Supporting Information

For

Ruthenium-Catalyzed Deoxygenative Hydroboration of Carboxylic Acids: A DFT Mechanistic Study

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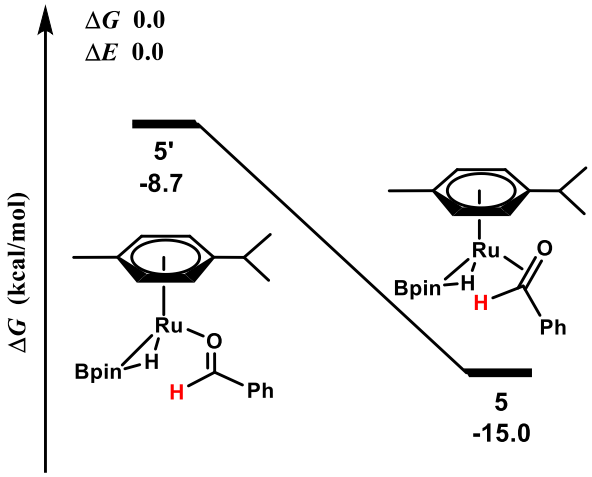
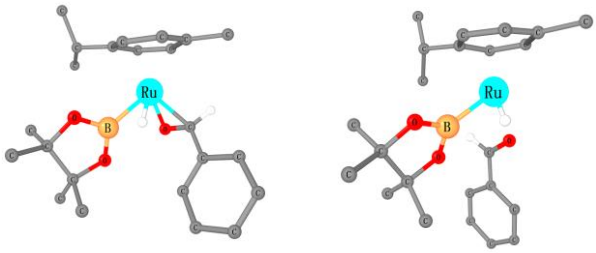


Figure S1. The Gibbs free energy profiles along reaction pathway of intermediate **5** and **5'**. (The numbers are free energies)

As shown in Figure S1, the PhCHO of the intermediate **5** can be coordinated with the central Ru atom in the form of side-on and end-on, respectively. The relative free energy of intermediate **5** and **5'** is -15.0 and -8.7 kcal/mol, respectively. Obviously, intermediate **5** is more stable.



		5	5'
Bond length:	Ru-C	2.14	3.02
	Ru-O	2.11	2.20
Atom distance:	C-H	2.50	3.50
Gibbs free energy:		-15.0	-8.7

Figure S2. The geometric structure diagram and energy of intermediates **5** and **5'** (In this structure, the hydrogen atom on the saturated carbon atom has been omitted.)

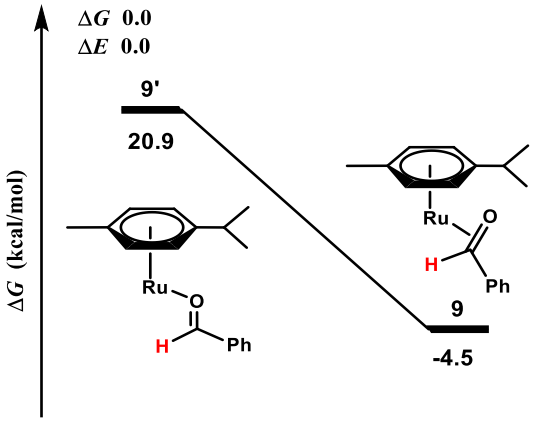


Figure S3. The Gibbs free energy profiles along reaction pathway of intermediate **9** and **9'**. (The numbers are free energies)

As shown in Figure S3, the PhCHO of the intermediate **9** can be coordinated with the central Ru atom in the form of side-on and end-on, respectively. The relative free energy of intermediate **9'** and **9** is 20.9 and -4.5 kcal/mol, respectively. Obviously, intermediate **9** is more stable. At the same time, intermediate **9** can remove PhCHO to form intermediate **11**.

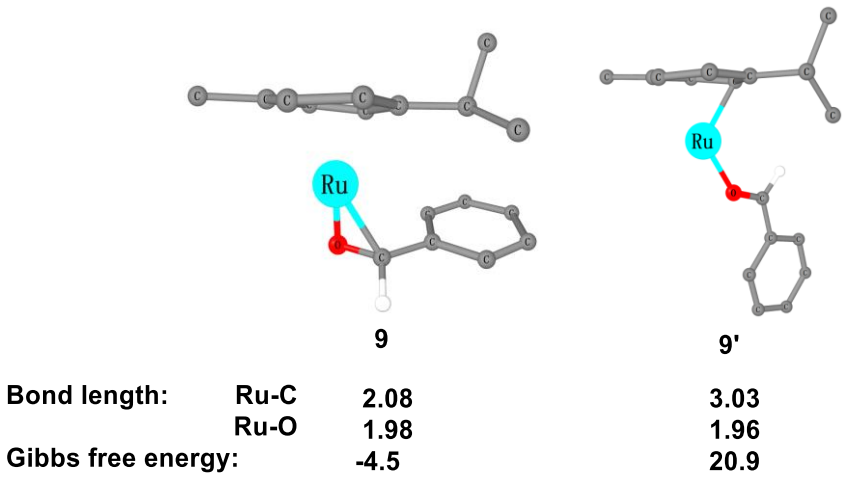


Figure S4. The geometric structure diagram and Gibbs free energy of intermediates **9** and **9'** (In this structure, the hydrogen atom on the saturated carbon atom has been omitted.)

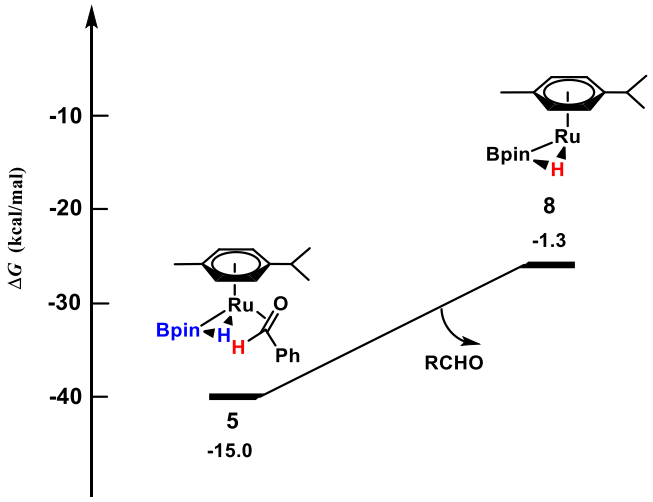


Figure S5. The Gibbs free energy profiles along reaction pathway for formation of intermediate **8+RCHO**. (The numbers are free energies)

As shown in Figure S5, it is possible that intermediate **5** release the PhCHO to give intermediate **8**, which is an endothermic reaction with an increase of energy by 13.7 kcal/mol. From the viewpoint of thermodynamics, it is possible to release PhCHO under the experimental conditions of 60°C, and the existence of PhCHO was also observed in the experiment.

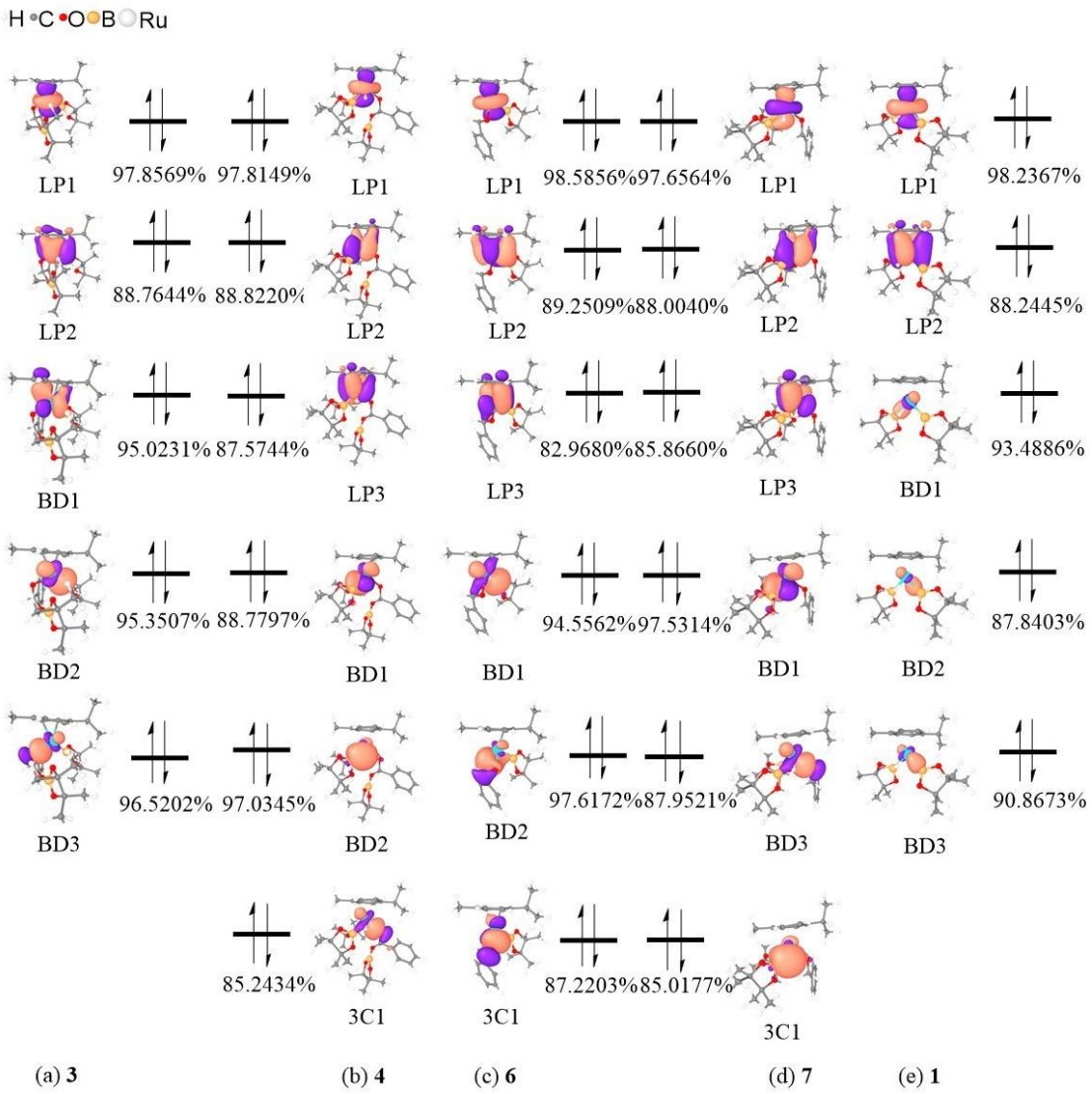


Figure S6. The NLMOs of in (a) **3**, (b) **4**, (c) **6**, (d) **7** and (e) **1**. (The values below the orbitals are percent from parent NBO)

Intermediates **3**, **4**, **6**, **7** and **1** are important species along reaction pathway, we analyze the oxidation state of Ru through the NLMO (Natural Localized Molecular Orbital) method in Figure S6.[1] In **3**, three lone pair d orbitals and two bonds (BD) are found for Ru center. Therefore, we can think the Ru center is divalent. As for **4**, there are three lone pair electron orbits, two BD orbits, and one three-center orbits. The *d* orbitals of Ru center of **6** and **7** are similar to those of **3** and **4** above. It should be noted that in **4** and **7**, the 3C features a Ru-H-B three-center bond, implying that Ru center provide two electrons to HBpin moiety to form μ-H structure. The Ru-B^1/Ru-B^3 distances of **4** and **7** are 2.105 Å/2.132 Å and 2.076 Å/2.129 Å, respectively (see Table

S4). These difference between Ru-B^1 and Ru-B^3 are within 0.05 Å for **4** and **7**. Hence, **4** and **7** should be Ru(IV) species while the second HBpin coordinates with Ru center in **4** and **7**. In **1**, The NLMO orbit show that there are two lone pair electron orbits, three BD orbits, it indicates that a lone pair of electrons is involved in the formation of BD orbitals, the oxidation state of Ru increases from Ru(II) to Ru(IV).

Reference

(1) Reed, A. E., Natural localized molecular orbitals. *J. Chem. Phys.* **1985**, *83* (4), 1736-1740.

Table S1. Electronic energies in (E_{ele}, in a.u.; at ωB97X-D/BS-II), and thermal correction energies (E_{therm}, in a.u., calculated at 298.15 K and 1 atm).

