

## Supporting Information

### Hydrogenation of CO<sub>2</sub> to methanol by the diphosphine–ruthenium(II) cationic complex: a DFT investigation to shed light on the decisive role of carboxylic acids as promoters

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### S1. Selection of the computational protocol.

The optimization of the complex **Ru2<sup>+</sup>** has been performed using several exchange–correlation functionals, including functionals developed to properly take into consideration weak interactions such as M06-L and  $\omega$ -B97XD, to test the reliability of the B3LYP results. Furthermore, both LANL2DZ and SDD effective core potentials (ECPs) were tested for describing Ru atom. Geometric parameters that include calculated bond distances and angles were compared to the experimental ones reported by Sun and co-workers,<sup>12</sup> and all the values are listed in table S1. According to our results, the inclusion of dispersion forces is not really beneficial, while the well-known B3LYP functional shows the best overall fitting of the selected parameters. Moreover, the use of SDD pseudo potential over LANL2DZ leads to bond distances that are closer to the experimental values. Based on those observations, B3LYP/SDD method has been selected for our DFT study. However, the search of critical transition states along with the check of very

	Exp	M06L/ LANL2DZ	B3LYP/ SDD	B3LYP/ LANL2DZ	$\omega$ -B97XD/ LANL2DZ	$\omega$ -B97XD/ SDD
<b>Ru1–Cl1</b>	2.409	2.491	2.433	2.439	2.453	2.446
<b>Ru1–P2</b>	2.328	2.335	2.342	2.394	2.328	2.333
<b>Ru1–P1</b>	2.329	2.358	2.362	2.407	2.362	2.359
<b>Ru1–C4</b>	2.221	2.248	2.284	2.316	2.286	2.243
<b>P3–O1</b>	1.480	1.505	1.498	1.503	1.502	1.502
<b>P1–Ru1–Cl1</b>	87.8	102.6	89.1	84.8	101.3	101.7
<b>P2–Ru1–Cl1</b>	85.1	88.7	88.4	84.4	89.3	89.0
<b>P1–Ru1–P2</b>	86.8	85.7	92.7	89.6	86.0	86.0

high energy barriers were calculated using  $\omega$ -B97XD functional to confirm the reliability of the B3LYP functional.

Table S1. DFT optimized geometrical structure of cationic portion of **Ru2<sup>+</sup>**. Selected bond lengths (Å) and angles (°) compared with available experimental values<sup>12</sup>

## S2. Scan calculations

The computational protocol used for the scan calculations discussed below is the same described in the “Computational Details” section of the main text. Therefore, Ru metal center, has been described using the relativistic compact Stuttgart/Dresden (SDD) effective core potential<sup>34</sup>. The standard 6-31G\* basis sets of Pople and co-workers were employed for the rest of the atoms, except C and H atoms of phenyl rings on which the smaller 3-21G basis were used. B3LYP functional has been selected. In order to get a better estimation of the energy associated to the maxima of each scan calculation, the corresponding structures have been used to run single point calculations performed using the bigger 6-311+G\*\* basis sets for all the atoms but Ru, for which SDD was kept. Single point calculations included also the effect of the solvent following the method described in the main text.

### S2.1. Scan\_1

In **scan\_1**, shown in figure S1, the H<sub>2</sub> molecule approaches to the metal center moving in between the p-cymene molecule and one phenyl ligand of Ru. The relaxed scan calculation involves 10 steps in which the initial Ru-H<sub>2</sub> distance in **1\_H<sub>2eq</sub>\*** is set to 3.830 Å and is decreased by 0.200 Å to the final bond distance of 1.830 Å in **2\_H<sub>2eq</sub>\***. The scan calculation underlines the presence of a maximum **ts1\_H<sub>2eq</sub>\***, whose structure has been used as starting structure for the search of a transition state. However, all our attempts, that include also the use of ω-B97XD and M06-L functionals, have failed and no stationary point with a unique imaginary frequency has been intercepted.

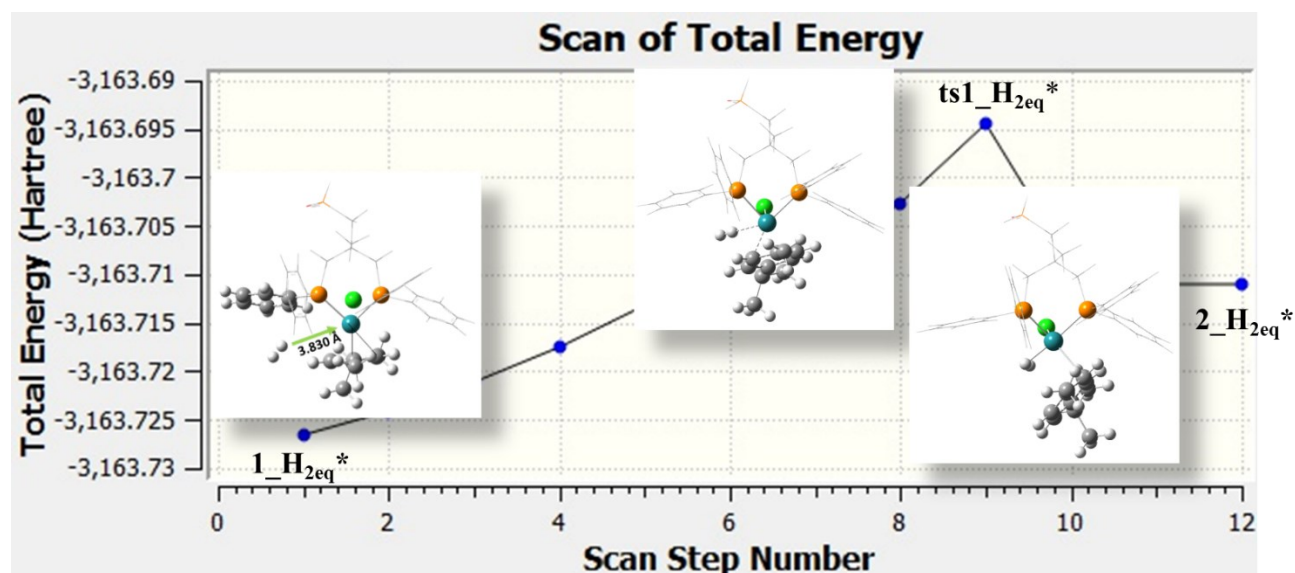


Figure S1. Calculated **Scan\_1** and related structures.

### S2.2. Scan\_2

In **scan\_2**, shown in figure S2, the H<sub>2</sub> molecule approaches to the metal center from the axial direction. The relaxed scan calculation involves 9 steps in which the initial Ru-H<sub>2</sub> distance in **1\_H<sub>2eq</sub>\*** is set to 3.500 Å and is decreased by 0.200 Å to the final bond distance of 1.700 Å in **2\_H<sub>2eq</sub>\***. The scan calculation underlines the presence of a maximum **ts1\_H<sub>2eq</sub>\***, whose structure has been used as starting structure for the search of a transition state, which, also in this case, was not found. The following steps of the investigated reaction mechanism are discussed in the main text.

