.21412900
H	-0.29155400	2.55112100	-1.31485600	C	-1.17571900	1.00695800	-2.33752900	C	-0.65802900	3.48940500	0.72242300
H	0.45347400	4.16428000	-1.39896500	H	-2.25999600	-3.09313000	2.60408500	H	-1.28087200	2.85685300	0.06957100
H	0.97155900	2.89990400	-2.51458000	H	0.13531700	-2.78803800	2.31463100	H	-1.33665200	4.11655600	1.31596800
C	-1.15470200	0.03366200	-0.92569400	N	-2.69731600	-1.28480900	1.64452400	H	-0.07577100	4.16686900	0.08283100
Ru	0.59974800	-0.36724100	0.11900500	H	0.02929900	-1.09978100	2.86045300	C	-0.64455200	1.89000400	2.63880600
O	-0.55610600	-2.72127900	-0.43573800	H	-2.15985900	-1.67707000	3.64540200	H	-0.05850300	1.33052400	3.38089400
H	-0.50003100	-2.46108600	0.85920300	C	-2.45591700	1.25786700	-2.83529900	H	-1.27854600	2.58743400	3.20293000
O	-0.26233600	-1.98751900	1.83553000	H	-2.57400900	1.83108700	-3.75954100	H	-1.31568100	1.18138300	2.12879600
H	-3.65707700	1.02678900	2.16290800	H	-4.58622400	0.99941100	-2.55403400	C	-0.98939200	0.26624100	-1.16181200
C	-1.81283800	-3.03922100	-0.87857000	H	-0.31136800	1.39748900	-2.88640800	Ru	0.80783900	-0.11483600	-0.19050100
H	-2.12316500	-4.07043000	-0.59075300	C	2.32569800	1.04512700	-1.21671600	C	0.53022500	-2.76257600	-1.61283800
H	-2.61600000	-2.36646500	-0.49344800	C	1.44108200	1.90160900	-0.51696900	H	0.76571500	-1.59127100	-1.32559600
H	-1.90382600	-2.99789600	-1.98640600	C	1.17263500	1.74359900	0.88022400	H	0.07207100	-2.56932700	-2.61550300
H	0.47601500	-2.51616800	2.15693100	C	1.86968500	0.67558800	1.53346300	H	1.58685600	-3.10821100	-1.75070800
				C	2.79901800	-0.16012000	0.86824300	O	-0.19224800	-3.35736100	-0.71868500
				C	2.97875500	-0.03170100	-0.53579100	H	-0.43618500	-2.35400600	0.18913800
α -TS2 _b				H	2.44596300	1.15439800	-2.29684900				
				H	0.87378100	2.63814500	-1.09010400				
N	-0.53022800	-1.42478300	0.83873600	H	1.65088700	0.46699400	2.58403000	α -TS4 _b			