Complex	E_{therm}	E_{ele}	ΔE	ΔG
1	0.5381	-1307.1219	0.0	0.0
2	0.6314	-1726.743533	11.1	15.6
2'	0.6322	-1726.738692	14.1	19.1
3	0.6393	-1726.7555	3.6	13.0
4	0.8178	-2138.618263	0.8	21.7
5	0.4650	-1240.7924	-19.2	-15.0
5'	0.4605	-1240.7779	-10.1	-8.7
6	0.4654	-1240.7740	-7.7	-3.2
7	0.6528	-1652.667521	-29.8	-8.3
8	0.3575	-895.2034	-32.4	-28.9
9	0.2844	-828.8971	4.0	-4.5
10	0.4686	-1240.7886	-16.8	-10.4
11	0.1753	-483.2635	18.8	8.6
12	0.6516	-1652.7137	-58.7	-38.0
1'	0.5381	-1307.117012	-67.2	-50.8
TS2-3	0.6289	-1726.7257	22.3	25.2
TS4-5	0.8168	-2138.6139	3.5	23.8
TS5-6	0.4630	-1240.7737	-7.5	-4.5
TS7-8	0.6507	-1652.6578	-23.7	-3.5
TS3-9	0.6353	-1726.7242	23.2	30.2
TS6-10	0.4666	-1240.7670	-3.3	2.0
HBPIN	0.1603	-411.8583	/	/
BpinOBpin	0.3262	-897.8577	/	/
PhCH$_2$OBpin	0.2668	-757.4684	/	/
PhCOOBpin	0.2464	-831.4976	/	/
PhCHO	0.0807	-345.5404	/	/

The convergence criteria and integration parameters used default values (Force: Maximum 0.000450, RMS 0.000300; Displacement: Maximum 0.001800, RMS 0.001200).

Table S2. Calculated imaginary frequencies of transition states at ωB97X-D/BS-I level.

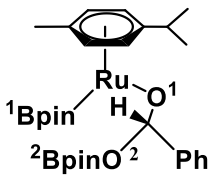
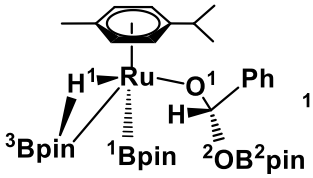
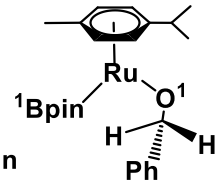
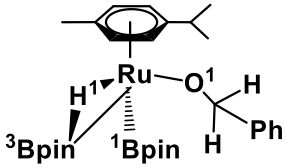
Complex	Imaginary frequencies
TS2-3	*556.87*
TS4-5	*241.16*
TS5-6	*424.67*
TS7-8	*121.37*
TS3-9	*307.65*
TS6-10	*174.11*

Table S3. Calculated free energies of stationary points at singlet and triplet states along reaction pathway (method: ωB97X-D/6-311++G(d, p) unit: kcal/mol).

Intermediates	**1**	**2**	**6**	**7**	**TS5-6**
singlet state	0.0	-13.2	-28.2	-37.1	-29.5
triplet state	10.2	6.5	-5.8	-12.0	-4.3

We have compared the free energies of some key intermediates at triplet state as shown in Table S3. It indicates these intermediates at triplet state own higher energy than those at singlet state. Therefore, the reaction should occur at singlet state.

Table S4. The geometric parameter of intermediates **3**, **4**, **6** and **7**. (unit: bond length in angstrom)

 **3**	 **4**	 **6**	 **7**	
Intermediate	Atom/ bond	**3**	**4**	**6**	**7**
NBO Charge	Ru	0.32	0.02	0.07	0.05
	B^1	0.98	0.93	0.99	0.91
Wiberg bond indexes	$Ru-B^1$	0.803	0.625	0.782	0.633
Bond lengths	O^1-B^1	3.052	2.754	2.913	2.812
	$Ru-B^1$	2.047	2.105	2.058	2.076
	$Ru-B^3$	~	2.132	~	2.129
	$Ru-H^1$	~	1.627	~	1.640
	B^3-H^1	~	1.410	~	1.411

The bond lengths, Wiberg bond indexes and NBO charges of intermediate **3** and **4** are summarized in Table S4. The length of the O^1-B^1 bond for the intermediate **3** is 3.052 Å, and 2.754 Å for intermediate **4**. The Wiberg bond index of the $Ru-B^1$ bond is 0.803 for the intermediate **3**, and 0.625 for intermediate **4**. It implies that the $Ru-B^1$ bond of **4** is weaker and more susceptible to be cleaved than that of **3**. Based on NBO

charge analysis, the charge on B^1 atom decreases from 0.9787 to 0.9298 after the coordination of the second HBpin, which is more likely to be attacked by nucleophiles. The bond lengths, Wiberg bond indexes and NBO charges of intermediate 6 and 7 are summarized in Table S4. The length of O1-B1 bond for the intermediate 6 is 2.913 Å, and 2.812 Å for intermediate 7. The Wiberg bond index of the Ru-B^1 bond is 0.782 for the intermediate 6, and 0.633 for intermediate 7. Therefore, the Ru-B^1 bond in 7 is weaker and more susceptible to cleavage. From the perspective of NBO charge, after inserting the second molecule HBpin, the charge on B^1 atom is reduced from 0.9894 to 0.9091, which is more likely to be attacked by nucleophiles.

Figure S7. Typical geometric structure diagram.

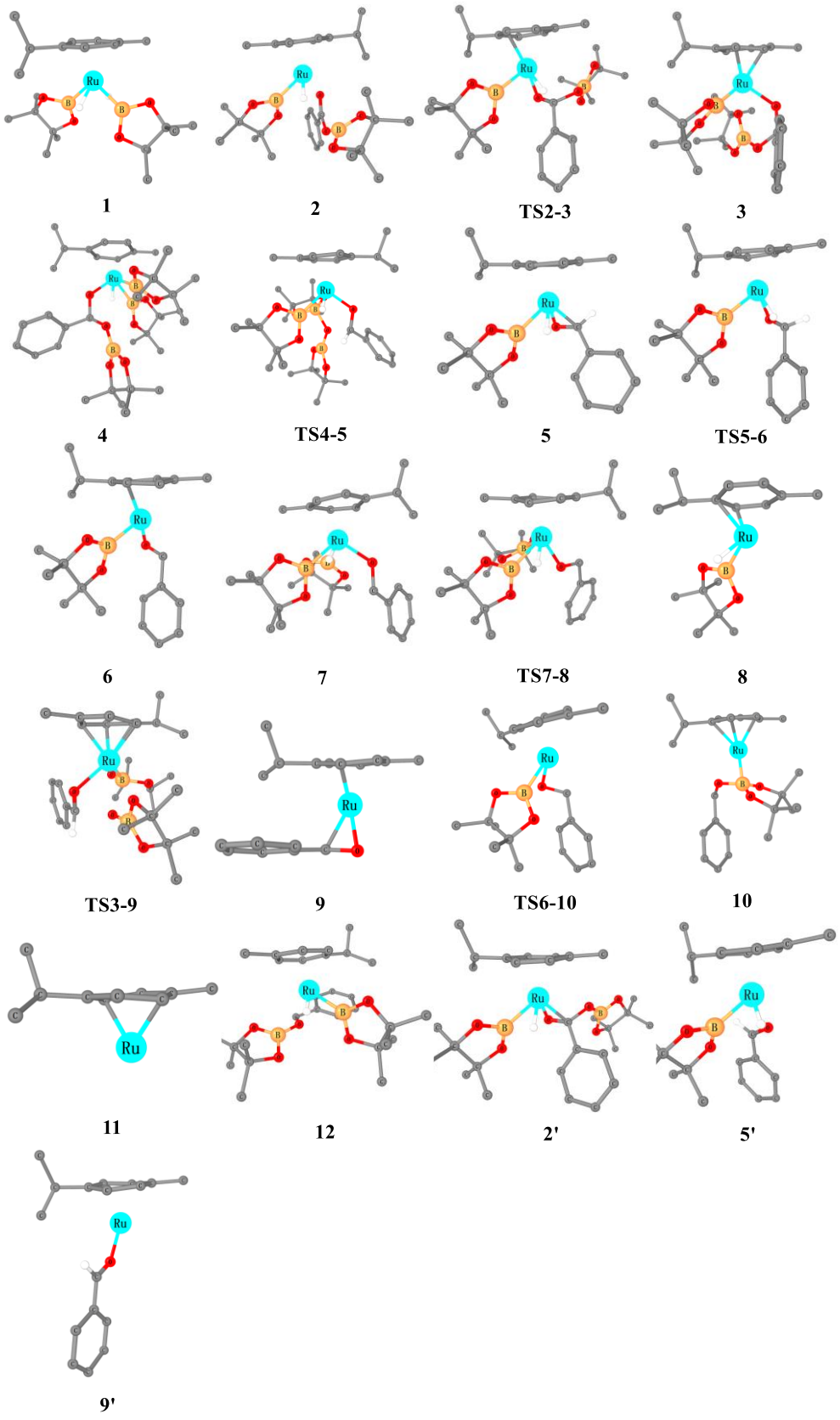


Figure S8. The IRC calculations of **TS2-3**, **TS5-6**, **TS7-1** and **TS6-9**.

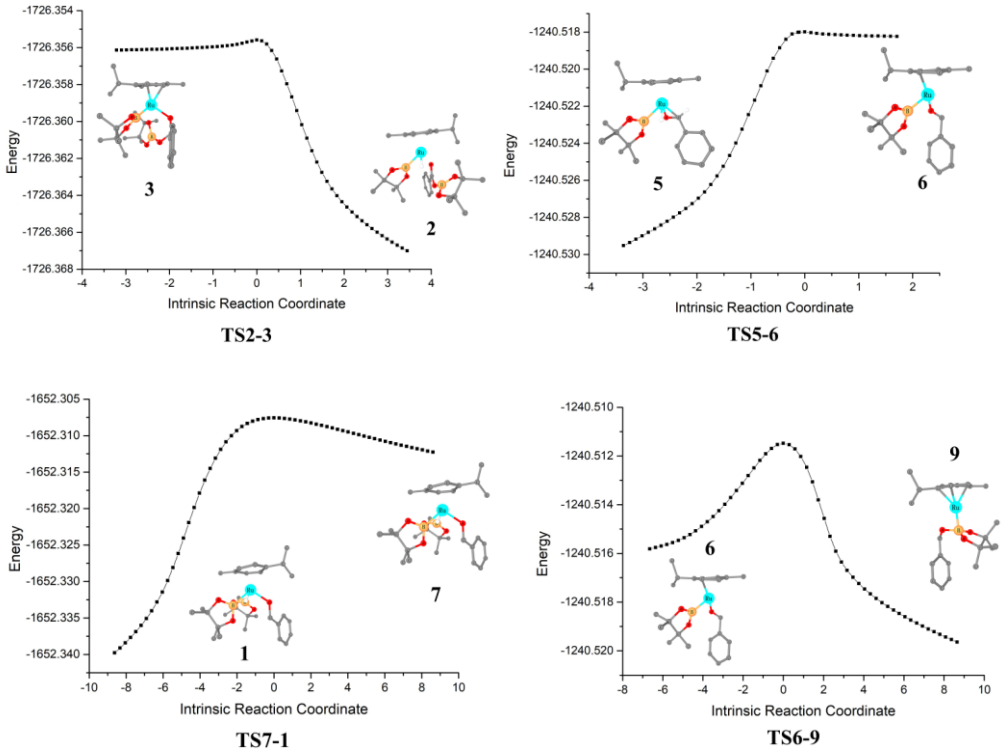
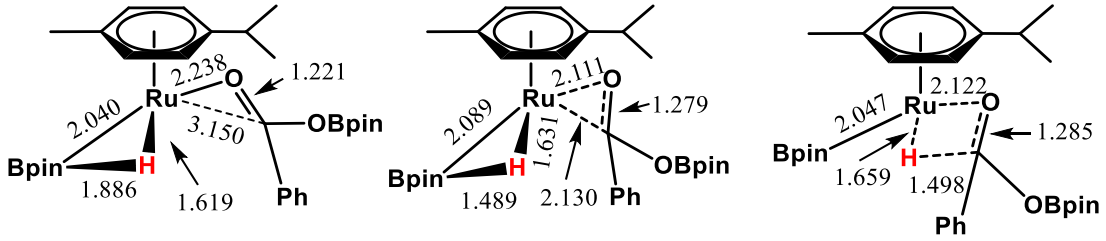


Figure S9. The geometric parameters and Gibbs free energy of intermediates **2, 2'** and **TS2-3**. (unit: bond length in angstrom, energy in kcal/mol)



	2	**2'**	**TS2-3**
Energy	**15.6**	**19.1**	**25.2**

It should be noted that there are two possible coordination modes with Ru center for carbonyl compounds such as PhCOOBpin, PhCHO. One is η^1 end-on coordination mode that only O atom of carbonyl group of PhCOOBpin moiety coordinates with Ru center (see **2** in Figure S9), another is η^2 side-on coordination mode that both C and O atoms of carbonyl group coordinate with Ru center (see **2'** in Figure S9). The intermediate **2'** with the C=O side-on coordination is 3.5 kcal/mol higher than **2**. In the hydride transfer step in stage 1, intermediate **2** will isomerize into **2'** firstly, then the bridged hydride is transferred to C atom of carbonyl group to form **3** via **TS2-3**. In the hydride transfer step in stage 2, the structure of **5** owning C=O η^2 side-on coordination mode is 6.3 kcal/mol lower than that of **5'** owning C=O η^1 end-on coordination mode. It is to say, PhCHO prefers side-on coordination with Ru center.