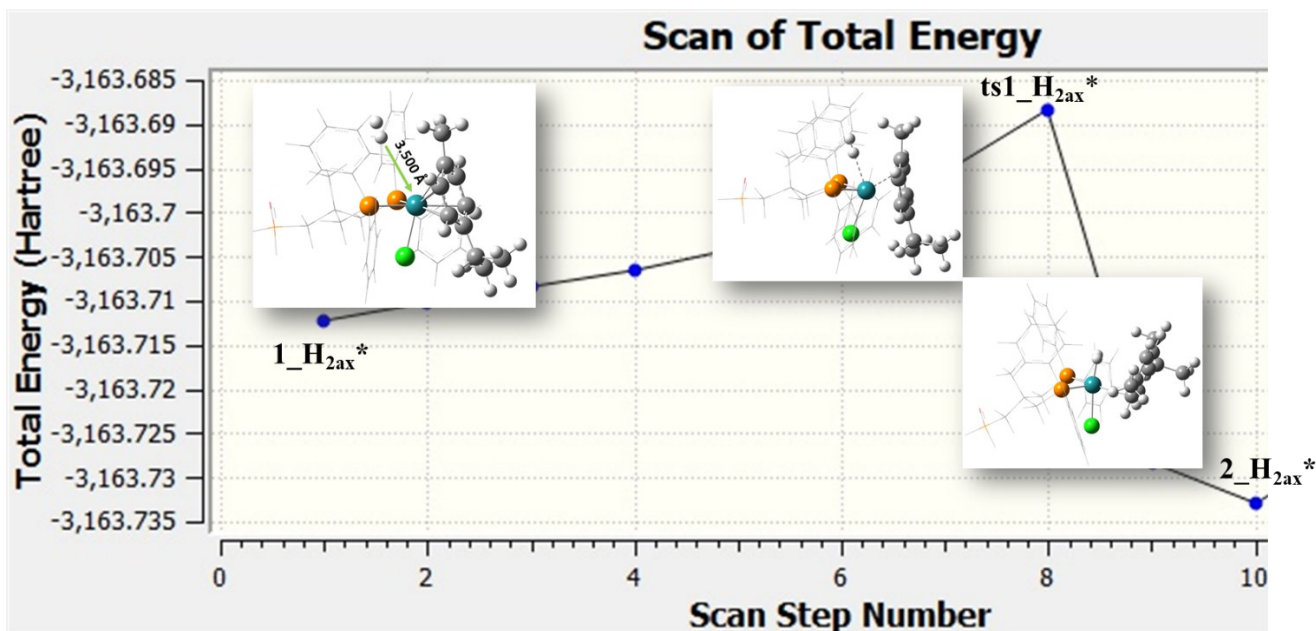


Figure S2. Calculated **Scan\_2** and related structures.

### S2.3. Scan\_3

In **scan\_3**, shown in figure S3, carbon dioxide approaches to the metal center from the equatorial direction. The relaxed scan calculation involves 8 steps in which the initial Ru-O distance in **1\_CO<sub>2eq</sub>\*** is set to 3.200 Å and is decreased by 0.100 Å to the final bond distance of 2.400 Å in **2\_CO<sub>2eq</sub>\***. The scan calculation underlines the presence of a maximum **ts1\_CO<sub>2eq</sub>\***, whose structure has been used as starting structure for the search of a transition state, with no success. As discussed in the main text, the coordination of a hydrogen molecule in axial position leads to the formation of **3\_H<sub>2ax</sub>** intermediate and the reaction does not continue.

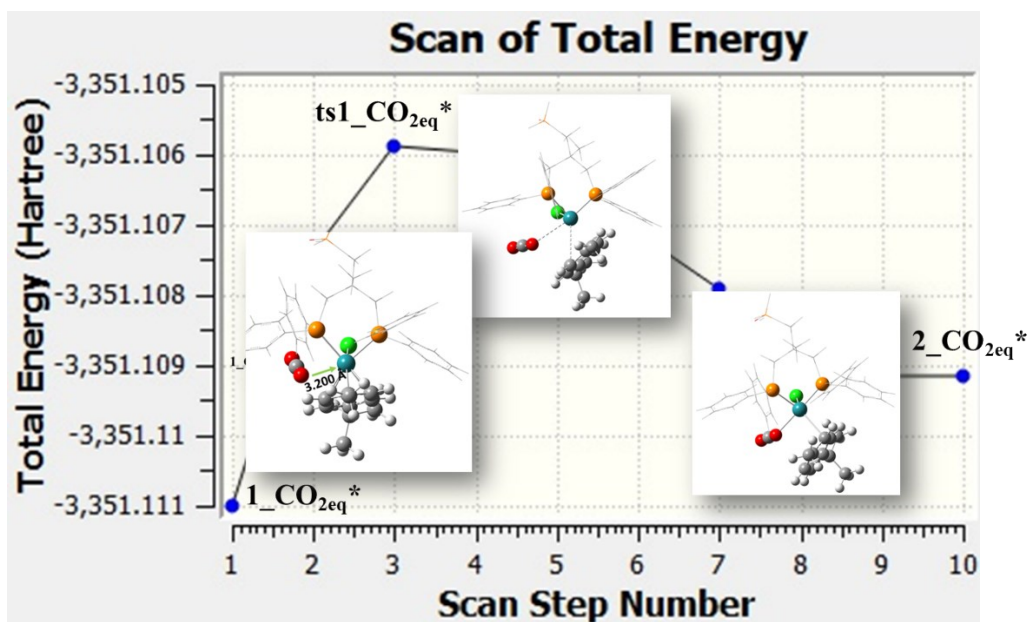


Figure S3. Calculated **Scan\_3** and related structures.

#### S2.4. Scan\_4

In **scan\_4**, shown in figure S4, carbon dioxide approaches to the metal center from the axial direction. The relaxed scan calculation involves 10 steps in which the initial Ru-O distance in  $1\_CO_{2eq}^*$  is set to 4.174 Å and is decreased by 0.200 Å to the final bond distance of 2.174 Å in  $2\_CO_{2ax}^*$ . The scan calculation underlines the presence of a maximum  $ts1\_CO_{2eq}^*$ , whose structure has been used as starting structure for the search of a transition state, which has been identified. The further details of the reaction mechanism are discussed in the main text.

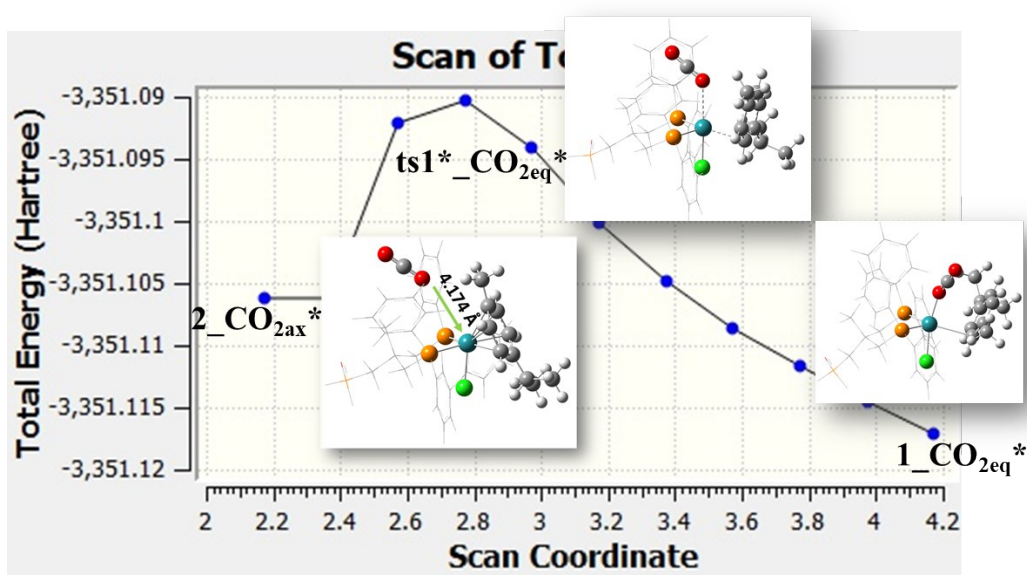


Figure S4. Calculated **Scan\_4** and related structures

### S3. Potential spontaneous proton transfer from one acetic acid molecule to chloride for the production and release of HCl.

To investigate the potential spontaneous proton transfer from a molecule of acetic acid to the chloride, with consequent formation and release of HCl, the Ru<sup>2+</sup> cation complex has been optimized in presence of a molecule of the acid, as in **Ru<sup>2+</sup>+CH<sub>3</sub>OH** shown in figure S5a. Our calculations show that no spontaneous proton occurs during the relaxation. The same result has been obtained also using ωB97XD functional to better taking into account the weak interactions. Moreover, the structure of the complex in which acetate anion has replaced the chloride anion while HCl has been formed and released, as in figure 5b, is 18.2 kcal/mol less stable than the starting complex, **Ru<sup>2+</sup>+CH<sub>3</sub>OH**.