				C	1.97474000	1.26560300	1.84734600	C	-3.56709000	1.75941200	-0.79163400
N	1.75938200	-1.19876500	-1.53709800	C	2.15929500	1.69484100	0.53534200	C	-4.32370500	-0.47370300	-0.27540700
C	2.31450300	-1.49161100	-0.22451000	C	1.00523300	1.82815700	-0.26837900	C	-4.59393000	2.28681100	-0.02008100
C	1.30268500	-1.87978900	0.73092000	C	-0.27458800	1.63712100	0.26851500	H	-2.89515300	2.41918200	-1.34585800
C	1.60777200	-2.48937900	1.95720800	C	-0.44878700	1.25347800	1.61873000	C	-5.35141200	0.06458300	0.49561500
H	2.65731000	-2.65627900	2.21646500	H	0.59953200	0.70302000	3.41090700	H	-4.25612600	-1.55778400	-0.38913200
C	4.10492500	-0.98711100	-1.42005000	H	2.84149400	1.11290000	2.49488000	C	-5.48960700	1.44406600	0.64270700
C	0.58182200	-2.86941600	2.81052500	H	1.10283600	2.21091700	-1.29152800	H	-4.70715500	3.37162300	0.05385100
C	2.88762100	-0.60639300	-2.27706800	H	-1.15171600	1.91202000	-0.31838600	H	-6.06197400	-0.60939200	0.98171900
C	-1.05574200	-2.03452600	1.21507200	C	-1.81448500	1.09415600	2.19743600	H	-6.30059300	1.85873400	1.24498700
H	4.66523000	-1.84320600	-1.83917900	H	-2.36119900	2.04997200	2.21253700				
H	2.91944400	-0.97912500	-3.30859700	H	-2.43117100	0.40370800	1.60200700				
N	3.58030100	-1.34679700	-0.11346100	H	-1.77585800	0.70967800	3.22490100	N-1			
H	2.74229800	0.48320600	-2.33022200	C	3.50922500	2.14115700	0.01160900				
H	4.83587600	-0.16733700	-1.33679300	H	3.61662500	1.73822400	-1.01230500	C	1.27504100	-1.07207100	-0.87861100
C	-0.74924400	-2.64591100	2.42797400	C	3.53978800	3.66490400	-0.11222600	O	2.55157200	-1.12268600	-0.62150300
H	-1.56112600	-2.94786400	3.09676600	H	3.42370100	4.13813000	0.87484700	H	0.79271400	-2.04911000	-1.16112900
H	0.80528500	-3.34546800	3.76789500	H	4.49402000	4.01096500	-0.53616100	H	1.41928000	0.78932900	0.78716600
H	-2.10630000	-1.84309300	0.96437500	H	2.73179100	4.04551500	-0.75287600	H	0.93831800	-0.34170700	-1.66761400
C	-0.03977800	-1.60288600	0.34192000	C	4.68789000	1.64648600	0.83420600	H	1.62739500	2.25251400	1.30745600
Ru	-0.37782200	-0.48435700	-1.26408800	H	4.65532400	0.55715500	0.98311700	Na	3.77301500	0.37050700	0.07954500
C	-2.13127400	-1.45621900	-1.94007700	H	5.63730500	1.89887600	0.33978200	O	2.10270000	1.52316600	0.90245500
H	-2.50440500	-2.20614400	-1.21709600	H	4.71412900	2.12433500	1.82575500	N	0.45123500	-0.59538400	0.36957800
H	-2.36798200	-1.77797800	-2.97204700	H	1.49451900	-2.08884700	-1.95840000	C	-0.89914600	-0.27976400	0.17974400
H	-0.83042300	-1.78917100	-2.15642300	N	-2.32407500	-0.09880500	-1.68014600	C	-1.93025900	-0.96030600	0.84887800
C	0.69771600	1.03854400	2.37417700	C	-3.38534900	0.36526000	-0.91236900	C	-1.25296900	0.77296400	-0.68583000

C	-3.26286400	-0.59820300	0.66718800	C	-2.78703000	-1.37044900	-0.07827900	H	1.16320400	2.22245900	-0.44971900
H	-1.67296300	-1.78619500	1.51928700	H	-0.76598300	-2.11460900	-0.21208300	C	3.47550300	-0.22190000	0.09609500
C	-2.58669900	1.11769800	-0.87601700	C	-3.02632400	1.01015000	0.12155500	H	3.00389900	-2.29311000	0.50972500
H	-0.45951200	1.32894500	-1.19252800	H	-1.21307200	2.16487700	0.13060400	H	3.58629400	1.88577300	-0.34773700
C	-3.60311800	0.43784500	-0.20131700	C	-3.61335700	-0.25047600	0.04389600	H	4.55743500	-0.36513400	0.12888100
H	-4.04511400	-1.14176700	1.20375100	H	-3.22652300	-2.36885100	-0.15134300	Na	-2.63441300	-0.71501800	0.82028500
H	-2.83666200	1.93901700	-1.55304900	H	-3.65539400	1.90041600	0.20433900	H	-1.57007700	-2.62968200	-1.39669300
H	-4.64893000	0.71549900	-0.34966700	H	-4.69918200	-0.36112000	0.07005300				
H	0.54958100	-1.32722700	1.07245100								