Atomic cartesian coordinates of intermediates and transition states (presented in Å).

1 and **1'**

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.01457200	-0.82523400	-0.28368900
C	1.65822800	-2.29819200	-1.07641300
C	0.52524700	-2.41798100	-1.89942000
C	1.55782400	-2.43134000	0.33023500
C	-0.74694700	-2.74456000	-1.34948600
C	0.29560500	-2.81294000	0.87158200
C	-0.82475200	-2.99721800	0.04165500
H	2.60868800	-2.00885700	-1.51137500
H	0.61470300	-2.24379900	-2.96562900
H	-1.78510000	-3.24154700	0.48182000
H	0.18965000	-2.94981600	1.94110100
C	2.01657700	2.97295800	-0.28982600
C	3.22011200	1.97349100	-0.28176300
C	1.68475300	3.51909800	1.10177200
H	2.43230100	4.24079400	1.44502800
H	0.71126600	4.01315000	1.05767500
H	1.61398000	2.70871300	1.83281100
C	3.85369900	1.79169100	-1.66326000
H	4.41583800	2.67805800	-1.97213200
H	4.54159400	0.94215900	-1.62822700
H	3.08823900	1.58186300	-2.41567500
C	2.14223700	4.11779100	-1.28589200
H	2.21974900	3.74761400	-2.30964800
H	1.25787100	4.75762100	-1.22398400
H	3.02350000	4.72884900	-1.06331400
C	4.29532800	2.26722400	0.75568100
H	3.88445400	2.24684200	1.76647700
H	5.08311300	1.51102400	0.69441500
H	4.74928900	3.24804100	0.57950100
O	2.57681100	0.73669800	0.05829500
O	0.92682200	2.12885200	-0.68148200
B	1.22973400	0.83226700	-0.30104100
C	-1.96721100	-2.86859900	-2.22012700
H	-1.80772600	-2.37407100	-3.18090900
C	2.79650600	-2.27490100	1.19102100

H	3.48761700	-1.65159800	0.61477400
C	3.44059000	-3.64898600	1.42370300
C	2.53674300	-1.54558000	2.50959600
H	2.77846400	-4.29406200	2.01232000
H	3.65036000	-4.15686400	0.47715400
H	4.38250400	-3.54449900	1.97090300
H	2.08480500	-0.57018700	2.31981800
H	1.88014200	-2.11878500	3.17343600
H	3.48264800	-1.39511100	3.03882300
H	-2.20043400	-3.92167600	-2.41054700
H	-2.81963800	-2.39245300	-1.73145900
H	0.18379200	0.18194200	0.95001400
C	-4.03572400	0.30540100	0.35006500
C	-3.36714800	1.70380000	0.55040100
C	-4.34236400	-0.40307400	1.67221100
H	-5.18616500	0.05848000	2.19369900
H	-4.59441500	-1.44648200	1.46301500
H	-3.47039200	-0.38845500	2.33228900
C	-3.46457000	2.59588400	-0.69054700
H	-4.47668500	2.98617200	-0.83492600
H	-2.77728000	3.43628500	-0.56717000
H	-3.16531400	2.04884300	-1.58896200
C	-5.26880500	0.30804800	-0.54294300
H	-5.03123700	0.66282700	-1.54736700
H	-5.67142800	-0.70552200	-0.62648900
H	-6.04914300	0.94966400	-0.12036700
C	-3.83325600	2.46712900	1.78252900
H	-3.61874200	1.91440000	2.69886900
H	-3.31424400	3.42770300	1.83779000
H	-4.90970300	2.66248800	1.73142800
O	-1.98662700	1.35488600	0.71022800
O	-2.98792700	-0.43355000	-0.29597400
B	-1.76837800	0.15399000	0.05426200
H	-0.70353400	0.27930500	-1.21195700

2

Coordinates (Angstroms)

	X	Y	Z
Ru	0.70034300	-1.32522000	0.05003500
C	2.87193900	-2.02759300	-0.38802100
C	1.85492600	-2.71809600	-1.12134600
C	2.82126900	-1.94733000	1.00586200
C	0.82192700	-3.43994400	-0.44964100
C	1.72277500	-2.59820500	1.66073800

C	0.80373400	-3.41377800	0.97892400
H	3.66695900	-1.52331800	-0.92756200
H	1.89041200	-2.73457900	-2.20479100
H	0.02623800	-3.93678600	1.52336100
H	1.60960700	-2.47851300	2.73358000
C	-3.19997400	-0.24807000	-1.25255100
C	-2.92258600	-1.42100600	-2.25093600
C	-2.96765100	1.13379400	-1.86931300
H	-3.73773300	1.38248400	-2.60592700
H	-2.99328600	1.88180700	-1.07281300
H	-1.98512000	1.19441200	-2.34546500
C	-3.59056800	-2.73200000	-1.82705100
H	-4.67591800	-2.69726400	-1.96200600
H	-3.19053900	-3.54609700	-2.43771200
H	-3.37409900	-2.95463500	-0.77810600
C	-4.55579300	-0.28677200	-0.55921600
H	-4.69329400	-1.21552300	-0.00280700
H	-4.62304900	0.54328800	0.15035700
H	-5.36845800	-0.18741800	-1.28673100
C	-3.24898500	-1.11325700	-3.70589900
H	-2.66789000	-0.26410000	-4.06938400
H	-3.00963000	-1.97995900	-4.32863200
H	-4.31445900	-0.89002300	-3.82644500
O	-1.50568700	-1.60164800	-2.12122600
O	-2.18057200	-0.45810700	-0.26992100
B	-1.10933300	-1.12639300	-0.87107200
C	-0.14635400	-4.28849400	-1.22501000
H	-0.39204900	-3.81380200	-2.17612100
C	3.84998900	-1.16388300	1.79587000
H	4.56673100	-0.76167700	1.06758100
C	4.62737900	-2.07905000	2.75109600
C	3.22573700	0.02253000	2.54064800
H	3.96408700	-2.49678700	3.51645600
H	5.08856500	-2.91380900	2.21501900
H	5.41679800	-1.52103900	3.26490900
H	2.70556300	0.69022800	1.84882600
H	2.49615500	-0.31861500	3.28286200
H	3.99894100	0.58928800	3.07117500
H	0.28568300	-5.27770900	-1.41262200
H	-1.07946900	-4.41735700	-0.67047800
H	0.52440100	-0.21786900	-1.11821400
C	-4.22544400	1.92676300	3.79406900
C	-3.53022600	0.72728900	3.93976900
C	-2.41560300	0.47056800	3.15235100

C	-1.99443400	1.41767600	2.21721000
C	-2.69169000	2.61800600	2.06902500
C	-3.80634300	2.87121300	2.85993800
H	-5.09892400	2.12419200	4.40789000
H	-3.86321900	-0.00961200	4.66329200
H	-1.86890100	-0.46215700	3.23291700
H	-2.36083300	3.34096300	1.33244600
H	-4.34823500	3.80448200	2.74667300
C	-0.83113200	1.09456200	1.36149300
O	-0.64688200	1.95993500	0.36991600
O	-0.13446700	0.10996000	1.55091800
C	2.66505500	2.63395300	-0.85950800
C	1.69742800	3.19752800	-1.97079100
C	3.36615100	1.34315500	-1.27069900
H	4.11278900	1.52967400	-2.04805300
H	3.86948600	0.92733300	-0.39403200
H	2.64510800	0.60000700	-1.61750100
C	1.46450700	4.70490400	-1.85783000
H	2.35959600	5.27022200	-2.13191600
H	0.65363700	4.98864600	-2.53301500
H	1.17328100	4.98444500	-0.84130200
C	3.68173300	3.63452800	-0.32777000
H	3.20020600	4.51120900	0.10812200
H	4.28448900	3.15718500	0.44922500
H	4.35305000	3.96141000	-1.12806000
C	2.08295200	2.82868500	-3.39550700
H	2.10429100	1.74682300	-3.53363900
H	1.35118500	3.24594200	-4.09202600
H	3.06631500	3.23964800	-3.64466300
O	0.43999300	2.56276600	-1.65492700
O	1.75073900	2.30893400	0.21412800
B	0.51876500	2.18116100	-0.35147100

2'

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.86589200	-0.83432800	-0.40462400
O	0.38837000	0.11561700	1.00213700
C	-1.18545000	-2.95360600	0.51641100
C	0.00107800	-2.96928900	-0.26551300
C	-2.41054500	-2.55419500	-0.04391000
C	-0.00830700	-2.69646600	-1.65673400
C	-2.37875100	-2.09137000	-1.39350100
C	-1.20804100	-2.20050500	-2.20029500

H	-1.12042900	-3.20929800	1.56695700
H	0.94241600	-3.21489600	0.21239000
H	-1.24778700	-1.89613800	-3.24020300
H	-3.28277600	-1.67733500	-1.82539600
C	0.97168700	0.20875700	-0.13269200
C	1.16655900	1.52832600	-0.81589300
C	1.85009500	1.61285700	-2.03036000
C	0.66853200	2.68782000	-0.22177700
C	2.02507100	2.84520700	-2.65078200
H	2.23937300	0.70836300	-2.48733500
C	0.84948100	3.91795300	-0.84372600
H	0.12982500	2.59859900	0.71431300
C	1.52487900	4.00270900	-2.05926100
H	2.55310900	2.90263100	-3.59805600
H	0.46521900	4.81916300	-0.37412600
H	1.66397200	4.96556600	-2.54148000
C	1.24032300	-2.83769500	-2.47572900
H	2.08658400	-2.39452900	-1.94628300
C	-3.71551100	-2.54131200	0.71966500
H	-4.26456200	-1.66976200	0.34927300
C	-3.53290000	-2.37834800	2.22794100
C	-4.52501900	-3.80288700	0.38729300
H	-3.10468500	-3.27805000	2.68377700
H	-2.87592600	-1.53262600	2.45311400
H	-4.50148600	-2.20329800	2.70515700
H	-4.69189800	-3.89895900	-0.68972500
H	-4.00065100	-4.70188600	0.72949200
H	-5.50078100	-3.77137500	0.88170900
H	1.45670200	-3.89620200	-2.65402900
H	1.13214700	-2.34203200	-3.44321200
C	-4.34987300	1.56510800	0.32687600
C	-3.24276200	2.55339400	0.82503600
C	-5.04288300	0.82579900	1.47309800
H	-5.68118900	1.49622400	2.05564800
H	-5.67167200	0.03119900	1.06110000
H	-4.31012700	0.37058600	2.14410900
C	-2.91344800	3.64434000	-0.19803700
H	-3.72304700	4.37488600	-0.28621400
H	-2.00784600	4.16481700	0.12184500
H	-2.71580300	3.21360000	-1.18365400
C	-5.39150300	2.18293200	-0.59665900
H	-4.93175900	2.59024300	-1.49843700
H	-6.11602600	1.42159000	-0.89838700
H	-5.93322000	2.98566100	-0.08523900