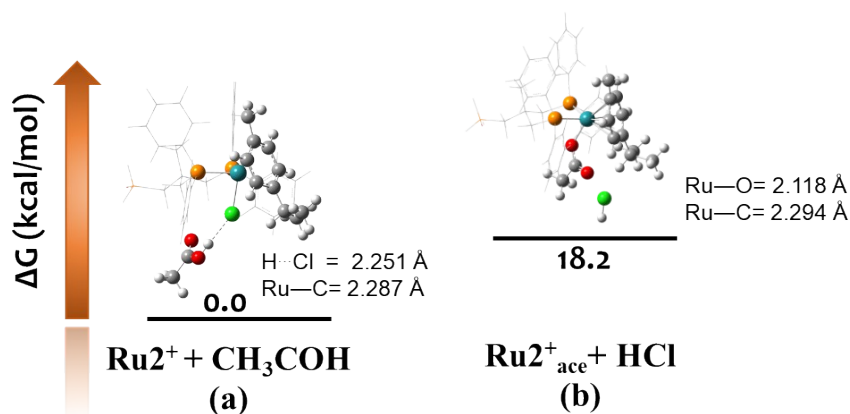


Figure S5. Optimized structures of **Ru<sup>2+</sup>+CH<sub>3</sub>OH** and **Ru<sup>2+</sup><sub>ace</sub>+HCl**. Energies are in kcal/mol and relative to the most stable intermediate **Ru<sup>2+</sup>+CH<sub>3</sub>OH**.

Starting from **Ru<sup>2+</sup><sub>ace</sub>+HCl**, a relaxed scan calculation, **Scan\_5**, has been performed in which the H<sub>2</sub>-Ru distance is decreased from 1.908 to 1.608 Å, as shown in figure S6. The scan shows that *p*-cymene is not released as a consequence of the hydrogen coordination. Those findings further support that the active specie formation occurs following the mechanism presented previously.

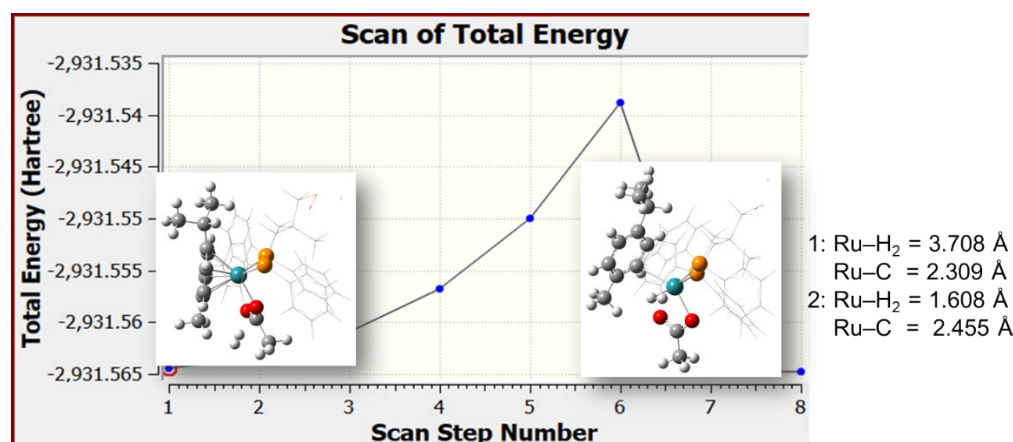


Figure S6. Calculated **Scan\_5** and related structures.

### S4. Further investigated mechanisms for the methanol production.

#### S4.1.

Figure S7 shows the B3LYP gas-phase zero-point-corrected energy profile for the hydrogenation reaction of formate by an uncoordinated H<sub>2</sub> molecule that leads to the production of formic acid. The computed energy barrier is very high and corresponds to 68.7 kcal/mol. To test the reliability of the B3LYP results, the discussed stationary points have been re-optimized using the exchange–correlation functional  $\omega$ -B97XD, whose calculated energy barrier is 67.7 kcal/mol. Such calculations have demonstrated that the energetics is not significantly influenced by the inclusion of dispersion corrections. Due to the prohibitive energy barrier, this reaction is not likely to take place and the further steps were not investigated.

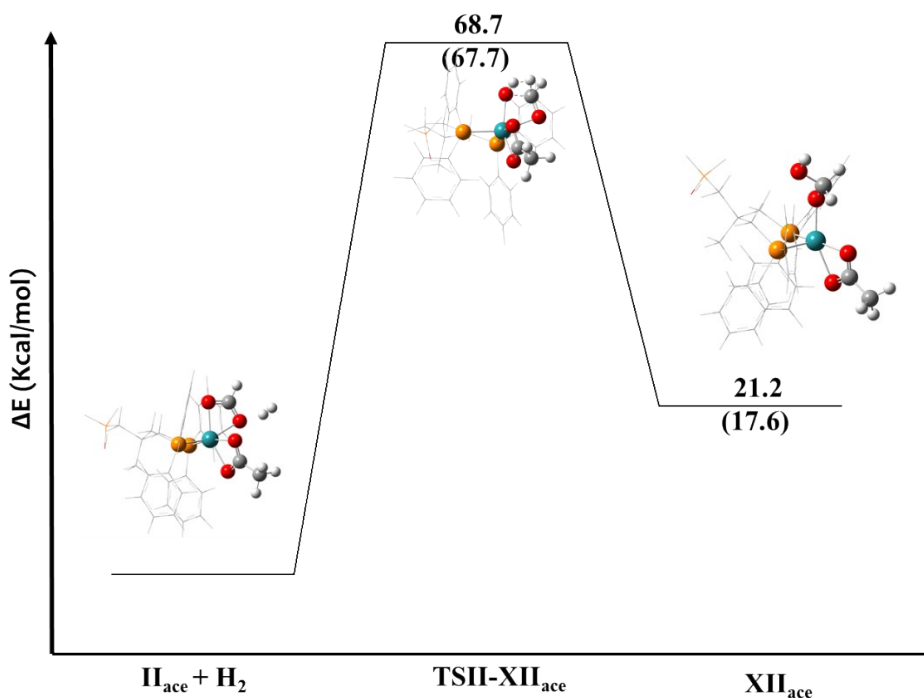


Figure S7. Calculated B3LYP gas-phase zero-point-corrected energy profile for the hydrogenation reaction of formate by an uncoordinated H<sub>2</sub> molecule.  $\omega$ -B97XD calculated values are shown in parenthesis. Energies are in kilocalories per mole.

#### S4.2.

As mentioned in the main text, the carboxylic acid plays a decisive role in replacing the p-cymene ligand, and favoring the formation of the metal-hydride active specie and the release of HCl. Furthermore, it has been observed that in presence of carboxylic acid the CO<sub>2</sub> molecule coordinate to the metal center via a C–Ru bond that activates the molecule toward the nucleophilic attack of the metal-coordinated hydride, which leads to the formation of formate. We have also investigated if the carboxylic acid has a direct role in the formate-to-methanol conversion. In this regard, the heterolytic breaking of an uncoordinated H<sub>2</sub> molecule that leads to a proton transfer to one oxygen of the formate and a hydride attack to the carboxylic carbon of the acetate has been investigated. The transition state **TSII-XIII<sub>ace</sub>** has been intercepted. A unique imaginary frequency of  $-1306.19i$  cm<sup>-1</sup> is calculated along a computed energy barrier of 61.1 kcal/mol. The formed **XIII<sub>ace</sub>** intermediate is 47.6 kcal/mol less stable than the previous one. Because of the high energy barrier and the endergonic process involved, the reaction has not been taken



in consideration for further investigation. The corresponding calculated B3LYP gas-phase zero-point-corrected energy profile along with the optimized structures of intermediates and transition state are reported in figure S8. Also in this case, the intermediates and transition state have been optimized using  $\omega$ -B97XD functional and very similar values have been obtained, confirming that this mechanism is not likely to occur.