N-4

				N-3							
N-2								C	-1.40979700	-1.36508200	0.59476200
				C	-1.26639900	1.53783300	-0.21094500	O	-2.65900800	-1.65964400	0.09466700
C	1.24158700	1.41059000	-0.27853900	O	-2.67099500	1.41839200	0.13556800	H	-1.43917700	-0.62521800	1.41896300
H	0.97409200	1.78835400	-1.29166500	H	-1.20814000	1.92196600	-1.26008000	H	-0.98417900	-2.29743300	1.01251700
H	0.88661500	2.16428400	0.44562700	H	-0.81113700	2.32661600	0.43513300	H	-1.86575700	0.69024800	-0.81768500
H	2.86322700	0.43514700	-0.69347700	H	-1.38634400	-1.15581400	-0.89387400	H	-0.65369200	-1.36609200	-1.31011300
O	2.82479200	-1.13772000	-0.84328600	O	-2.03666000	-1.92019800	-0.94815900	O	-2.75522000	1.03107600	-0.60632300
H	1.08090600	-0.59281700	-0.57501400	H	-3.12904100	2.21549900	-0.14902100	H	-3.07570800	-0.80264600	-0.11664900
H	3.17114200	-1.57014700	-1.62521200	N	-0.71880100	0.26017400	-0.01181600	N	-0.56264700	-0.81338700	-0.46050400
Na	2.65453500	-0.72200800	1.18703700	C	0.64017000	0.15505600	0.01367900	C	0.74911900	-0.40840900	-0.20381000
O	2.61198500	1.25784100	-0.12844900	C	1.22781600	-1.11660500	0.26793300	C	1.63914900	-0.23295700	-1.27930600
N	0.58555300	0.13361200	-0.01409200	C	1.54673800	1.22582600	-0.21616200	C	1.20574300	-0.12258400	1.09425900
C	-0.80248000	0.03786700	-0.02495300	C	2.60134200	-1.29569200	0.30750100	C	2.93351500	0.22280000	-1.06429900
C	-1.40585900	-1.23286500	-0.11328400	H	0.55853200	-1.96818800	0.43519600	H	1.29683200	-0.45600900	-2.29393900
C	-1.64133500	1.16190000	0.08181800	C	2.92595700	1.03182200	-0.16668700	C	2.50551300	0.34024500	1.29558200

H	0.55084700	-0.26446900	1.95536800	C	3.23545200	0.75620700	0.27511100	C	-2.84266800	1.35825700	0.08863800
C	3.37915200	0.51794000	0.22582200	H	1.73449100	2.01240400	1.19549500	H	-0.83770900	2.13786200	0.24468500
H	3.60391500	0.34855700	-1.91799900	C	2.44260000	-1.30491000	-0.69168100	C	-3.03553400	-1.02445100	-0.13101000
H	2.83825400	0.55569900	2.31394300	H	0.29962800	-1.66819100	-0.49107200	H	-1.20028300	-2.14546700	-0.13179300
H	4.39667700	0.87569600	0.39317700	C	3.49525400	-0.43271600	-0.40586300	C	-3.64682600	0.22451000	-0.04942300
C	-2.61054700	2.15369100	0.22116500	H	4.05228600	1.44554900	0.50344900	H	-3.30057500	2.34812000	0.16433100
H	-2.15292900	3.01029100	-0.30364600	H	2.63843300	-2.24167100	-1.21987100	H	-3.64713400	-1.92572500	-0.22498100
H	-3.60853500	2.46710900	0.55361900	H	4.51443000	-0.68031300	-0.71071500	H	-4.73425600	0.31512400	-0.08424300
H	-2.00527700	1.95265900	1.12417900	H	-0.53396900	1.16763800	1.46693800				