C	-3.50539600	3.17879900	2.18799500
H	-3.57443900	2.41849700	2.96759100
H	-2.68497900	3.85329800	2.44648800
H	-4.43418100	3.75893100	2.17523200
O	-2.09348300	1.70019100	0.92008400
O	-3.58372600	0.60558000	-0.42085500
B	-2.26311300	0.65672600	0.02899000
H	-1.29775400	0.57490200	-1.10224400
O	2.04964500	-0.67487400	-0.38053200
C	4.88595500	0.36593800	1.52062000
C	5.48085100	-0.63111300	0.46277700
C	4.69476100	-0.27164500	2.89776800
H	5.65185700	-0.42793100	3.40379200
H	4.07849300	0.39109400	3.50980400
H	4.18011900	-1.23332200	2.81708100
C	6.09491500	0.08407200	-0.74304300
H	7.03537500	0.57819400	-0.48356800
H	6.29357500	-0.65273100	-1.52547000
H	5.40626500	0.83309600	-1.14560000
C	5.63297800	1.68550300	1.64680300
H	5.63003300	2.23456600	0.70400300
H	5.14996300	2.30941600	2.40298400
H	6.66957300	1.51313300	1.95414800
C	6.45709800	-1.65310000	1.02563300
H	5.98531200	-2.27825000	1.78535600
H	6.81304000	-2.30449600	0.22304300
H	7.32371000	-1.15294600	1.46961800
O	4.30349800	-1.31567000	-0.00903900
O	3.57474400	0.62511100	0.98742300
B	3.25711000	-0.44818400	0.19906900

3

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.80591400	-0.89594700	-0.63469000
O	-0.10867500	-0.09747700	-2.30571700
C	2.53479400	-2.02129800	0.25059200
C	2.86440100	-2.13117600	-1.15097900
C	1.33342900	-2.53278900	0.78758200
C	1.91500100	-2.54340000	-2.06237200
C	0.33697800	-2.94553100	-0.15331100
C	0.59522900	-2.82815600	-1.53832000
H	3.28884600	-1.64649500	0.93092900
H	3.84057800	-1.79887700	-1.49106100

H	-0.20309900	-3.04153600	-2.24100800
H	-0.64346400	-3.25047000	0.19411400
C	-1.00889400	0.89224000	-2.35259600
C	-2.45579200	0.49377900	-2.06428500
C	-3.45543700	1.46495000	-1.97299800
C	-2.80853500	-0.84905600	-1.98553100
C	-4.78512400	1.09638500	-1.79383100
H	-3.18203000	2.51430700	-2.03409600
C	-4.13743200	-1.22278100	-1.80434300
H	-2.02207200	-1.59095800	-2.05321400
C	-5.13000700	-0.25228000	-1.71080300
H	-5.55345400	1.86042800	-1.72087300
H	-4.39703700	-2.27484000	-1.73093400
H	-6.16719300	-0.54143200	-1.56976000
C	2.11161400	-2.48880300	-3.54677700
H	3.13123500	-2.19237000	-3.80363500
C	1.09381800	-2.68168000	2.27472700
H	0.00733900	-2.73005400	2.40728100
C	1.61215000	-1.50659500	3.10619600
C	1.69135900	-4.01244500	2.75225200
H	2.70322800	-1.42125000	3.05342100
H	1.17248900	-0.56432400	2.76731200
H	1.35330500	-1.65359400	4.15974600
H	1.29012400	-4.85583500	2.18239100
H	2.78022000	-4.01120300	2.63117400
H	1.46753500	-4.17802000	3.81055400
H	1.90158700	-3.45641800	-4.01293600
H	1.41610800	-1.75005400	-3.96189000
C	-1.71336100	1.06309900	2.19793100
C	-2.45508700	-0.32467700	2.11261700
C	-2.42000200	2.19492900	1.45401800
H	-3.34551500	2.48913900	1.95775300
H	-1.74955100	3.05818700	1.41569000
H	-2.64749400	1.91089100	0.42614500
C	-2.24066000	-1.20594000	3.34481300
H	-2.76227200	-0.80832200	4.22014500
H	-2.63123300	-2.20574300	3.13578500
H	-1.17944100	-1.29801800	3.58909000
C	-1.37458200	1.51596100	3.61422200
H	-0.72621900	0.80154400	4.12557600
H	-0.85628000	2.47797400	3.57469000
H	-2.28650800	1.64828800	4.20520500
C	-3.94283200	-0.22340000	1.80291100
H	-4.11678300	0.27838600	0.85039700

H	-4.37131600	-1.22701300	1.73276400
H	-4.46714900	0.31896100	2.59692800
O	-1.80665500	-0.97982700	1.00785100
O	-0.48308200	0.80664200	1.49658200
B	-0.64164200	-0.31610000	0.69112800
H	-0.99061200	1.33714100	-3.36322400
O	-0.71621000	2.03027300	-1.48627200
C	2.05906900	3.32756800	0.31197100
C	2.63806600	1.96737900	-0.20883000
C	1.67813500	3.28156400	1.79291100
H	2.56182200	3.27271500	2.43784500
H	1.09353400	4.17625300	2.02469400
H	1.06468500	2.40255600	2.00215100
C	3.43321900	2.09427000	-1.50748500
H	4.41005700	2.55471500	-1.33513300
H	3.58267200	1.09292800	-1.92144500
H	2.89017600	2.68804700	-2.24756400
C	2.95242900	4.52774300	0.02821100
H	3.10454600	4.67072600	-1.04285400
H	2.48524400	5.43120500	0.42798100
H	3.92727600	4.40603400	0.51166100
C	3.43644300	1.20293600	0.83115500
H	2.79174100	0.84034500	1.63322300
H	3.93667400	0.35034200	0.36786100
H	4.20662300	1.85405200	1.25626500
O	1.42316500	1.25402500	-0.54788600
O	0.84915200	3.46728900	-0.44312900
B	0.44543700	2.21993100	-0.85154700

4

Coordinates (Angstroms)

	X	Y	Z
Ru	2.09331400	0.15898700	-0.34202700
O	0.75344600	1.67928500	-0.04421800
C	4.06815200	1.10489200	-1.27764400
C	4.04032100	-0.32566900	-1.32113500
C	3.83900000	1.77166300	-0.07198700
C	3.99510000	-1.11568500	-0.14340400
C	3.67154500	0.98080400	1.10965300
C	3.81252600	-0.41978200	1.07802700
H	4.15795200	1.65841100	-2.20446300
H	4.11039400	-0.82804300	-2.27996100
H	3.68549700	-0.97700600	1.99890600
H	3.41841400	1.46331200	2.04544800

C	0.36192600	-1.01326500	3.36799700
C	-0.07320300	-2.28907900	2.55754900
C	-0.78838600	-0.06764000	3.70970000
H	-1.46510700	-0.51260700	4.44560500
H	-0.36753100	0.84670600	4.13679900
H	-1.35533400	0.20912300	2.82182100
C	0.82812700	-3.50245700	2.80058200
H	0.71538900	-3.89794700	3.81404900
H	0.56177400	-4.29205700	2.09300300
H	1.88054700	-3.24910200	2.63907100
C	1.16647000	-1.31255100	4.62918100
H	2.08225900	-1.86538400	4.40868900
H	1.44558800	-0.37259200	5.11263900
H	0.56992300	-1.89430900	5.33930500
C	-1.53639700	-2.67570900	2.72392200
H	-2.19172100	-1.85934500	2.41580900
H	-1.75717600	-3.55001600	2.10321900
H	-1.75198500	-2.93521200	3.76589500
O	0.13421300	-1.89386800	1.19145100
O	1.22112100	-0.33461400	2.43656300
B	0.95982200	-0.79062100	1.15563500
C	-0.53391100	1.61524700	-0.43221000
H	-0.68576800	1.12469500	-1.40589300
C	-1.13533300	3.01084200	-0.46067200
C	-0.79942500	3.93433400	0.53051000
C	-2.03749400	3.37467700	-1.45705800
C	-1.36572300	5.20331600	0.52595300
H	-0.08423800	3.63855600	1.29080000
C	-2.60664000	4.64702700	-1.46356600
H	-2.30768900	2.64753800	-2.21742100
C	-2.27273900	5.56303100	-0.47127600
H	-1.10072900	5.91809200	1.29977900
H	-3.31086600	4.92206400	-2.24351200
H	-2.71561000	6.55462700	-0.47376700
C	-4.62963800	-0.34903300	0.80814100
C	-4.60588300	0.33497000	-0.60988200
C	-5.72186500	0.16684800	1.73768800
H	-5.65983400	-0.35139800	2.69822600
H	-5.61230300	1.23623400	1.92338400
H	-6.71292000	-0.01890500	1.31087600
C	-5.32505500	-0.43999000	-1.70486100
H	-4.91369900	-1.44334200	-1.82716500
H	-6.39231900	-0.52814300	-1.47759900
H	-5.22081500	0.08830400	-2.65634500

C	-4.68121400	-1.87582100	0.74806600
H	-3.88196800	-2.26908000	0.11772200
H	-4.54061600	-2.27527100	1.75599500
H	-5.64223500	-2.23364700	0.36685600
C	-5.10584100	1.78230800	-0.58276600
H	-4.58406700	2.36671400	0.18033800
H	-4.89517000	2.24645900	-1.54940700
H	-6.18245500	1.83736500	-0.39786100
O	-3.20225000	0.38399100	-0.91324300
O	-3.35648000	0.02458600	1.35123700
B	-2.54094000	0.40785200	0.30111800
O	-1.28529100	0.82840100	0.53800900
C	4.09977000	-2.61293200	-0.19407100
H	3.59547700	-2.99063900	-1.08523300
C	3.69620900	3.27598800	0.02325400
H	3.11807100	3.46709000	0.93430500
C	2.91110900	3.88059900	-1.14260300
C	5.08163300	3.91849700	0.18382800
H	3.44994100	3.78181200	-2.09173900
H	1.93567000	3.39449100	-1.22219000
H	2.75603000	4.94907400	-0.96684900
H	5.61966200	3.50548100	1.04273700
H	5.69053200	3.75010100	-0.71115800
H	4.98344300	4.99846100	0.32812800
H	5.14910000	-2.92602600	-0.20821400
H	3.61701100	-3.06068300	0.67830300
C	-0.83853300	-2.41495700	-2.32568600
C	0.44524300	-3.31404000	-2.26730900
C	-1.10437300	-1.81302600	-3.70703600
H	-1.45201200	-2.56536400	-4.42136900
H	-1.87419900	-1.04431500	-3.59978100
H	-0.20384100	-1.33852400	-4.10772800
C	0.42419800	-4.31256700	-1.10914400
H	-0.31135900	-5.10537300	-1.27516700
H	1.41257700	-4.77323200	-1.01998500
H	0.19903000	-3.79627100	-0.17368300
C	-2.10086400	-3.06827100	-1.78714700
H	-1.97726600	-3.33607200	-0.73622800
H	-2.91907600	-2.34911700	-1.86361600
H	-2.36238500	-3.96331400	-2.36097600
C	0.78798600	-4.02200500	-3.57057900
H	0.94469000	-3.31108300	-4.38371400
H	1.70618000	-4.60230900	-3.44339700
H	-0.01322100	-4.71127100	-3.85593600

O	1.47632400	-2.35093300	-1.97868900
O	-0.49669600	-1.32275000	-1.46526400
B	0.87320200	-1.26190000	-1.36156600
H	1.31825100	0.01403400	-1.76493500

5

Coordinates (Angstroms)

	X	Y	Z
Ru	0.08336900	-1.07559500	-0.15584500
O	-1.00043600	-0.66858200	-1.92278700
C	1.92671500	-2.26977100	-0.91360300
C	0.82935100	-3.15651900	-0.72458700
C	2.36846100	-1.44587200	0.13518100
C	0.20590500	-3.33057300	0.53786000
C	1.62031500	-1.49006200	1.35168700
C	0.58506000	-2.44779500	1.56872000
H	2.38558100	-2.20863400	-1.89236400
H	0.47708800	-3.73595400	-1.57157200
H	0.08379500	-2.48505200	2.52935300
H	1.87178200	-0.79328600	2.14327600
C	-1.82091000	-1.25926400	-1.11707200
H	-1.98711600	-2.34468300	-1.24621500
C	-2.98975900	-0.55618100	-0.51963000
C	-3.88670400	-1.26964900	0.27738500
C	-3.21164000	0.80254800	-0.75598500
C	-4.97936800	-0.63302500	0.85594700
H	-3.71964300	-2.33134400	0.44865700
C	-4.30674400	1.43627400	-0.18027700
H	-2.49884200	1.34244100	-1.36972700
C	-5.19144300	0.72502300	0.62951100
H	-5.66750900	-1.19617400	1.47947200
H	-4.47612700	2.49344100	-0.36557100
H	-6.04582300	1.22443200	1.07623400
C	-0.88307100	-4.34679000	0.73167800
H	-1.43963400	-4.50271100	-0.19616600
C	3.53835800	-0.49518600	0.01819300
H	3.24928200	0.39713400	0.58297900
C	3.83207600	-0.07068400	-1.41985700
C	4.77718800	-1.11406700	0.68165100
H	4.24860900	-0.89582000	-2.00832000
H	2.92394700	0.28410200	-1.91644500
H	4.56894900	0.73743200	-1.42744900
H	4.58454600	-1.36892300	1.72809200
H	5.08143700	-2.02817900	0.16024600