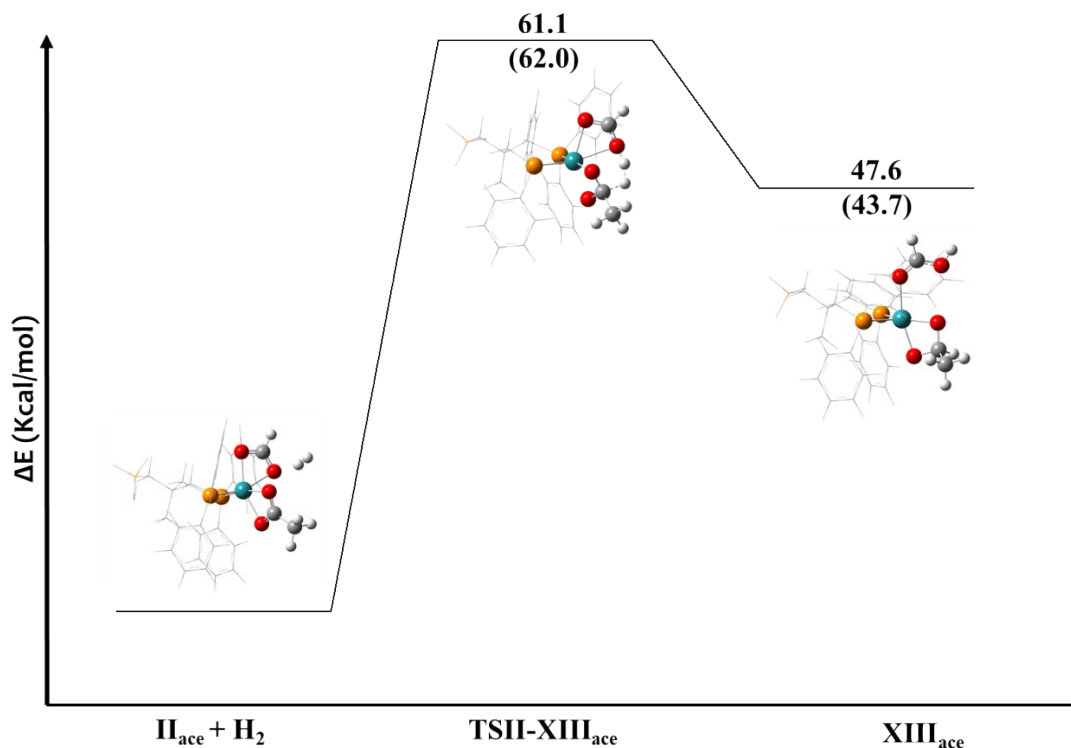


Figure S8. Calculated B3LYP gas-phase zero-point-corrected energy profile for the heterolytic breaking of an uncoordinated  $\text{H}_2$  molecule.  $\omega$ -B97XD calculated values are shown in parenthesis. Energies are in kilocalories per mole.

### S5. Evaluation of the thermal corrections to free Gibbs energies at the experimental temperature (160°C) vs the room temperature.

The effect of the thermal corrections at the experimental temperature (160°C) has been evaluated by comparing the values of the  $\delta E$ s for the methanol production assisted by both the acetate and hexanoate anions. Therefore, the geometries of the  $\text{II}_{\text{ace}}$  and  $\text{TSVI}_{\text{ace}}$ , and those of  $\text{X}_{\text{hex}}$  and  $\text{TSX}_{\text{hex}}$  have been fully relaxed at the experimental temperature, and the optimized structures have been used to run single point calculations considering the solvent effects as described in the computational method. The values at both 25 and 160° C are reported in table S2.



Table S2. Calculated  $\delta E$ s at room temperature and experimental temperature (160°C)

	T=25° C		T=160° C	
Energy barrier	$I_{\text{ace-TSVI}_{\text{ace}}}$	$I_{\text{hex-TSVI}_{\text{hex}}}$	$I_{\text{ace-TSVI}_{\text{ace}}}$	$I_{\text{hex-TSVI}_{\text{hex}}}$
Free energy (kcal/mol)	24.9	22.6	23.7	20.6

The computed energy barriers at 160° C are very similar to those computed at room temperature and confirm the lower energy barrier in presence of hexanoate anion. Based on those results, all the calculations have been performed including room temperature.

### S6. Details concerning the approach used to calculate the Gibbs free energy in solution.

Following the procedure proposed by Wertz<sup>1</sup> and previously adopted<sup>2</sup> to properly handle the change of translational and rotational entropy occurring when a solute is transferred from the gas phase into the solution phase, Gibbs free energies in solution for each species, have been calculated as:

$$G_{298K} = E_{\text{elec}} + G_{\text{solv}} + \text{ZPE} + H_{\text{vib}} + 6 kT - T(S_{\text{vib}}) - T[0.54 \times (S_{\text{rot}} + S_{\text{trans}} - 14.3) + 8.0],$$

where  $T=298K$  and the term  $6kT$  accounts for the potential and kinetic energies of the translational and rotational modes. Such procedure involves decomposition of the solute solvation into three steps: (1) the solute is treated as an ideal gas and compressed from 1 atm (1 mol, 24.5 L) to 55.5 mol/L; (2) then the solute is transferred to a hypothetical 55.5 mol/L solution, which has the intermolecular interaction of a dilute solution; (3) finally this hypothetical solution is diluted to 1M (1 mol, 1L). In the first step, due to the compression, the entropy loss of solute is:

$$\Delta S = 1.987 \ln \left( \frac{V_{\text{fin}}}{V_{\text{init}}} \right) = 1.987 \ln \left( \frac{1}{\frac{55.5}{24.5}} \right) = -14.3 \text{ e.u.}$$

In the second step the assumption by Wertz is that the solute loses 46% of its translational and rotational entropies, that means only 54% of translational and rotational entropies is conserved. Finally, due to the dilution of the solution in the third step the entropy gain is:

$$\Delta S = 1.987 \ln \left( \frac{V_{\text{fin}}}{V_{\text{init}}} \right) = 1.987 \ln \left( \frac{1}{55.5} \right) = 8 \text{ e.u.}$$

Therefore, from calculated gas-phase translational and rotational entropies, the entropies in solution can be calculated as:

$$0.54 \times (S_{\text{rot}} + S_{\text{trans}} - 14.3) + 8.0$$

By using the ideal gas translational entropy, the Wertz approximation and the continuum solvation free energies, free energies at standard (1M) concentration can be calculated.

### S7. Cartesian coordinates (Å) and zero-point corrected energies, (Hartrees) of optimized structures of stationary points for the hydrogenation of CO<sub>2</sub> in absence of acid.

H2

Zero-point energy = -1.168366

H	0.00000000	0.00000000	0.37139700
H	0.00000000	0.00000000	-0.37139700

HCl

Zero-point = -460.794043

Cl	0.00000000	0.00000000	0.07144400
H	0.00000000	0.00000000	-1.21454100

p-cymene

Zero-point = -389.318915

C	-2.20652800	0.06478700	-0.00999400
C	-1.60628900	-1.19826500	0.00056700
C	-0.21719600	-1.33636600	0.00821500
C	0.62510300	-0.21957000	0.00341500
C	0.02169600	1.04697100	-0.01054600
C	-1.36409800	1.18543800	-0.01822000
H	-2.23195700	-2.08775200	0.00140700
H	0.21940800	-2.33251700	0.01429700
H	0.64090000	1.94037500	-0.01948600
H	-1.80119600	2.18136200	-0.03259700
C	-3.70889300	0.22136700	0.01011700
H	-4.21048800	-0.68929600	-0.32989800
H	-4.07427700	0.43745500	1.02196800
H	-4.03495900	1.04592300	-0.63208800
C	2.13930600	-0.38222500	0.00795100
H	2.34525800	-1.46076400	0.02283900
C	2.78265800	0.19157100	-1.26831800
H	2.62590900	1.27347800	-1.34001700
H	3.86342400	0.01199900	-1.27250400
H	2.35687100	-0.26627600	-2.16641700
C	2.77897200	0.22590200	1.27003100
H	2.35046000	-0.20727200	2.17900900
H	3.85964600	0.04620200	1.28221700
H	2.62261600	1.30941800	1.31195500

Ru2+

Zero-point = -3161.806090

Ru	0.84007800	-0.79679300	0.38878400
P	1.13053400	1.40280700	-0.36053700
P	-1.47855400	-0.61167700	-0.01999500
C	-1.88724200	0.27209500	-1.59984400
H	-1.46325200	-0.35882300	-2.38442000
H	-2.97450700	0.22567700	-1.68970400
C	0.13282000	1.86698500	-1.86513300
C	-1.41935900	1.74135800	-1.82472700
C	-1.90146500	2.16630500	-3.25106700