N-TS3

N-TS2

N-TS1

								C	1.27714100	-1.43987800	-0.13177900
				C	1.26129500	-1.35428600	0.31823900	O	2.68680900	-1.27252400	-0.06845400
C	-1.35133200	1.33502900	-0.75971600	H	1.00536700	-1.69987900	1.34867500	H	0.99790700	-1.94885600	-1.08329400
O	-2.58631300	1.34735500	-0.56437600	H	0.86033000	-2.11927100	-0.37473200	H	1.00970300	-2.14137800	0.68290800
H	-0.76133300	2.28292400	-0.70161600	H	2.90005600	-0.21654000	0.67587800	H	1.37772100	0.66642700	-0.66745600
H	-1.08808600	-0.40711600	0.82516600	O	2.98972600	1.07588100	0.81560000	O	2.42019200	1.25003300	-0.99506900
H	-0.89331200	0.62990600	-1.49977400	H	1.00259200	0.64886400	0.61345500	H	2.90125500	-0.65318600	-0.79736600
H	-1.66504300	-2.30380800	1.19581100	H	3.48198500	1.35819300	1.58837000	N	0.66430900	-0.15260900	0.01690000
Na	-3.56752100	-0.53859800	-0.13557200	Na	2.63691800	0.64206500	-1.23615700	C	-0.70838100	-0.07009900	0.00501900
O	-1.98965800	-1.55320400	0.69554000	O	2.60508900	-1.18567900	0.12784600	C	-1.32430800	1.20584300	0.01946500
N	-0.44958900	0.50527300	0.69902000	N	0.56075900	-0.08316900	0.04030800	C	-1.56276500	-1.19671700	-0.01024000
C	0.88117900	0.19867000	0.38531500	C	-0.83171200	-0.01370500	0.04306000	C	-2.70431300	1.34148300	0.03334800
C	1.93713500	1.07709200	0.66478800	C	-1.45950400	1.24422800	0.13549300	H	-0.68296500	2.09324100	0.01538800
C	1.14306400	-0.99651500	-0.30378100	C	-1.64843400	-1.15179000	-0.08027100	C	-2.94826600	-1.04602800	0.00882500

H	-1.13733000	-2.20301000	-0.03709600	C	2.37133800	1.17234100	-0.70372500	C	3.35240200	0.62722000	0.19363000
C	-3.53649800	0.21660200	0.03297300	H	0.38320100	1.83907400	-0.18960500	H	4.00890700	-1.27128300	-0.60212200
H	-3.14272700	2.34377000	0.04425000	C	3.30873800	0.14234200	-0.64555700	H	2.40285200	2.42069700	0.93520400
H	-3.57957100	-1.93935300	0.00013900	H	3.69643800	-1.85817800	0.07592000	H	4.36567200	0.99908600	0.35862200
H	-4.62273300	0.32681900	0.04575400	H	2.61308700	2.09904200	-1.23262200	C	-2.81804800	1.76531500	-0.18819200
Na	2.55420600	0.80696800	1.11301100	H	4.28715600	0.25493700	-1.11781200	H	-2.29448000	2.58202100	-0.72062400
H	2.32065100	1.75983000	-1.80212500					H	-3.88440300	2.05585200	-0.14563900
								H	-2.45340700	1.78601900	0.86405100

N-TS5

N-TS4

				C	-1.36720700	-1.22929700	0.90552500	N-TS6			
C	-1.23744000	0.65534000	1.44590300	O	-2.62941400	-1.38471200	0.59151100				
H	-0.79515100	1.64374700	1.67357200	H	-1.09457100	-0.38763400	1.58964100	C	-1.12339500	1.61114200	-0.37017600
H	-3.44533300	0.11920000	-0.38520600	H	-0.85078300	-2.14355400	1.26287100	O	-2.06086100	1.23102300	1.26971400
H	-2.15743500	0.44861900	2.00486700	H	-1.34207900	-0.01214300	-0.77985100	H	-2.07040800	1.89788100	-0.83340100
H	-4.28819200	-1.15625300	-0.07682300	H	-0.60943100	-1.57900400	-1.06558400	H	-0.50787100	2.44650800	-0.01459000
Na	-1.43778600	-0.71925400	-0.95570400	O	-2.63840000	0.54470600	-0.81917400	H	-1.41992600	-0.38545400	-0.53721300
O	-3.68652300	-0.78409200	-0.72634200	H	-2.87314100	-0.42665800	-0.05406300	C	0.74479600	0.14750000	-0.39103300
H	-2.18836700	2.16839300	-0.10845900	N	-0.56874900	-0.78978900	-0.41923600	C	1.03690900	-1.17615600	-0.02701700
O	-2.14044900	1.20701900	-0.11593400	C	0.76441700	-0.31783700	-0.23879200	C	1.78381000	1.09077500	-0.41526200
N	-0.47404100	-0.38434900	1.16355200	C	1.86172500	-1.12122200	-0.55528900	C	2.33489700	-1.53865000	0.31976400
C	0.76805700	-0.14921800	0.58787500	C	0.95919500	0.95688200	0.30203500	H	0.22360400	-1.90546100	-0.00225300
C	1.72752800	-1.18796000	0.61905700	C	3.15322700	-0.64328100	-0.34510400	C	3.07847800	0.71897100	-0.06405800
C	1.11901500	1.03506900	-0.10559600	H	1.70199000	-2.11964600	-0.97200000	H	1.58011600	2.11548500	-0.73705700
C	2.97266700	-1.04009600	0.02063700	C	2.25316600	1.42292600	0.51721600	C	3.36267400	-0.59538800	0.30655800
H	1.46488500	-2.10665800	1.15069300	H	0.09336700	1.58057200	0.53927000	H	2.54447100	-2.57200100	0.60672800