H	5.61558300	-0.41141000	0.65235900
H	-0.45782400	-5.31001800	1.03287900
H	-1.58547700	-4.02543800	1.50421100
C	1.29893100	2.96776000	0.62402500
C	0.01150400	3.24783400	-0.22121100
C	2.58343500	3.09267200	-0.19763500
H	2.79608600	4.13563000	-0.44953600
H	3.42388100	2.70563900	0.38564900
H	2.51338400	2.51685700	-1.12385300
C	-1.19889900	3.61891400	0.64067500
H	-1.09129100	4.61358900	1.08322700
H	-2.09412400	3.61096000	0.01413000
H	-1.34934500	2.88928000	1.44146600
C	1.41627100	3.78753000	1.90186900
H	0.58152800	3.59267600	2.57705100
H	2.34244900	3.52982900	2.42326300
H	1.44203300	4.85799800	1.67283100
C	0.18633700	4.26554700	-1.34004200
H	0.93410800	3.93838800	-2.06403700
H	-0.76166600	4.39344300	-1.86897100
H	0.48546200	5.23782100	-0.93466500
O	-0.25740200	1.96193300	-0.79712600
O	1.13140900	1.58383200	0.97692900
B	0.26891900	1.00153400	0.04650800
H	-0.70471200	0.08558100	0.68110200

5'

Coordinates (Angstroms)

	X	Y	Z
Ru	1.29287500	-0.73190000	0.55818100
O	-0.57596600	-1.85218900	0.21721300
C	2.59749500	-1.26682000	-1.28660300
C	2.97531500	-2.22941200	-0.29075100
C	2.66401200	0.11622100	-1.03541200
C	3.37157800	-1.85294400	0.99067300
C	3.01333800	0.51823100	0.29565000
C	3.29023900	-0.45008100	1.29976000
H	2.27114200	-1.62598900	-2.25644900
H	2.91458700	-3.28425200	-0.54030500
H	3.52758400	-0.11143100	2.30229300
H	3.01940000	1.57128000	0.55354600
C	-1.35368300	-1.51723100	-0.66716000
H	-0.98571300	-0.99697800	-1.56412000

C	-2.79851100	-1.76993800	-0.59674100
C	-3.61689900	-1.32874600	-1.63852400
C	-3.35785400	-2.38524000	0.52726800
C	-4.99368400	-1.50701300	-1.56295200
H	-3.17153400	-0.83598700	-2.49886800
C	-4.73208400	-2.56434300	0.59914100
H	-2.70042100	-2.70248400	1.32988200
C	-5.54836300	-2.12556200	-0.44473800
H	-5.63378100	-1.16309600	-2.36875100
H	-5.17334900	-3.03929600	1.46925000
H	-6.62330600	-2.26378100	-0.38194000
C	3.81917500	-2.84559700	2.02599900
H	3.50374500	-3.85851300	1.76330500
C	2.38443800	1.15841200	-2.10093200
H	2.28517600	2.11865500	-1.58007000
C	1.07267600	0.91320000	-2.85168800
C	3.57347500	1.25726400	-3.06579900
H	1.09355900	-0.03587500	-3.39888600
H	0.23297200	0.88932600	-2.15051600
H	0.89896400	1.70886100	-3.58389300
H	4.50380700	1.46145600	-2.52762600
H	3.70284800	0.31678400	-3.61239800
H	3.41796000	2.05679100	-3.79734700
H	4.91137900	-2.84435000	2.11952700
H	3.39866200	-2.60173600	3.00474900
C	-0.68285700	3.05382100	0.84834800
C	-1.88179800	2.09271000	0.55348600
C	-0.19695900	3.79603800	-0.40038600
H	-0.90680300	4.56431800	-0.72159000
H	0.75737200	4.27882600	-0.17301800
H	-0.03594700	3.09964700	-1.22861100
C	-2.67694200	1.71603500	1.80643000
H	-3.28134400	2.55118200	2.17319500
H	-3.34303200	0.88452900	1.55879100
H	-2.00610900	1.38673500	2.60472200
C	-0.92399400	4.04343800	1.98089100
H	-1.12233800	3.52794800	2.92207500
H	-0.03773200	4.66866800	2.11894500
H	-1.77171700	4.69753100	1.75029900
C	-2.82805500	2.55054300	-0.54815600
H	-2.30289400	2.67966000	-1.49670400
H	-3.60963300	1.79817400	-0.69191800
H	-3.30893500	3.49742900	-0.28169500
O	-1.20232600	0.91166400	0.11494200

O	0.35422900	2.14293600	1.23411700
B	0.08126300	0.89011800	0.68987400
H	0.65475600	-0.49821200	2.01777500

6

Coordinates (Angstroms)

	X	Y	Z
Ru	0.98866900	-0.90093300	-0.04714300
O	-0.26792700	-1.58584800	-1.57211900
C	2.98092100	-0.68323400	-1.02807400
C	3.02842600	-2.05021500	-0.59499300
C	2.81057700	0.38091200	-0.11390900
C	2.74463200	-2.38874500	0.72220100
C	2.49363800	0.03597700	1.23740300
C	2.37312500	-1.32238300	1.61406500
H	3.12869800	-0.46779700	-2.07919900
H	3.20726100	-2.82813000	-1.32936600
H	2.07956300	-1.56051200	2.63111500
H	2.26250900	0.82001500	1.94788100
C	-0.86745700	-2.13212900	-0.52904900
H	-0.60666600	-3.18491800	-0.31019600
C	-2.36153800	-1.91189100	-0.37917700
C	-3.04009600	-2.37354200	0.74617300
C	-3.06531000	-1.28243400	-1.40153300
C	-4.41611000	-2.19974500	0.85834500
H	-2.48807800	-2.86435200	1.54582000
C	-4.44336400	-1.11988500	-1.29739200
H	-2.50811000	-0.91234400	-2.25371000
C	-5.12146800	-1.57361800	-0.16737500
H	-4.93733600	-2.55373700	1.74249900
H	-4.99009100	-0.63126500	-2.09863900
H	-6.19562900	-1.43909500	-0.08411600
C	2.72286100	-3.81298500	1.20090300
H	2.73377500	-4.51404000	0.36343500
C	2.95116500	1.83557500	-0.50800000
H	2.28149600	2.39297900	0.15385300
C	2.52892800	2.12211500	-1.94913900
C	4.39331300	2.29115400	-0.24542300
H	3.24192400	1.71078300	-2.67242000
H	1.54272200	1.69716100	-2.15916100
H	2.48530100	3.20237600	-2.11609000
H	4.67872700	2.12580900	0.79799400
H	5.09526400	1.73862900	-0.87982500
H	4.50578100	3.35759100	-0.46364000

H	3.59319300	-4.02109700	1.83236600
H	1.82709300	-4.00663800	1.79809200
C	-0.88509900	2.87399900	0.75619100
C	-2.06412300	2.07205900	0.11588200
C	-0.25487600	3.87512400	-0.21460100
H	-0.92022500	4.72217900	-0.40588300
H	0.67337000	4.26015800	0.21785500
H	-0.01665900	3.39576800	-1.16784100
C	-2.98544600	1.43173700	1.15777800
H	-3.59463000	2.18165300	1.67172700
H	-3.64894900	0.72338300	0.65684800
H	-2.40637200	0.87894500	1.90326000
C	-1.21227000	3.55884800	2.07546000
H	-1.53076100	2.83678600	2.82894200
H	-0.32598400	4.07629200	2.45336800
H	-2.00758400	4.29927100	1.93975100
C	-2.88923400	2.83280500	-0.91186000
H	-2.27394800	3.16853000	-1.74852100
H	-3.66709000	2.17276400	-1.30532400
H	-3.37321600	3.70311400	-0.45620500
O	-1.36729000	1.00902600	-0.55011300
O	0.08121500	1.83469200	1.00004200
B	-0.18943500	0.77741400	0.12957600
H	-0.49476100	-1.54620900	0.58597300

7

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.27151200	-1.35548200	-0.26904000
O	1.65834000	-0.18557900	-1.19636600
C	0.84696800	-3.67989200	-0.60248800
C	-0.45623000	-3.44336800	-0.05368000
C	1.96995200	-3.10744900	-0.01445000
C	-0.63081900	-2.83543800	1.21659000
C	1.78014400	-2.32971000	1.17773100
C	0.52676000	-2.27253700	1.81524200
H	0.94540200	-4.23207100	-1.53088000
H	-1.33139300	-3.81961100	-0.57167800
H	0.42269100	-1.72771500	2.74784100
H	2.62105400	-1.81187100	1.62080600
C	0.04016900	2.43027600	1.69487300
C	-0.96331600	1.61921100	2.58396700
C	-0.64120400	3.36256900	0.69219900
H	-1.11459400	4.21602700	1.18724600

H	0.11973100	3.73312400	-0.00023600
H	-1.38674700	2.81957700	0.10661000
C	-0.33563800	1.09782400	3.87752900
H	-0.15829500	1.90206700	4.59709000
H	-1.01400000	0.36990200	4.33222500
H	0.61841400	0.60242500	3.67363600
C	1.12219600	3.18468500	2.45496200
H	1.72673900	2.51494100	3.06966400
H	1.78802600	3.67124100	1.73730400
H	0.67943800	3.95187800	3.09907200
C	-2.27227100	2.33367200	2.88475300
H	-2.80228600	2.58988900	1.96566200
H	-2.92040200	1.69072500	3.48732300
H	-2.08618100	3.25544000	3.44513900
O	-1.23866500	0.46255600	1.76550100
O	0.66300600	1.38801000	0.93119500
B	-0.19517000	0.32623800	0.85478500
C	1.37418800	0.96421000	-1.91332300
H	1.50566100	0.78710300	-2.99956600
C	2.25931300	2.13800200	-1.52513800
C	2.07899800	3.38086000	-2.13616300
C	3.23714800	2.01242700	-0.54149400
C	2.84896100	4.47954900	-1.76486600
H	1.31620600	3.49056900	-2.90519700
C	4.01558000	3.10589100	-0.17147900
H	3.34588000	1.04870800	-0.05723700
C	3.82310700	4.34570700	-0.77714600
H	2.68998700	5.44071600	-2.24584900
H	4.77232000	2.99341400	0.60054600
H	4.42724000	5.19969700	-0.48488300
C	-1.97176500	-2.75688700	1.88650700
H	-2.76592600	-2.84418700	1.14422800
C	3.34500700	-3.28400200	-0.62289700
H	3.18819500	-3.56405100	-1.67122100
C	4.07188200	-4.44044100	0.07947000
C	4.17569100	-1.99680200	-0.60446300
H	4.22773700	-4.21203100	1.13967200
H	3.50556200	-5.37466800	0.01371500
H	5.05357500	-4.60076600	-0.37660900
H	3.59057200	-1.16070900	-0.99994600
H	4.50306600	-1.74927000	0.41205800
H	5.07863400	-2.13424500	-1.20659400
H	-2.07715600	-3.56090300	2.62266200
H	-2.08363300	-1.79285800	2.38745700