H	-1.73637900	3.24256400	-3.37325500
H	-1.31728300	1.66087100	-4.03200700
P	-3.67962100	1.82532100	-3.64768100
H	-3.92662900	2.75651500	-4.68773000
H	-3.60809100	0.60827400	-4.37393100
O	-4.65241000	1.82582600	-2.50195600
H	0.40233300	2.90288800	-2.09899600
H	0.51770000	1.23438900	-2.66748400
C	-2.03423400	2.72985800	-0.81279700
H	-1.76712000	2.49498000	0.21646400
H	-1.67317400	3.74326400	-1.01805800
H	-3.12243100	2.72885300	-0.89263500
C	-2.63168800	0.10030900	1.23043000
C	-3.92250100	0.53182200	0.86167500
C	-2.27792400	0.12852100	2.58823400
C	-4.81308800	0.99246000	1.83260200
H	-4.24573600	0.53504100	-0.17213900
C	-3.17427200	0.58314900	3.55835200
H	-1.29653900	-0.20996100	2.88548100
C	-4.44453900	1.01944500	3.18007600
H	-5.79710300	1.33034100	1.53053900
H	-2.88296700	0.59283400	4.60287300
H	-5.14330100	1.37553800	3.92745900
C	-2.21425300	-2.28827400	-0.26435900
C	-1.95707200	-3.03218000	-1.43281500
C	-2.98899200	-2.87224200	0.75646400
C	-2.46532700	-4.32497500	-1.57049500
H	-1.34288200	-2.61849400	-2.22128700
C	-3.48459300	-4.17018400	0.61352300
H	-3.22383900	-2.31031000	1.65183200
C	-3.22525900	-4.89909200	-0.54847200
H	-2.26764100	-4.88195800	-2.47914800
H	-4.08524800	-4.60324000	1.40489200
H	-3.61864200	-5.90234300	-0.66060500
C	0.88987800	2.82058000	0.78400100
C	1.34258000	4.10432800	0.41809500
C	0.19177000	2.66561900	1.98999300
C	1.10183500	5.19831200	1.24878800
H	1.89300600	4.24562100	-0.50531700
C	-0.04972900	3.76485100	2.81875300
H	-0.19149400	1.69270000	2.26379300
C	0.40636100	5.03093700	2.45048100
H	1.45571000	6.18062600	0.95900100
H	-0.60298700	3.63171600	3.74127900
H	0.21888100	5.88428000	3.09104700
C	2.87668400	1.62160100	-0.91026800
C	3.30715200	1.17952900	-2.17513300
C	3.83319800	2.13273400	-0.00925000

C	4.65736800	1.25084000	-2.52582200
H	2.60351400	0.75502600	-2.87817800
C	5.18179100	2.19354700	-0.36464000
H	3.52176700	2.50884400	0.95860100
C	5.59735100	1.75238500	-1.62334600
H	4.97222000	0.91310600	-3.50636500
H	5.90349800	2.59724400	0.33607500
H	6.64334000	1.80609900	-1.90037600
Cl	0.98837700	-1.36320600	-1.97907200
C	1.42357800	-0.90229200	2.69229300
C	0.62001300	-2.01576500	2.32517400
C	1.02145100	-2.92741200	1.31146100
C	2.24210900	-2.74456000	0.61307900
C	2.98162100	-1.55506300	0.87276500
C	2.56555400	-0.65172600	1.87865000
H	-0.29832300	-2.21429700	2.86807900
H	0.38243600	-3.76959900	1.07241300
H	3.86384300	-1.32337300	0.29128100
H	3.16348100	0.23411700	2.06545700
C	1.19204600	-0.10279600	3.94781200
H	0.16201700	-0.16538200	4.30305200
H	1.83056800	-0.50788300	4.74220900
H	1.45552600	0.94881800	3.81601900
C	2.69922000	-3.79677000	-0.38392700
H	1.84256700	-3.98941200	-1.04082100
C	3.88532900	-3.37067300	-1.25762200
H	4.79500100	-3.23023400	-0.66225400
H	4.09662300	-4.15627000	-1.98826000
H	3.67328300	-2.45068000	-1.80711600
C	3.02634700	-5.10193400	0.37979700
H	2.17480500	-5.46872100	0.96012200
H	3.30633300	-5.88232200	-0.33341200
H	3.86804200	-4.95670400	1.06539700

1\_Heq

Zero-point = -3162.973534

Ru	-0.81743400	0.81147800	0.36370300
P	-1.18927100	-1.39154000	-0.33644700
P	1.49324700	0.53134800	-0.04402200
C	1.86261800	-0.40030100	-1.60678300
H	1.46085700	0.23195500	-2.40212600
H	2.95062400	-0.39624500	-1.69985000
C	-0.21710900	-1.92347400	-1.83486800
C	1.33875500	-1.85498000	-1.80307600
C	1.79835600	-2.32311700	-3.22331800
H	1.59237500	-3.39439600	-3.32568800
H	1.23058600	-1.80985600	-4.01122200
P	3.58650200	-2.05658400	-3.63128600

H	3.79372100	-3.01241300	-4.65756900
H	3.55879100	-0.84895800	-4.37590600
O	4.56300000	-2.07695000	-2.48882600
H	-0.52620000	-2.95307500	-2.04664400
H	-0.58207400	-1.29328500	-2.64834400
C	1.91991800	-2.84875500	-0.77639100
H	1.67223200	-2.58250500	0.24999000
H	1.51438300	-3.84960700	-0.95889400
H	3.00638000	-2.89600300	-0.86469800
C	2.61788400	-0.20345900	1.21917200
C	3.88367000	-0.70887300	0.85753200
C	2.27151500	-0.17400200	2.57881900
C	4.75586300	-1.18529700	1.83760600
H	4.20123400	-0.75667900	-0.17696300
C	3.14961000	-0.64472500	3.55785000
H	1.31085400	0.22354300	2.87035600
C	4.39421400	-1.15518000	3.18685400
H	5.72028800	-1.57992600	1.54119200
H	2.86469700	-0.60887100	4.60356500
H	5.07870200	-1.52398200	3.94125700
C	2.30771900	2.16631200	-0.32888900
C	2.04812000	2.91089300	-1.49713900
C	3.16084000	2.71241400	0.64880200
C	2.63286000	4.16521300	-1.67767100
H	1.37559700	2.52639100	-2.25235500
C	3.73609500	3.97211500	0.46224400
H	3.39478900	2.15062000	1.54414200
C	3.47528200	4.70066100	-0.69996700
H	2.43167400	4.72208100	-2.58564300
H	4.40032400	4.37351600	1.21878500
H	3.93083800	5.67267200	-0.84662600
C	-0.99375100	-2.79032200	0.83943600
C	-1.49477100	-4.06486600	0.50572900
C	-0.28375700	-2.63296600	2.03824600
C	-1.28966300	-5.14728700	1.36078400
H	-2.05474100	-4.20738500	-0.41173200
C	-0.07815600	-3.72074900	2.89145100
H	0.13669800	-1.66885900	2.28766500
C	-0.58219900	-4.97751700	2.55512000
H	-1.68062000	-6.12249100	1.09568900
H	0.48486400	-3.58645300	3.80788700
H	-0.42260900	-5.82199700	3.21470700
C	-2.94478800	-1.55965900	-0.87445500
C	-3.36464600	-1.12900400	-2.14688300
C	-3.91512400	-2.01738500	0.04036700
C	-4.71802000	-1.15914700	-2.49125600
H	-2.64936200	-0.74473700	-2.86127300
C	-5.26657900	-2.03709200	-0.30891600

H	-3.61333500	-2.38439200	1.01474600
C	-5.67150000	-1.60759400	-1.57507800
H	-5.02476300	-0.83095900	-3.47759800
H	-5.99924500	-2.39999700	0.40265700
H	-6.71992800	-1.62945600	-1.84719000
Cl	-0.95478900	1.33366400	-2.01525000
C	-1.38015300	0.99301100	2.66878300
C	-0.55420600	2.07779900	2.26591400
C	-0.94294300	2.97043400	1.23129300
C	-2.17394100	2.79703800	0.54727300
C	-2.93679600	1.63193500	0.84252800
C	-2.53217100	0.74579300	1.86904500
H	0.37268900	2.27005800	2.79653500
H	-0.28937300	3.79387300	0.96847300
H	-3.82816100	1.40427500	0.27352400
H	-3.14828100	-0.12095300	2.08417900
C	-1.16026800	0.22469600	3.94575000
H	-0.12872600	0.27851800	4.29775500
H	-1.78960000	0.66391500	4.72927100
H	-1.44382800	-0.82508700	3.84439400
C	-2.61638300	3.83342800	-0.47237100
H	-1.76085900	3.99215800	-1.13967300
C	-3.81738500	3.41067300	-1.32711200
H	-4.72580100	3.30599400	-0.72253800
H	-4.01644900	4.18121700	-2.07695800
H	-3.62968300	2.47193300	-1.85330100
C	-2.91077100	5.16352000	0.26114300
H	-2.04730700	5.52675700	0.82568900
H	-3.18031500	5.93156300	-0.46928800
H	-3.74996300	5.05258100	0.95616600
H	1.64360200	5.71937200	1.81806400
H	1.17234500	6.08439600	2.26323200