H	3.87772900	1.46366600	-0.09436000	H	-4.64203600	1.53517900	-2.18879200	C	-1.14500000	0.20894500	-0.96483000
H	4.38083200	-0.88399600	0.57586300	H	-0.52726500	0.56253200	-3.00513300	Ru	0.60166400	-0.49357000	-0.11453900
N	-0.57191900	0.47451500	-0.75654500	C	2.15651600	-0.23361300	-1.58582200	C	-2.86358600	-0.36905500	2.26057500
C	-3.55259700	-1.17336100	-0.42863300	C	1.70490100	1.03397600	-1.10249700	N	-2.04608100	-0.18475300	1.19584800
H	-3.44998800	-1.96794600	-1.18730300	C	1.71846900	1.36155700	0.28242600	H	-3.91308700	-0.09375100	2.21897500
H	-4.31027800	-1.51853400	0.29547600	C	2.13597500	0.32023700	1.16216900	O	0.02038200	-2.39048000	-0.63342000
H	-3.97957000	-0.28762300	-0.94204700	C	2.67186900	-0.92129600	0.70369000	C	-1.27870500	-2.83239100	-0.63871800
O	-2.33657400	-0.91645600	0.20116900	C	2.65887900	-1.21846700	-0.67855700	H	-1.29895800	-3.90901300	-0.90048800
H	-2.31676100	0.14804300	0.89211200	H	2.08010300	-0.46930000	-2.64933700	H	-1.80136100	-2.75681000	0.34376400
H	-1.36246100	1.10229900	1.92593000	H	1.26878300	1.73901200	-1.81561100	H	-1.93481200	-2.32499800	-1.38092800
				H	2.03138500	0.48406100	2.24075800				
				H	2.97391000	-1.68661400	1.42099700				
Ru7-5				C	2.95548800	-2.59252700	-1.16740700	Ru7-TS3			
				H	3.59613200	-3.14588900	-0.47014200				
N	-0.79572100	-0.60961700	1.47456000	H	1.99303300	-3.12835500	-1.25083700	N	0.90537900	-1.26126800	-1.12531700
C	-2.26806500	0.28067900	-0.11970300	H	3.43101900	-2.58142800	-2.15642300	C	0.58894200	-1.37979100	1.18436100
C	-3.51594800	0.75170000	-0.52711100	C	1.25025400	2.68491600	0.84196200	C	0.97823500	-1.61524900	2.50141100
H	-4.35828100	0.79334900	0.16821400	H	0.70938300	2.44635800	1.77763100	H	1.99458900	-1.94552800	2.73477700
C	-2.10366800	-0.93534000	3.26990400	C	2.45188100	3.55280800	1.20826200	C	2.99376900	-2.05606900	-1.40676700
C	-3.67344100	1.16402100	-1.84792800	H	3.03983500	3.80793600	0.31327400	C	0.04544900	-1.42294100	3.51933400
C	-0.81692600	-1.06821400	2.72689400	H	2.13449100	4.49641800	1.67494000	C	1.83993500	-1.55975700	-2.03415600
C	-1.35320900	0.62039000	-2.28829600	H	3.12822600	3.04351800	1.90935500	C	-1.62087900	-0.76794000	1.87880800
H	0.08945700	-1.47853500	3.16578900	C	0.28925500	3.42980400	-0.06925200	H	1.63493600	-1.40336500	-3.09078600
H	-2.43903600	-1.21463600	4.26395800	H	-0.56481000	2.80388600	-0.36601400	H	3.91565600	-2.38427400	-1.87748700
C	-2.59192800	1.09102200	-2.72834200	H	-0.10535600	4.32395100	0.43285700	C	-1.25078000	-1.00584500	3.20265500
H	-2.71802500	1.40219500	-3.76871000	H	0.78555600	3.77752000	-0.98841100	H	-1.98206700	-0.85811600	4.00206500