H	0.33538100	1.30052200	-1.78961900
C	-3.86791300	-0.41985900	-0.92157100
C	-3.26761900	0.83129000	-1.64840500
C	-4.30900700	-0.12789400	0.51366900
H	-5.18933900	0.52117400	0.53839300
H	-4.56719000	-1.07145100	1.00244100
H	-3.49661900	0.33288300	1.07998700
C	-3.29436000	0.71354800	-3.17371100
H	-4.30949500	0.80642200	-3.57026300
H	-2.68065500	1.51239800	-3.59729200
H	-2.87530900	-0.24252000	-3.49975100
C	-4.98468600	-1.12084700	-1.68324600
H	-4.64407000	-1.47945300	-2.65610500
H	-5.33826300	-1.98114200	-1.10853500
H	-5.83040800	-0.44221600	-1.83430500
C	-3.85799300	2.16470700	-1.21409900
H	-3.72465100	2.32817800	-0.14345200
H	-3.36133500	2.97984400	-1.74725800
H	-4.92774200	2.20592900	-1.44297300
O	-1.88536800	0.78255900	-1.25493700
O	-2.73179400	-1.30072000	-0.85196200
B	-1.58145300	-0.52458500	-0.90772200
H	-0.54284700	-1.10050300	-1.66955700

8

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.97159400	-0.70198500	-0.50651400
C	-1.48641800	0.28827500	1.32405200
C	-2.08505200	-0.98643600	1.49511000
C	-1.81214400	1.11382600	0.19461000
C	-2.94170600	-1.48416500	0.48807100
C	-2.79547800	0.63606400	-0.73770200
C	-3.35607100	-0.63771200	-0.58573200
H	-0.76891300	0.65439100	2.05069200
H	-1.81320700	-1.61386000	2.33584900
H	-4.05050000	-1.01858400	-1.32630900
H	-3.07917400	1.25017400	-1.58434000
C	3.28228100	-0.74307500	-0.37497000
C	2.98170000	0.42701100	0.61991700
C	3.70708700	-0.24764400	-1.75972600
H	4.71340200	0.18172100	-1.74582300
H	3.69829300	-1.09098000	-2.45488200
H	3.00860700	0.50655600	-2.13340300

C	3.01340300	-0.01585300	2.08562300
H	4.03333500	-0.21116800	2.42992800
H	2.58690100	0.77983600	2.70250100
H	2.41466900	-0.91949300	2.23105200
C	4.27244600	-1.77872200	0.13939100
H	3.90914700	-2.25804800	1.04990600
H	4.42068600	-2.55462800	-0.61659700
H	5.24231300	-1.31444700	0.34704300
C	3.84103400	1.66963400	0.43005900
H	3.70698700	2.09731700	-0.56495300
H	3.55787300	2.42794700	1.16529800
H	4.90100600	1.43551400	0.57396400
O	1.61975800	0.74888700	0.30303900
O	1.98976100	-1.35601400	-0.51734800
B	1.02863000	-0.38871600	-0.24356800
C	-3.49308000	-2.88271100	0.58403500
H	-2.84193800	-3.52341900	1.18310500
C	-1.20944400	2.50260400	0.11200000
H	-0.22674100	2.43249800	0.59092700
C	-2.08355900	3.48102700	0.90949300
C	-0.98421200	2.99798900	-1.31590200
H	-3.07569000	3.57551700	0.45339600
H	-2.21891500	3.14546100	1.94235900
H	-1.62663000	4.47524400	0.93150900
H	-0.39020100	2.27873900	-1.88469600
H	-1.92965200	3.16644000	-1.84398900
H	-0.45065600	3.95290700	-1.29660500
H	-4.48256600	-2.87010700	1.05360800
H	-3.59902000	-3.33333900	-0.40631600
H	-0.01331000	-0.00493700	-1.61427700

9

Coordinates (Angstroms)

	X	Y	Z
Ru	1.06735300	-0.66574900	-0.37163300
C	1.43907600	1.51707400	-0.87535000
C	2.67354600	0.83727800	-0.73457900
C	0.45948600	1.38823500	0.13429200
C	3.08271200	0.20380100	0.48315800
C	0.80686400	0.60624400	1.28775200
C	2.12790400	0.09370800	1.49929600
H	1.21586500	2.02440700	-1.80481000
H	3.36331300	0.83530800	-1.57276700
H	2.35509800	-0.45160900	2.40888100

H	0.04337100	0.43652200	2.04166800
C	4.45476800	-0.39710700	0.60624700
H	4.76701300	-0.85368900	-0.33670500
C	-0.91082400	2.02595600	0.05439400
H	-1.61868500	1.30698900	0.48188000
C	-1.35764200	2.32285900	-1.37565700
C	-0.93522100	3.29482200	0.91882900
H	-0.78709400	3.14977700	-1.81409900
H	-1.24305900	1.44017400	-2.01042300
H	-2.41302500	2.60801400	-1.38199700
H	-0.68058700	3.07573200	1.96020500
H	-0.21911500	4.03462000	0.54418400
H	-1.93119000	3.74723800	0.90206300
H	5.19004700	0.37282200	0.86422700
H	4.47982100	-1.16665700	1.38073500
C	-4.23882400	-0.21501100	0.79415800
C	-3.29167300	-0.82964400	1.61297400
C	-2.13103000	-1.36480000	1.06608900
C	-1.89206300	-1.28849700	-0.31167100
C	-2.86281600	-0.70204900	-1.12839000
C	-4.02252200	-0.16237500	-0.58087200
H	-5.14285400	0.20596100	1.22289300
H	-3.46305700	-0.89721800	2.68356300
H	-1.38875900	-1.85107600	1.69141600
H	-2.69706000	-0.65355600	-2.20209500
H	-4.76062900	0.29918000	-1.23039200
C	-0.61331200	-1.77669800	-0.89264200
O	0.24028400	-2.45000900	-0.11023400
H	-0.68580500	-2.09267000	-1.94288500

9’

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.93866800	-0.71473200	-0.36327800
O	-1.00720400	-0.48297300	-0.22848700
C	2.88463400	0.28458100	-1.08243800
C	3.12127000	-1.07553400	-0.74399500
C	2.18873100	1.11489300	-0.18010100
C	2.87835500	-1.60433100	0.56081500
C	1.81538100	0.53465900	1.08660400
C	2.23848600	-0.77149000	1.49586800
H	3.15662800	0.65154300	-2.06625200
H	3.54782000	-1.73371900	-1.49453800
H	2.01586800	-1.13133200	2.49474900

H	1.25620800	1.13987000	1.79473400
C	-1.84963700	0.19163400	0.41184300
C	-3.27896100	0.02396100	0.22243100
C	-4.17425000	0.80984400	0.96395000
C	-3.78974000	-0.91206600	-0.69188500
C	-5.54501800	0.66338500	0.79751600
H	-3.78665900	1.53700400	1.67323500
C	-5.16045100	-1.05343100	-0.85343700
H	-3.09682200	-1.51863300	-1.26519300
C	-6.04343100	-0.26858100	-0.11125200
H	-6.22730500	1.27671600	1.37791100
H	-5.54597100	-1.77992700	-1.56228200
H	-7.11473600	-0.38400700	-0.24136500
C	3.28119600	-3.01410800	0.89819300
H	3.10963400	-3.68366800	0.05118600
C	1.89407200	2.56596500	-0.50333300
H	2.09640500	2.69929300	-1.57320200
C	2.83986200	3.48481000	0.28206400
C	0.42893400	2.94032600	-0.26398800
H	2.67803600	3.37334100	1.35991200
H	3.88703800	3.24659200	0.07393100
H	2.66762500	4.53438900	0.02311300
H	-0.23512200	2.28061800	-0.82908100
H	0.16491100	2.86497900	0.79688700
H	0.24411900	3.97413200	-0.57182900
H	4.34678300	-3.06300900	1.15030900
H	2.71192700	-3.39324200	1.75016400
H	-1.49674400	0.93395900	1.13660300

10

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.35775400	0.18016800	-0.27378400
O	0.34853000	-1.18097700	0.08984300
C	-3.42959800	-0.78506300	-0.98394300
C	-3.40195100	0.47840300	-1.54775300
C	-3.05095600	-0.96596300	0.39663800
C	-2.97903300	1.59930400	-0.75070500
C	-2.88722700	0.17497100	1.24504100
C	-2.85292900	1.46567100	0.66342400
H	-3.66511200	-1.65021800	-1.59475500
H	-3.60802900	0.62151700	-2.60326900
H	-2.66478800	2.34370900	1.27205300
H	-2.74185000	0.04044800	2.31143600

C	1.03932600	-1.71970200	-1.04135300
H	0.58772400	-2.70045200	-1.22630400
C	2.51651200	-1.84595100	-0.77027200
C	3.44785200	-1.40159000	-1.70791700
C	2.96711300	-2.38554200	0.43610800
C	4.81326000	-1.50356800	-1.45157200
H	3.10062400	-0.95788100	-2.63727700
C	4.32907300	-2.48126300	0.69682200
H	2.24141000	-2.70178200	1.17858400
C	5.25589000	-2.04193400	-0.24688400
H	5.52989500	-1.15161800	-2.18719300
H	4.67054500	-2.89470900	1.64074700
H	6.31926200	-2.11582600	-0.04156900
C	-2.86339100	2.95338600	-1.39999400
H	-2.26120800	2.89947000	-2.31196200
C	-3.05416200	-2.35058200	1.02017400
H	-2.57819200	-2.25281100	2.00347000
C	-2.24682200	-3.38008300	0.22651100
C	-4.50049500	-2.81866400	1.23319400
H	-2.65572900	-3.52964700	-0.77870800
H	-1.20823100	-3.05651300	0.13599400
H	-2.26810700	-4.34873300	0.73570900
H	-5.06784100	-2.09669000	1.82814900
H	-5.01395200	-2.94047500	0.27286200
H	-4.52379100	-3.78329200	1.75001300
H	-3.85463600	3.33281100	-1.67248600
H	-2.39899100	3.67693200	-0.72685800
C	2.10112600	1.69703200	1.26601800
C	1.49967100	2.22279000	-0.09911200
C	3.52168900	1.14476700	1.12057700
H	4.25019300	1.94237500	0.94463400
H	3.78820300	0.62973000	2.04678100
H	3.58847400	0.42026300	0.30712100
C	0.42375900	3.28939200	0.08818700
H	0.84899400	4.22748900	0.45572800
H	-0.05164700	3.47824200	-0.87771000
H	-0.34306700	2.94509700	0.78656000
C	2.06561600	2.72540800	2.39142900
H	1.04194700	3.02262500	2.62527400
H	2.50559700	2.29021100	3.29253800
H	2.64308700	3.61741100	2.12610300
C	2.54153200	2.70709100	-1.09968200
H	3.23386500	1.90682800	-1.36662600
H	2.04461600	3.04966100	-2.01171300

H	3.11265300	3.54480600	-0.68668600
O	0.88225500	1.04120800	-0.64818000
O	1.24844400	0.60343000	1.62161600
B	0.57931500	0.19551300	0.47262900
H	0.87373400	-1.09309100	-1.92314600

11

Coordinates (Angstroms)

	X	Y	Z
Ru	0.70776800	-1.03546700	-0.25576900
C	-0.17915500	0.67129900	-1.13891200
C	1.18204200	1.11397200	-0.98909600
C	-1.05062400	0.35665900	-0.02948500
C	1.79925600	0.94914200	0.25317100
C	-0.43446300	0.22107600	1.22559100
C	0.99395700	0.36893300	1.30357400
H	-0.62272700	0.70319600	-2.13189300
H	1.72892200	1.50481100	-1.84086200
H	1.47843100	0.15778500	2.25424700
H	-0.99661500	-0.05245400	2.11104100
C	3.23000300	1.33290300	0.51210600
H	3.79750000	1.39154800	-0.41993700
C	-2.53966900	0.21061400	-0.26364700
H	-2.66109000	-0.19055600	-1.27846100
C	-3.21065200	1.59154300	-0.21859000
C	-3.21606100	-0.76172400	0.70298300
H	-3.09757800	2.03748700	0.77565300
H	-2.76181200	2.27524200	-0.94540900
H	-4.28058700	1.51228800	-0.43693900
H	-2.69662800	-1.72416600	0.71345900
H	-3.22593600	-0.36587800	1.72441200
H	-4.25719700	-0.92766100	0.41014300
H	3.28627600	2.30880800	1.00873800
H	3.71944400	0.60359400	1.16347400

TS2-3

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.32916000	-0.84401200	-0.48069800
O	0.56834400	0.56236900	0.83093100
C	0.31201200	-2.86884100	0.33219800
C	1.36216700	-2.57745300	-0.60010800
C	-1.03761300	-2.94607900	-0.06453100