Ts1\*\_H2eq

Zero-point = -3162.931453

Ru	-0.89186300	0.84687600	0.31963600
P	-1.02830000	-1.37289300	-0.40179600
P	1.47410800	0.71451600	0.01024100
C	1.98409500	-0.24261700	-1.50373500
H	1.59295300	0.36070500	-2.32661900
H	3.07309900	-0.16205800	-1.53065000
C	0.02666900	-1.86399400	-1.85352600
C	1.56970600	-1.71946000	-1.74874500
C	2.12021200	-2.12694300	-3.15564700
H	1.98424600	-3.20601000	-3.28909600
H	1.56086800	-1.63017900	-3.96006800
P	3.90610700	-1.74532900	-3.46807900
H	4.20941000	-2.63680500	-4.52794000

H	3.84340300	-0.50549900	-4.15534800
O	4.83029000	-1.77077700	-2.28329000
H	-0.22986800	-2.90798500	-2.06480200
H	-0.33328800	-1.25669200	-2.68639900
C	2.16917200	-2.70214400	-0.72166600
H	1.89681900	-2.45780500	0.30276400
H	1.80643800	-3.71591800	-0.92194800
H	3.25769600	-2.70692100	-0.79543500
C	2.52738400	0.06842900	1.37988400
C	3.79923200	-0.48343300	1.12942800
C	2.11828900	0.23511600	2.71310100
C	4.61407800	-0.88073100	2.19138900
H	4.16932300	-0.61726300	0.12022900
C	2.93988400	-0.15479100	3.77345900
H	1.15639800	0.68367500	2.91814900
C	4.18887600	-0.72076300	3.51237700
H	5.58586800	-1.31100100	1.98092800
H	2.61045200	-0.00951000	4.79645400
H	4.82994900	-1.02662500	4.33043900
C	2.34236500	2.31120900	-0.33227800
C	2.29020800	2.90656400	-1.60709800
C	3.03634200	2.97129400	0.69722400
C	2.92969700	4.12335100	-1.84375800
H	1.72269800	2.44773500	-2.40671200
C	3.66635200	4.19424800	0.45474700
H	3.10627000	2.52560900	1.68159300
C	3.61814700	4.77100000	-0.81497100
H	2.88431700	4.56780000	-2.83114300
H	4.20472500	4.68650600	1.25615200
H	4.11403900	5.71569100	-1.00306400
C	-0.72716700	-2.73188200	0.80236300
C	-1.11000200	-4.05104800	0.48224300
C	-0.01405500	-2.50436600	1.98806500
C	-0.79678800	-5.10416300	1.34125600
H	-1.65843000	-4.25398800	-0.43043600
C	0.30156500	-3.56312100	2.84426300
H	0.33146500	-1.50853200	2.22591200
C	-0.09217400	-4.86269400	2.52471100
H	-1.09884800	-6.11284200	1.08535100
H	0.86711300	-3.36975700	3.74846200
H	0.15338200	-5.68448000	3.18655700
C	-2.73660700	-1.73056700	-1.00680000
C	-3.15154600	-1.30801100	-2.28465500
C	-3.67733500	-2.36177300	-0.16698700
C	-4.46860600	-1.50965700	-2.70335900
H	-2.46316900	-0.79659200	-2.94290300
C	-4.99396700	-2.55324300	-0.59038500
H	-3.37690500	-2.73349400	0.80561400



C	-5.39358000	-2.12669100	-1.85876100
H	-4.76918300	-1.18253500	-3.69189400
H	-5.70126700	-3.04652100	0.06617800
H	-6.41404700	-2.28090300	-2.18817300
Cl	-1.00061400	1.31455000	-2.07147300
C	-1.68930800	0.72253400	2.63974400
C	-1.10359200	1.99971000	2.45712700
C	-1.62572200	2.92135000	1.52584100
C	-2.68456000	2.57993100	0.65330300
C	-3.17614300	1.24888800	0.72211600
C	-2.69390200	0.35713500	1.70630100
H	-0.30242200	2.32204900	3.11485200
H	-1.17820800	3.90468100	1.46298700
H	-3.94440600	0.91083500	0.03987300
H	-3.13873400	-0.62892400	1.77397600
C	-1.41427700	-0.12084800	3.85652600
H	-0.39637200	0.00275100	4.23097000
H	-2.09484600	0.19301700	4.65755400
H	-1.58789500	-1.18108700	3.66710200
C	-3.23148700	3.61623500	-0.31324100
H	-2.36329700	4.00401800	-0.86285900
C	-4.22939500	3.05819300	-1.33560800
H	-5.14873700	2.70753500	-0.85223300
H	-4.51309600	3.85050300	-2.03363300
H	-3.79799700	2.23965700	-1.91682300
C	-3.85743800	4.78891400	0.47699800
H	-3.14973000	5.24932000	1.17235900
H	-4.19126200	5.56336000	-0.21927200
H	-4.72850300	4.45452900	1.05053300
H	-0.26084400	2.87868400	-0.34855000
H	-0.03591100	3.56620900	-0.56459700

2\_H2eq

Zero-point = -3162.951069

Ru	0.69552500	-0.75416400	-0.00811300
P	0.60741400	1.56490100	-0.30561300
P	-1.57722600	-0.93041000	-0.20700800
C	-2.35342200	0.21177600	-1.43484900
H	-1.94926300	-0.13504100	-2.39147600
H	-3.42533300	-0.00625600	-1.45193000
C	-0.65185800	2.14292500	-1.54992200
C	-2.14482200	1.75347800	-1.34950700
C	-2.90928900	2.34904300	-2.57545900
H	-2.66202100	3.41208400	-2.70201300
H	-2.60286800	1.83772300	-3.49531500
P	-4.75313100	2.26126400	-2.47098400
H	-5.09113200	3.46583200	-1.80443600

H	-5.12811300	2.55980100	-3.80493800
O	-5.33683600	1.01043000	-1.87462700
H	-0.56008400	3.23366000	-1.59744400
H	-0.31201600	1.74177400	-2.50888700
C	-2.71237800	2.37865900	-0.05966000
H	-2.20459900	2.02459300	0.83555400
H	-2.60099500	3.46803000	-0.08453900
H	-3.77147500	2.14095000	0.06182600
C	-2.50978500	-0.75266400	1.36323400
C	-3.87726000	-0.41658700	1.37539900
C	-1.86846800	-1.05132100	2.57802100
C	-4.56958500	-0.35581200	2.58649500
H	-4.40962500	-0.20659500	0.45420400
C	-2.56691100	-0.99104300	3.78593200
H	-0.82608800	-1.35316300	2.57407200
C	-3.91788500	-0.63694300	3.79060100
H	-5.62135400	-0.09559700	2.58632900
H	-2.06305800	-1.22952100	4.71588900
H	-4.46369800	-0.59119700	4.72541600
C	-2.11729600	-2.58970200	-0.79814600
C	-1.85098000	-3.00002500	-2.11962400
C	-2.77004400	-3.48019100	0.07485000
C	-2.23603200	-4.26905100	-2.55211000
H	-1.32318700	-2.34578300	-2.80118400
C	-3.14549000	-4.75072400	-0.36635400
H	-2.99776200	-3.18221400	1.09002000
C	-2.88154200	-5.14725700	-1.67804400
H	-2.02908400	-4.57097400	-3.57208300
H	-3.65219600	-5.42437900	0.31455800
H	-3.17845100	-6.13201000	-2.01841900
C	0.34085500	2.63519800	1.16474100
C	0.52174600	4.02912800	1.07101500
C	-0.09638000	2.08680900	2.38122200
C	0.27230200	4.84685500	2.17299100
H	0.87233200	4.47140700	0.14511200
C	-0.34653000	2.90993300	3.48236400
H	-0.27741300	1.02209400	2.46165700
C	-0.16079200	4.28926100	3.38011700
H	0.41696600	5.91760000	2.09116700
H	-0.69484800	2.47392000	4.41157300
H	-0.35416400	4.92834100	4.23324300
C	2.19507000	2.20673100	-0.98668400
C	2.47595500	2.15907600	-2.36454600
C	3.19444500	2.66937200	-0.10613300
C	3.71866000	2.57528300	-2.84654900
H	1.74481600	1.77612000	-3.06343400
C	4.43726300	3.07531500	-0.59471400
H	2.99646500	2.73396000	0.95743700