H	0.33062100	-1.60280800	4.55776500	C	3.25733200	2.74139000	-0.96799600	H	-4.65832800	2.32687700	-1.41908700
H	-2.63354100	-0.41867500	1.65062600	H	3.19067500	3.65017100	-0.35022800	H	-0.44413100	2.07894100	-2.26650900
C	-0.70673900	-0.94160300	0.82662900	H	4.32021600	2.56892600	-1.19334100	C	2.14872700	0.50586000	-1.48151100
Ru	-1.06531700	-0.56050600	-1.06450300	H	2.74594600	2.95472900	-1.91742700	C	1.74318900	1.29574500	-0.36614900
H	3.28820400	-2.35028600	0.811178100	C	3.41056600	1.23061900	1.03004300	C	1.79267600	0.80779800	0.97264300
C	-2.96194800	-1.58152900	-1.07737500	H	2.93714800	0.42137800	1.60664500	C	2.12978800	-0.56172900	1.11873800
H	-3.16159800	-2.03421900	-0.08254100	H	4.44125400	0.92478600	0.79931100	C	2.55129200	-1.38096400	0.03186300
H	-3.34952600	-2.22424500	-1.89756400	H	3.47920300	2.10742500	1.69251300	C	2.53927000	-0.85688100	-1.28817300
H	-1.63627200	-2.08170900	-1.34834900	N	1.44570600	-1.56089800	0.08356000	H	2.10688500	0.92136300	-2.49050200
O	-3.11099200	-0.28279500	-1.21129700	C	2.70517800	-2.04689700	-0.05322400	H	1.37692000	2.31096700	-0.55314400
C	-0.74919100	2.39434900	1.34334400					H	2.05474700	-1.01109900	2.11510100
C	0.62378400	2.13251400	1.19665300					H	2.81815100	-2.42587800	0.20155900
C	1.16227300	1.75764300	-0.02533900	Ru7-6				C	2.92360800	-1.70515100	-2.45616300
C	0.27188000	1.62641100	-1.12249500					H	2.72360900	-2.76685700	-2.26571300
C	-1.10079400	1.88807600	-0.97736200	N	-0.93017700	-1.50306900	0.65193900	H	2.37259700	-1.41405600	-3.35891500
C	-1.63127000	2.28638800	0.27896400	C	-2.35533200	0.10511700	-0.29450900	H	3.99768700	-1.60069800	-2.67397700
H	-1.13418300	2.68127500	2.32636800	C	-3.60002300	0.71368400	-0.45814100	C	1.41272800	1.67290000	2.15273900
H	1.27246900	2.22851900	2.07118100	H	-4.48778000	0.32317700	0.04626800	H	1.46056100	1.02381500	3.04561900
H	0.68665400	1.44142900	-2.11951600	C	-2.32593100	-2.77390400	1.87345900	C	2.42491300	2.79868300	2.34356600
H	-1.74982700	1.93489900	-1.85746100	C	-3.69398100	1.83467800	-1.27798500	H	2.41410700	3.49152900	1.48793800
C	-3.09371700	2.54101500	0.42438500	C	-1.00143200	-2.56277100	1.46400200	H	2.19957000	3.38961700	3.24302100
H	-3.44788200	3.30178200	-0.28778800	C	-1.31803600	1.68383300	-1.73729100	H	3.45035600	2.41556600	2.44149600
H	-3.66188700	1.62490100	0.20345700	H	-0.09900500	-3.12058000	1.70162700	C	-0.00829300	2.21295400	2.04976800
H	-3.35133800	2.87975300	1.43618800	H	-2.70260000	-3.55216300	2.53006700	H	-0.74401000	1.39813100	1.99508900
C	2.64327200	1.54395200	-0.24354800	C	-2.54877800	2.31590800	-1.91750600	H	-0.25671500	2.84205400	2.91700600
H	2.74307300	0.67461700	-0.91931900	H	-2.61950700	3.19260100	-2.56716200	H	-0.14723500	2.82942900	1.14798200

C	-1.16878600	0.55926500	-0.90859900
Ru	0.53861900	-0.48657400	-0.44514500
C	-3.05945100	-1.77553700	1.25596300
N	-2.19131000	-1.02782600	0.52960000
H	-4.12015300	-1.54486400	1.27486300
H	-0.06141600	-1.31929100	-1.69728700