C	1.07498200	-2.22906900	-1.91537800
C	-1.34048500	-2.54738300	-1.40587100
C	-0.31044000	-2.12787400	-2.27906200
H	0.57530500	-3.06526400	1.36513100
H	2.38997500	-2.54676400	-0.25502400
H	-0.57128500	-1.78924500	-3.27610300
H	-2.37448400	-2.50440300	-1.72579900
C	0.64854000	1.18388900	-0.29139600
C	0.11040500	2.59320700	-0.39448100
C	0.07951300	3.25986200	-1.61674600
C	-0.33802200	3.22683000	0.75994200
C	-0.40944000	4.55973400	-1.68787300
H	0.43693900	2.75668900	-2.51026600
C	-0.81191000	4.53326200	0.69033100
H	-0.32627300	2.67597900	1.69206500
C	-0.85385700	5.19959500	-0.53230300
H	-0.44097400	5.07469600	-2.64293300
H	-1.15820000	5.02914000	1.59214900
H	-1.23418300	6.21524800	-0.58654500
C	2.14237000	-1.86295100	-2.90475400
H	3.09433200	-1.68251000	-2.40452300
C	-2.15461300	-3.40050200	0.85038400
H	-3.05394400	-2.88228500	0.50206000
C	-1.93876400	-3.01843000	2.31456000
C	-2.36627500	-4.91206300	0.68907100
H	-1.11659700	-3.58348600	2.76777900
H	-1.71635300	-1.95146200	2.41008300
H	-2.84100400	-3.23894800	2.89298600
H	-2.56034700	-5.17633900	-0.35497600
H	-1.47915800	-5.46455900	1.01831700
H	-3.21756900	-5.24777800	1.28948200
H	2.26530400	-2.66009000	-3.64613900
H	1.86650100	-0.94724400	-3.43489500
C	-4.43194200	0.13691100	0.25042300
C	-3.72819300	1.50239600	0.52986100
C	-4.79621200	-0.61536900	1.53246300
H	-5.63679800	-0.14444300	2.05095100
H	-5.08123700	-1.64027900	1.27712600
H	-3.94279200	-0.65760700	2.21492900
C	-3.74395300	2.44058200	-0.68098800
H	-4.73922400	2.86205800	-0.85290800
H	-3.04138100	3.25821300	-0.50176800
H	-3.42335000	1.91585300	-1.58557300
C	-5.63734000	0.21280200	-0.67585500

H	-5.35949200	0.60269900	-1.65644100
H	-6.06510800	-0.78428800	-0.81399300
H	-6.41114100	0.85937800	-0.24869700
C	-4.20745500	2.24143600	1.77072100
H	-4.04703100	1.65078800	2.67453600
H	-3.65001100	3.17665800	1.87247700
H	-5.27250900	2.48363800	1.69031500
O	-2.36967400	1.09074900	0.73043800
O	-3.38504100	-0.60322600	-0.40317500
B	-2.15940300	-0.06028700	-0.00726700
H	-0.34685700	0.62070400	-1.25959100
O	1.85374400	1.04674100	-1.01529500
C	4.35763000	0.52776100	1.46647400
C	4.99083700	-0.14694300	0.19993800
C	3.63929600	-0.47052800	2.37816700
H	4.34638200	-1.10362500	2.92204200
H	3.03586800	0.08743900	3.09713900
H	2.95662800	-1.10445200	1.80458300
C	6.05192900	0.72314400	-0.47385400
H	6.97131800	0.76474000	0.11693000
H	6.28693900	0.29884600	-1.45322900
H	5.68462800	1.74231700	-0.62203100
C	5.31206300	1.39424900	2.27334000
H	5.70930500	2.21498100	1.67376900
H	4.78480200	1.82326900	3.12895300
H	6.14752400	0.79600100	2.65111500
C	5.52455500	-1.55341100	0.42712900
H	4.73881400	-2.22954300	0.76987600
H	5.93660900	-1.95101500	-0.50434600
H	6.32244300	-1.54289800	1.17616800
O	3.86317100	-0.21617000	-0.69625500
O	3.34251900	1.36197100	0.88259400
B	2.97090600	0.74701900	-0.28257200

TS3-9

Coordinates (Angstroms)

	X	Y	Z
Ru	0.70546600	-1.02997800	-0.60641600
O	-0.29919600	-0.20591300	-2.34528300
C	2.34563300	-2.11936900	0.32811100
C	2.51725300	-2.65804100	-1.00311500
C	1.16987000	-2.32879500	1.09480400
C	1.42138600	-3.13235200	-1.68897000
C	0.03264100	-2.81466900	0.37886900

C	0.14075200	-3.06762900	-1.01122100
H	3.20264700	-1.66479400	0.80955100
H	3.48755200	-2.59656200	-1.48555300
H	-0.75135300	-3.34509300	-1.56346000
H	-0.93321000	-2.87441000	0.86833300
C	-1.15652900	0.71413700	-2.27205800
C	-2.60573400	0.45291100	-2.04655100
C	-3.50821200	1.51446300	-2.08555500
C	-3.06842500	-0.84429900	-1.84455200
C	-4.86706200	1.28359500	-1.90896500
H	-3.13485900	2.52463800	-2.23110000
C	-4.42671400	-1.07895600	-1.67287500
H	-2.34797700	-1.65309000	-1.81212700
C	-5.32696200	-0.01582600	-1.70243900
H	-5.56801900	2.11206700	-1.92971400
H	-4.78685500	-2.09024900	-1.51096300
H	-6.38837900	-0.19920200	-1.56509000
C	1.47323700	-3.57217000	-3.12232300
H	2.47067700	-3.43491200	-3.54630900
C	1.08414600	-2.06445400	2.58132500
H	0.08825000	-1.64732400	2.75903900
C	2.09994500	-1.04165800	3.08547500
C	1.19952100	-3.39258900	3.34132100
H	3.12677800	-1.41728100	3.00681700
H	1.99882800	-0.10697300	2.52914600
H	1.91274600	-0.82647800	4.14182400
H	0.44261600	-4.11021900	3.01005200
H	2.18465700	-3.84602500	3.18487800
H	1.06740400	-3.23079200	4.41577700
H	1.19968500	-4.62837900	-3.21683100
H	0.76421300	-2.98882000	-3.71794200
C	-1.19970000	1.19467500	2.54748300
C	-2.42752300	0.32678000	2.01714100
C	-1.36606600	2.70442200	2.34057600
H	-2.18597000	3.10722900	2.94326400
H	-0.44008000	3.20138600	2.64564700
H	-1.53953900	2.93828900	1.29010300
C	-2.87949800	-0.77705000	2.97632700
H	-3.29745100	-0.36934500	3.90178100
H	-3.65300900	-1.37134000	2.48192400
H	-2.05656200	-1.44989500	3.23199600
C	-0.83006900	0.94221500	4.00889000
H	-0.62839300	-0.11246800	4.20557100
H	0.07655000	1.50564400	4.24830900

H	-1.62644500	1.27474600	4.68214900
C	-3.64404400	1.15147900	1.59755400
H	-3.37670400	1.87583100	0.82771300
H	-4.39427400	0.48156000	1.16832900
H	-4.08934000	1.67534500	2.44997500
O	-1.92043800	-0.32616300	0.85315900
O	-0.10266000	0.75847000	1.73962200
B	-0.62252100	0.10427900	0.59574800
H	-0.96625700	1.63918400	-2.83961300
O	-0.78217300	1.58807000	-0.57774000
C	2.44114900	3.11684900	-0.35746500
C	2.77085700	1.68026900	-0.89143600
C	2.60752900	3.22459400	1.16058800
H	3.66021800	3.19822700	1.45657800
H	2.17800900	4.17386900	1.49048500
H	2.06880000	2.41586000	1.66484200
C	2.98084500	1.62067600	-2.40312900
H	3.94679800	2.04564500	-2.69003800
H	2.94625800	0.57393800	-2.71803900
H	2.18771600	2.15700300	-2.93083000
C	3.18915800	4.23359600	-1.06801800
H	2.95349200	4.25744600	-2.13344000
H	2.90839500	5.19679500	-0.63491300
H	4.26991900	4.10695300	-0.94786900
C	3.90368400	0.97645300	-0.16387100
H	3.65621300	0.80812800	0.88580700
H	4.09693100	0.00874800	-0.63461900
H	4.82018600	1.57185300	-0.22251900
O	1.52450400	1.01624000	-0.61398200
O	1.03274200	3.24646800	-0.62988400
B	0.49451700	1.98359700	-0.59360000

TS4-5

Coordinates (Angstroms)

	X	Y	Z
Ru	2.07203800	0.15052400	-0.47044300
O	0.84834500	1.81168200	-0.77343400
C	4.27006300	0.70991800	-1.12221700
C	4.10563300	-0.68081600	-0.83441100
C	3.88041300	1.66530000	-0.17954000
C	3.73330700	-1.14661600	0.45267600
C	3.38934300	1.20387300	1.08226000
C	3.37578400	-0.16331300	1.40705700
H	4.60500200	1.01022400	-2.10744100

H	4.32125000	-1.41090700	-1.60677200
H	3.01227800	-0.46371700	2.37973400
H	2.99374200	1.91574700	1.79634400
C	0.01108900	0.12760200	3.26030200
C	-0.21559300	-1.39186400	2.88077900
C	-1.27898300	0.88746800	3.59499300
H	-1.72934000	0.53027100	4.52698600
H	-1.03061700	1.94572000	3.72152200
H	-2.01494100	0.79941000	2.79641400
C	0.91272000	-2.32093800	3.34168600
H	0.93423500	-2.42982900	4.43027900
H	0.75444700	-3.30882700	2.89919400
H	1.88916100	-1.96570900	3.01175000
C	0.99760100	0.34575200	4.40829400
H	1.97439400	-0.10054300	4.21166300
H	1.14285200	1.41913700	4.55919800
H	0.61155700	-0.07942200	5.34075500
C	-1.53959800	-1.97060600	3.37904700
H	-2.38377700	-1.41218500	2.97760800
H	-1.62729000	-3.00959200	3.04514000
H	-1.58231300	-1.96165800	4.47364500
O	-0.22519500	-1.38912500	1.45601800
O	0.56490700	0.68829600	2.07538300
B	0.23350900	-0.13550300	0.95570100
C	-0.36229400	1.60408100	-1.11832600
H	-0.57628600	0.93344300	-1.96065100
C	-1.28293100	2.77737000	-0.98281500
C	-1.39499100	3.42372200	0.24981600
C	-1.98330500	3.24856800	-2.08791500
C	-2.22377100	4.53232900	0.37179600
H	-0.84442000	3.02561700	1.09745500
C	-2.79286500	4.37608700	-1.97031600
H	-1.89907800	2.72868000	-3.03819300
C	-2.91971700	5.01197900	-0.73916400
H	-2.32815700	5.02747300	1.33233600
H	-3.33318700	4.74934800	-2.83477900
H	-3.56220000	5.88191000	-0.64220700
C	-4.35992100	-0.47570300	0.65120500
C	-4.35608700	0.16537200	-0.78709000
C	-5.34474400	0.15386700	1.62849500
H	-5.25778300	-0.33999600	2.60010400
H	-5.14506700	1.21709000	1.76973300
H	-6.37276100	0.03082200	1.27323000
C	-5.14600500	-0.61145500	-1.83080700

H	-4.77988200	-1.63406000	-1.93547900
H	-6.20711000	-0.64570900	-1.56386700
H	-5.05337700	-0.11591600	-2.80062600
C	-4.53739000	-1.99271200	0.64771000
H	-3.83926200	-2.46765500	-0.04148700
H	-4.33579100	-2.37628900	1.65119200
H	-5.55656700	-2.27325400	0.36638500
C	-4.78873000	1.63237800	-0.78978500
H	-4.20386500	2.22383900	-0.07910100
H	-4.61307000	2.05154800	-1.78242800
H	-5.85078100	1.73871500	-0.55125500
O	-2.96170200	0.13515500	-1.14549600
O	-3.02957500	-0.19612100	1.11513600
B	-2.24683300	0.09611300	0.02652900
O	-0.94078000	0.49709000	0.11190600
C	3.72905200	-2.61044700	0.79006400
H	3.81501600	-3.21315700	-0.11359300
C	3.88005800	3.15313300	-0.46128500
H	3.06223700	3.57072900	0.13689900
C	3.58928000	3.49415100	-1.92303300
C	5.20033400	3.77214300	0.01915200
H	4.40187400	3.17732300	-2.58637100
H	2.65942900	3.01843100	-2.24407800
H	3.48268300	4.57688500	-2.03653400
H	5.37658700	3.56592200	1.07922400
H	6.04530900	3.36789700	-0.54900100
H	5.18635800	4.85745400	-0.11991500
H	4.56271000	-2.84382200	1.46098100
H	2.79425100	-2.88863900	1.27857700
C	-0.58529500	-2.90366900	-2.09538800
C	0.59792800	-3.72320600	-1.48219200
C	-0.47493400	-2.72560400	-3.61186900
H	-0.66396000	-3.66116400	-4.14649300
H	-1.21369300	-1.98541000	-3.92997900
H	0.51699300	-2.35685800	-3.88879700
C	0.27117900	-4.31526900	-0.10915100
H	-0.44969900	-5.13548700	-0.18283200
H	1.19362800	-4.70940100	0.32836000
H	-0.11939000	-3.53921900	0.55509600
C	-1.96899400	-3.41181900	-1.72658000
H	-2.09086100	-3.44426300	-0.64311800
H	-2.71988400	-2.73229100	-2.13903800
H	-2.14058400	-4.41360500	-2.13364400
C	1.17132700	-4.79562400	-2.39904100