C	4.70164100	3.03127500	-1.96596900
H	3.91758300	2.53806200	-3.91112100
H	5.19256700	3.43480900	0.09436700
H	5.66419100	3.35340100	-2.34469500
C	2.20580400	-1.59703500	2.67724400
C	2.68940900	-2.88443800	2.36125000
C	3.46868400	-3.10559000	1.23486900
C	3.80529400	-2.06182300	0.34507200
C	3.30323500	-0.78227800	0.63072400
C	2.51368900	-0.55032000	1.78481300
H	2.47064000	-3.71199800	3.03137600
H	3.84065400	-4.10744600	1.03661400
H	3.59055100	0.06410300	0.01850700
H	2.28181400	0.47147200	2.07272400
C	1.52146000	-1.34257100	3.99835900
H	0.78881200	-2.12109200	4.23380600
H	2.26010800	-1.34774400	4.80876600
H	1.02212800	-0.37122900	4.02140700
C	4.75145400	-2.34592100	-0.81346000
H	4.41765200	-3.29074600	-1.26497800
C	4.75092300	-1.27455700	-1.91114500
H	5.15825100	-0.32341100	-1.55081600
H	5.38422600	-1.60247200	-2.74071700
H	3.74636100	-1.09302700	-2.30158700
C	6.18201500	-2.57481800	-0.27330900
H	6.21728400	-3.37297900	0.47408700
H	6.85306200	-2.85028500	-1.09246300
H	6.57097300	-1.66156200	0.19012900
H	0.59092800	-2.54786100	0.38664200
H	1.03408500	-2.53488500	-0.27508300
Cl	0.87783300	-0.91373600	-2.38233100

Ts2\_H2eq

Zero-point = -3162.892622

Ru	0.62868200	-0.72917400	0.12555200
P	0.62934900	1.65089700	-0.37704100
P	-1.61560800	-0.90283400	-0.16839800
C	-2.38794600	0.31151000	-1.33384700
H	-1.97976800	0.04499500	-2.31681900
H	-3.45904300	0.09217800	-1.37077700
C	-0.74970500	2.28560000	-1.47257300
C	-2.20431700	1.84603000	-1.14269800
C	-3.10714500	2.52630300	-2.22074700
H	-2.91181600	3.60722300	-2.25385900
H	-2.86920600	2.13020100	-3.21553900
P	-4.92837100	2.34410900	-1.98702700
H	-5.24053800	3.36298400	-1.05312000

H	-5.41874300	2.90371200	-3.19379900
O	-5.43030600	0.96942200	-1.63974800
H	-0.68495200	3.37907800	-1.47205200
H	-0.51779400	1.95742900	-2.49120900
C	-2.63538500	2.33482900	0.25278600
H	-1.99809800	1.93935300	1.04279200
H	-2.58217200	3.42718400	0.30962800
H	-3.65503700	2.02064700	0.48937000
C	-2.58452300	-0.82382400	1.38666900
C	-3.98347700	-0.66798300	1.37658600
C	-1.91626100	-0.97173800	2.61277300
C	-4.68721700	-0.64262900	2.58147300
H	-4.52751100	-0.55868100	0.44431200
C	-2.62729400	-0.94580800	3.81499900
H	-0.84194900	-1.12958600	2.62197100
C	-4.01301700	-0.77774000	3.79918100
H	-5.76386400	-0.52147600	2.56801600
H	-2.10391400	-1.06485100	4.75705200
H	-4.56782000	-0.75961300	4.72965600
C	-2.16235000	-2.51573100	-0.88610600
C	-2.87127400	-2.63089300	-2.09366400
C	-1.84872300	-3.68814200	-0.16806100
C	-3.24408700	-3.88933500	-2.57666300
H	-3.15329900	-1.75472600	-2.66172700
C	-2.22556800	-4.93885200	-0.65388000
H	-1.31115700	-3.61752900	0.77109300
C	-2.92076400	-5.04265500	-1.86294700
H	-3.79377800	-3.96168800	-3.50765500
H	-1.98387800	-5.83062800	-0.08738400
H	-3.21359600	-6.01530000	-2.23957000
C	0.63853700	2.88382900	0.99361900
C	0.93840800	4.24002500	0.76243400
C	0.28319300	2.48080800	2.29213100
C	0.89072400	5.16185100	1.80859000
H	1.22340200	4.57072900	-0.23038200
C	0.23246600	3.40684500	3.33727900
H	0.01924500	1.44526700	2.48136100
C	0.53966400	4.74697200	3.09693700
H	1.12765000	6.20235100	1.62003600
H	-0.05005000	3.08356000	4.33259000
H	0.50378300	5.46586200	3.90663200
C	2.13235900	2.10271700	-1.35134000
C	2.20273900	1.84972100	-2.73474700
C	3.29230100	2.55859600	-0.69293200
C	3.39021000	2.06072200	-3.43915900
H	1.33455800	1.49169000	-3.27718600
C	4.47782200	2.76484700	-1.40154300
H	3.26340300	2.77260300	0.36938100

C	4.53038300	2.51835000	-2.77570900
H	3.42152500	1.87224800	-4.50610400
H	5.35624600	3.12851600	-0.88091000
H	5.44898200	2.68642000	-3.32468900
C	2.15382200	-1.46218500	2.81742500
C	2.65249500	-2.75909300	2.58789900
C	3.43934700	-3.04423400	1.48160400
C	3.76043300	-2.06010300	0.52585000
C	3.22934600	-0.77276400	0.71473100
C	2.44670100	-0.47119500	1.85851100
H	2.44215300	-3.54319300	3.31085800
H	3.82866000	-4.05113000	1.35621400
H	3.51689300	0.03521600	0.05171300
H	2.22589500	0.56753700	2.08712000
C	1.45509000	-1.13398800	4.11464300
H	0.68731500	-1.87500800	4.35967700
H	2.17389500	-1.13604500	4.94254600
H	0.99008500	-0.14540700	4.09135400
C	4.72599700	-2.40629300	-0.60240400
H	4.35406100	-3.33373800	-1.06250100
C	4.83180300	-1.34302500	-1.70279200
H	5.28012100	-0.41667800	-1.32849700
H	5.47323100	-1.71079500	-2.50899200
H	3.85987500	-1.09333700	-2.13532500
C	6.12728500	-2.71368500	-0.02617700
H	6.10011200	-3.51081600	0.72177800
H	6.80441100	-3.02695800	-0.82672400
H	6.55266100	-1.82240300	0.44774200
H	0.65511600	-2.33382600	0.41331500
H	0.82035800	-2.59712800	-1.41317400
Cl	0.96775400	-1.57039500	-2.22096100

### 3\_H2eq

Zero-point = -3162.897332

Ru	0.61286300	-0.70359900	0.22974100
P	0.64124600	1.64601200	-0.45150600
P	-1.62387500	-0.91072100	-0.08272000
C	-2.41478600	0.29504700	-1.24910800
H	-2.05646600	-0.01571300	-2.23883300
H	-3.48885400	0.10389600	-1.23935100
C	-0.77138500	2.25109900	-1.52080100
C	-2.21213100	1.83132700	-1.11492900
C	-3.15807600	2.48201200	-2.17482500
H	-2.98277200	3.56556000	-2.22875100
H	-2.94069700	2.07564800	-3.17020400
P	-4.96989400	2.27188300	-1.89719000
H	-5.28244700	3.28690400	-0.95987000
H	-5.49905100	2.81443900	-3.09467000