H	1.55731400	-4.36602100	-3.32533100
H	1.99484100	-5.30927300	-1.89453700
H	0.40805400	-5.54036800	-2.64740900
O	1.58796200	-2.70533100	-1.28507500
O	-0.40050100	-1.61104000	-1.50861500
B	0.93427700	-1.48048200	-1.14408200
H	1.55289800	-0.37053000	-1.91908300

TS5-6

Coordinates (Angstroms)

	X	Y	Z
Ru	0.96148200	-0.90809100	-0.06322200
O	-0.28927100	-1.59617900	-1.61688100
C	3.00851000	-0.70507300	-1.00679900
C	2.97393900	-2.07839200	-0.59958200
C	2.83193800	0.34432500	-0.08225100
C	2.65846400	-2.43636300	0.70884900
C	2.46380100	-0.01463500	1.25318500
C	2.30899200	-1.37648200	1.61126200
H	3.19442700	-0.47862700	-2.04942300
H	3.13332500	-2.84898100	-1.34632100
H	1.98995500	-1.62071500	2.61918900
H	2.23354200	0.76454500	1.96932700
C	-0.86944400	-2.11650400	-0.57051800
H	-0.57884700	-3.14433400	-0.28463000
C	-2.35263600	-1.88845300	-0.37885700
C	-3.00492100	-2.35965600	0.75836600
C	-3.08016700	-1.25276100	-1.38113300
C	-4.37773000	-2.18758800	0.90299600
H	-2.43300500	-2.85546200	1.54052600
C	-4.45567600	-1.09390300	-1.24513300
H	-2.54465000	-0.87716200	-2.24468200
C	-5.10682700	-1.55632400	-0.10294400
H	-4.87879000	-2.54886800	1.79575100
H	-5.02149000	-0.60162200	-2.03062700
H	-6.17911800	-1.42477800	0.00500000
C	2.58220100	-3.86957100	1.15440000
H	2.56620400	-4.54961900	0.29966100
C	3.00878900	1.80320800	-0.44444500
H	2.32781000	2.35849800	0.20794200
C	2.63163400	2.12168500	-1.89119400
C	4.44922800	2.23185000	-0.13181700
H	3.35639100	1.70944300	-2.60221500
H	1.64420900	1.71731600	-2.13342600

H	2.61119400	3.20514900	-2.04115900
H	4.70096900	2.04533800	0.91670100
H	5.16122300	1.67903700	-0.75460400
H	4.58386600	3.29986700	-0.32872900
H	3.44412700	-4.12758600	1.77900700
H	1.67914000	-4.04310500	1.74664200
C	-0.85494900	2.89333900	0.73195900
C	-2.04483100	2.11767900	0.08039300
C	-0.19341800	3.88084800	-0.23211100
H	-0.83531600	4.74511700	-0.42676000
H	0.74084500	4.24142700	0.20833300
H	0.04049000	3.39751400	-1.18442000
C	-2.98612800	1.49386900	1.11474000
H	-3.58490200	2.25464000	1.62496400
H	-3.65894400	0.79854900	0.60818400
H	-2.42327300	0.92919700	1.86368800
C	-1.17983000	3.58454700	2.04857300
H	-1.51653900	2.86819500	2.79962800
H	-0.28747700	4.08631100	2.43329700
H	-1.96098700	4.33886600	1.90695100
C	-2.84654000	2.89894600	-0.95045200
H	-2.21858600	3.22360300	-1.78207400
H	-3.63667100	2.25811400	-1.35114900
H	-3.31420900	3.77833800	-0.49519600
O	-1.36485100	1.04249600	-0.58345500
O	0.08551900	1.83318800	0.98368300
B	-0.19794900	0.78346900	0.10742100
H	-0.48792500	-1.38313000	0.62358300

TS6-10

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.26192800	-0.72875400	-0.19491700
O	0.23056500	-0.37785800	1.21259000
C	-3.40205600	-0.88375900	0.86385300
C	-3.40050900	-1.89800600	-0.08029600
C	-2.92245900	0.42799300	0.50946100
C	-2.92000900	-1.65264500	-1.41345800
C	-2.67736200	0.71805000	-0.86928600
C	-2.68842600	-0.32184600	-1.83783000
H	-3.68148700	-1.09625400	1.88954200
H	-3.66518800	-2.91114400	0.20493100
H	-2.42348800	-0.11816700	-2.86847900
H	-2.39256700	1.72507000	-1.15339700

C	0.71720200	-1.64763200	0.94302600
H	0.31540300	-2.38089400	1.65844000
C	2.22910000	-1.72630000	0.91219200
C	2.92762700	-2.32585900	-0.13158200
C	2.93699900	-1.18017200	1.98354700
C	4.31801200	-2.38386100	-0.10712700
H	2.38260300	-2.72277100	-0.98343600
C	4.32746600	-1.22809100	2.00594300
H	2.38990400	-0.70349800	2.79159500
C	5.02174000	-1.83238700	0.95999300
H	4.85255700	-2.84681800	-0.93097900
H	4.86878600	-0.79345800	2.84076100
H	6.10661500	-1.87052900	0.97570300
C	-2.81985600	-2.79225200	-2.39293400
H	-2.46643500	-3.70186000	-1.90054700
C	-2.82327800	1.54726800	1.52758100
H	-2.11615100	2.27262900	1.10907500
C	-2.25124000	1.08086600	2.86860300
C	-4.19141100	2.22087200	1.69646300
H	-2.93984000	0.40874700	3.39389800
H	-1.29842500	0.56671600	2.71707300
H	-2.08742000	1.94497000	3.51973200
H	-4.56956800	2.60682000	0.74454800
H	-4.92826200	1.51010700	2.08824000
H	-4.12391100	3.05545200	2.40110700
H	-3.79929200	-3.00559100	-2.83476100
H	-2.12522600	-2.55143400	-3.20071900
C	1.50645900	2.48064700	-0.35708400
C	2.19219600	1.49430900	-1.37013300
C	2.11936100	2.42108300	1.04367100
H	3.12204600	2.85841900	1.06396600
H	1.47955600	2.98542300	1.72761200
H	2.16930000	1.39099100	1.40145700
C	1.98802600	1.90289200	-2.83059100
H	2.56321600	2.79720100	-3.08931200
H	2.31455400	1.08193400	-3.47433200
H	0.93013500	2.09335500	-3.03289800
C	1.42561700	3.92634100	-0.82898600
H	0.86197300	4.01441400	-1.75955400
H	0.92351900	4.53156600	-0.06901200
H	2.42758100	4.33952200	-0.98536600
C	3.66625600	1.22362300	-1.09624400
H	3.81078700	0.77258900	-0.11286900
H	4.05443100	0.52424200	-1.84182600

H	4.24823400	2.14978200	-1.15639100
O	1.45873300	0.27595600	-1.17470900
O	0.17292600	1.94925200	-0.26699200
B	0.27571700	0.58566400	-0.52280400
H	0.36778200	-1.99629300	-0.10325300

TS7-8

Coordinates (Angstroms)

	X	Y	Z
Ru	0.48381400	-1.28944800	-0.33743500
O	1.00732400	0.54095000	-1.12205300
C	1.48550300	-3.52184100	-0.77974100
C	0.18645100	-3.47169600	-0.17603800
C	2.53650800	-2.79077800	-0.25196300
C	-0.01228700	-2.91456800	1.11507500
C	2.26569100	-2.00066400	0.92489000
C	1.07759400	-2.17820500	1.65716000
H	1.62719700	-4.09174600	-1.69256900
H	-0.64646200	-3.97453500	-0.65516800
H	0.95574900	-1.65277900	2.59755200
H	3.03281000	-1.34848900	1.32643700
C	0.14451400	1.90889900	2.45551400
C	-1.35364900	1.46364900	2.43144600
C	0.38469200	3.20919900	1.69337200
H	-0.02274000	4.06696800	2.23694800
H	1.45808200	3.36027400	1.55846600
H	-0.06309300	3.17345800	0.69870700
C	-1.71147800	0.50535400	3.56992700
H	-1.75708000	1.02160100	4.53310600
H	-2.68912600	0.05774200	3.37077900
H	-0.97668500	-0.30173800	3.64665900
C	0.76675300	1.99486700	3.84271100
H	0.74392900	1.03211400	4.35721100
H	1.81022300	2.30828600	3.75387500
H	0.24095400	2.73311300	4.45684300
C	-2.36719500	2.59753100	2.36694900
H	-2.23678100	3.18942500	1.45995300
H	-3.38074700	2.18478600	2.36425600
H	-2.27140600	3.25567000	3.23650900
O	-1.42523800	0.71441100	1.20693600
O	0.77964800	0.83602500	1.73526800
B	-0.15665000	0.26239200	0.88507800
C	2.21853000	1.16296300	-0.89789500
H	2.57916900	1.02744800	0.13787600

C	2.10798700	2.65368200	-1.16540300
C	3.15005300	3.51621100	-0.82038100
C	0.95730900	3.18141900	-1.74964600
C	3.04181500	4.88585500	-1.04073900
H	4.05022400	3.11075300	-0.36181900
C	0.84807300	4.55217000	-1.97245700
H	0.15031900	2.49780300	-1.99370000
C	1.88576700	5.40969400	-1.61644500
H	3.85606500	5.54712200	-0.75772200
H	-0.05556900	4.95475700	-2.42201000
H	1.79539800	6.47868500	-1.78509100
C	-1.31030500	-3.08860100	1.84930800
H	-2.13609900	-3.09718400	1.13565200
C	3.92650200	-2.87291500	-0.84513300
H	3.86764600	-3.56699600	-1.69224200
C	4.90450200	-3.46594400	0.17992600
C	4.42842500	-1.52909300	-1.37617700
H	5.03478500	-2.79107000	1.03250700
H	4.54943400	-4.42799200	0.56091200
H	5.88657100	-3.61788400	-0.27762100
H	3.75863000	-1.14551800	-2.14904500
H	4.48332000	-0.78161700	-0.57856500
H	5.42941400	-1.64087400	-1.80408600
H	-1.30959400	-4.02722200	2.41358100
H	-1.47802100	-2.26449600	2.54614100
H	3.01109700	0.77098700	-1.55986800
C	-3.79475500	-1.02233300	-0.89831400
C	-3.41205100	0.28517700	-1.69603300
C	-4.25248100	-0.75923500	0.53777700
H	-5.21613900	-0.24208900	0.56335300
H	-4.36703900	-1.71855100	1.05149100
H	-3.50508900	-0.16940100	1.06955300
C	-3.64473500	0.16957100	-3.20394900
H	-4.71022400	0.13044500	-3.44915900
H	-3.20602500	1.04313100	-3.69224700
H	-3.15662700	-0.72067800	-3.60963700
C	-4.80511200	-1.92292900	-1.59987000
H	-4.44669300	-2.24812400	-2.57784800
H	-4.98351500	-2.81382900	-0.99139400
H	-5.76048900	-1.40464800	-1.73018300
C	-4.05303800	1.56081600	-1.16323700
H	-3.76151700	1.73747100	-0.12745300
H	-3.71453200	2.41190500	-1.76004300
H	-5.14477400	1.50792500	-1.22885300

O	-1.99403000	0.38754100	-1.51101600
O	-2.53975500	-1.72445400	-0.82268200
B	-1.52376400	-0.80869300	-1.03862800
H	-0.43176500	-1.23249200	-1.71259000