O	-5.44453500	0.88930500	-1.53374500
H	-0.70202500	3.34343700	-1.56521000
H	-0.58193100	1.88080900	-2.53380800
C	-2.58340400	2.35893000	0.28321500
H	-1.92967400	1.95901000	1.05779900
H	-2.50046500	3.45013800	0.31945600
H	-3.60227200	2.07713400	0.56135500
C	-2.60923900	-0.87645400	1.46357900
C	-3.99146100	-0.60924300	1.47376200
C	-1.95409900	-1.16496700	2.67420900
C	-4.69122800	-0.61613800	2.68166600
H	-4.52990700	-0.39045500	0.55779700
C	-2.66148700	-1.16560400	3.87825500
H	-0.89662900	-1.41297400	2.66359700
C	-4.02987300	-0.88847700	3.88273100
H	-5.75539100	-0.41190200	2.68243500
H	-2.14937000	-1.39258800	4.80640400
H	-4.58126300	-0.89272400	4.81540000
C	-2.14460800	-2.50489000	-0.89412600
C	-3.30730000	-2.59856700	-1.68284100
C	-1.35502400	-3.66460600	-0.72272500
C	-3.65422700	-3.80664400	-2.29321100
H	-3.95974200	-1.74653000	-1.82499800
C	-1.70623900	-4.86782900	-1.34501700
H	-0.49686000	-3.62930400	-0.05726900
C	-2.85275400	-4.93923700	-2.13700900
H	-4.55616100	-3.85897600	-2.89162200
H	-1.09034300	-5.74737000	-1.19576300
H	-3.12619200	-5.87024300	-2.61846000
C	0.70340300	2.94335400	0.85928400
C	1.00930500	4.28426400	0.55803800
C	0.37738100	2.60606600	2.18422900
C	0.99738500	5.25442300	1.56082000
H	1.27093800	4.56560800	-0.45619100
C	0.36243300	3.57978400	3.18623200
H	0.11092800	1.58258600	2.42999700
C	0.67600400	4.90399100	2.87570900
H	1.23920500	6.28241800	1.31767100
H	0.10347900	3.30575900	4.20253500
H	0.66830700	5.66003800	3.65162200
C	2.11377500	2.04049200	-1.49588800
C	2.13660600	1.71134300	-2.86487400
C	3.29686000	2.52373500	-0.90197800
C	3.30097700	1.87544900	-3.61827200
H	1.25027100	1.32446000	-3.35548000
C	4.45959800	2.68224400	-1.65954700
H	3.30474300	2.79524800	0.14742000
C	4.46524000	2.36072200	-3.01883600

H	3.29605900	1.62796100	-4.67356800
H	5.35696500	3.06658400	-1.18842200
H	5.36616800	2.49119400	-3.60600000
C	2.22372900	-1.28567300	2.93079200
C	2.71081100	-2.59487800	2.76945800
C	3.44856300	-2.95836000	1.65047900
C	3.73460600	-2.04326500	0.62017300
C	3.21999700	-0.74056700	0.74774900
C	2.48395700	-0.36141600	1.89809900
H	2.52683400	-3.32949800	3.54940500
H	3.82604900	-3.97471100	1.57652800
H	3.49281100	0.02303400	0.02816000
H	2.27508500	0.69101700	2.06696200
C	1.55208900	-0.87121800	4.21767100
H	0.78480100	-1.59036600	4.52217000
H	2.28363600	-0.82333400	5.03289800
H	1.08796000	0.11478200	4.13772200
C	4.64656000	-2.47089300	-0.52536400
H	4.22092800	-3.39798700	-0.93683700
C	4.75648300	-1.45552600	-1.66978400
H	5.24367900	-0.53010400	-1.34487500
H	5.36335100	-1.87542500	-2.47727900
H	3.78292100	-1.19108600	-2.08951200
C	6.05593100	-2.81163700	0.01047300
H	6.02820200	-3.57837500	0.78934600
H	6.68982400	-3.18138500	-0.80138400
H	6.53308900	-1.92083900	0.43329200
H	0.62650500	-2.23456100	0.70897200
H	0.10044000	-2.65243300	-1.91512200
Cl	0.93807200	-1.63715700	-2.00398800

1\_H2ax

Zero-point= -3162.973764

Ru	-0.91236500	0.75198500	0.39502000
P	-1.01869400	-1.45700100	-0.37403900
P	1.41152700	0.76939800	-0.02359500
C	1.88608200	-0.06271600	-1.61281900
H	1.40589100	0.53604200	-2.39012600
H	2.96500200	0.07669500	-1.70665800
C	0.00861500	-1.82319700	-1.88518700
C	1.54448400	-1.56494900	-1.84898700
C	2.05551200	-1.93454800	-3.28065400
H	1.98402000	-3.02001600	-3.41158500
H	1.42641400	-1.47515900	-4.05512000
P	3.79570800	-1.43718200	-3.68081500
H	4.11822200	-2.33517300	-4.72933900
H	3.61548300	-0.22534500	-4.39689600



O	4.76989400	-1.36197300	-2.53875700
H	-0.17222900	-2.87649300	-2.12662600
H	-0.43228900	-1.21968500	-2.68113600
C	2.24594100	-2.50570300	-0.84803700
H	1.96516700	-2.30270500	0.18445100
H	1.97215600	-3.54449700	-1.06066900
H	3.32973400	-2.41137200	-0.93191500
C	2.62647800	0.14688200	1.21548500
C	3.94722800	-0.17181200	0.83810000
C	2.28222900	0.07876400	2.57414200
C	4.87737600	-0.56411300	1.80192900
H	4.26520400	-0.13930000	-0.19686400
C	3.21750600	-0.30737200	3.53713600
H	1.27751300	0.33291400	2.87718600
C	4.51806000	-0.63304900	3.15041700
H	5.88491000	-0.81598300	1.49352200
H	2.93274400	-0.34978200	4.58265100
H	5.24730400	-0.93583300	3.89215700
C	2.00028000	2.50501800	-0.25384900
C	1.67979900	3.23471800	-1.41555600
C	2.72185300	3.14432400	0.77284600
C	2.07485700	4.56770000	-1.54104400
H	1.10337100	2.77715500	-2.20826800
C	3.10374800	4.48135700	0.64221700
H	3.00452800	2.59653400	1.66317900
C	2.78252500	5.19580500	-0.51328200
H	1.82976800	5.11393700	-2.44464500
H	3.66490900	4.95724900	1.43797000
H	3.08792000	6.23022200	-0.61596800
C	-0.65703800	-2.85839100	0.75916800
C	-1.00154800	-4.17294300	0.38566100
C	0.02567100	-2.65260100	1.96646500
C	-0.67292900	-5.24791400	1.21146100
H	-1.53753000	-4.35437200	-0.53921500
C	0.35657200	-3.73215300	2.78998800
H	0.32665100	-1.65250700	2.24516300
C	0.00513200	-5.02991500	2.41562000
H	-0.94583400	-6.25439400	0.91716200
H	0.89674300	-3.55882300	3.71355700
H	0.25832700	-5.86792600	3.05387600
C	-2.74239400	-1.81680600	-0.92029900
C	-3.21261000	-1.40323200	-2.18065000
C	-3.64980000	-2.41231400	-0.02039600
C	-4.55329800	-1.58472200	-2.52815000
H	-2.54927900	-0.91668400	-2.88269800
C	-4.98979400	-2.58314700	-0.37244100
H	-3.30473500	-2.76781700	0.94380000
C	-5.44502800	-2.16952000	-1.62678900

H	-4.89854400	-1.26770200	-3.50537400
H	-5.67285700	-3.05072400	0.32729100
H	-6.48375700	-2.30869100	-1.90136800
C	-1.47589800	0.80798300	2.70760300
C	-0.79122400	1.99425200	2.32574900
C	-1.29432100	2.85565400	1.31458900
C	-2.50182500	2.54943700	0.63432200
C	-3.11433000	1.29386700	0.90579700
C	-2.59539300	0.44014800	1.90839800
H	0.11081800	2.28459300	2.85462600
H	-0.74641500	3.75655700	1.06405600
H	-3.97636600	0.97249800	0.33679800
H	-3.09964600	-0.49985000	2.10704700
C	-1.15493300	0.04445900	3.96602500
H	-1.30278100	-1.03034300	3.84054900
H	-0.13763100	0.22198700	4.31881600
H	-1.83243100	0.38133900	4.75997800
C	-3.07660200	3.54828000	-0.35608100
H	-2.25104600	3.83297700	-1.01918800
C	-4.21792800	2.99979200	-1.22095800
H	-5.10369800	2.76584500	-0.61898500
H	-4.51535500	3.75810300	-1.95044300
H	-3.91519000	2.10599500	-1.77128700
C	-3.53404700	4.80931200	0.41504100
H	-2.72094900	5.26322000	0.98888600
H	-3.90216600	5.55706200	-0.29307400
H	-4.34905500	4.57353300	1.10767700
H	2.52096000	-6.10231000	0.81091400
H	3.12446000	-6.47056700	0.58191400
Cl	-1.11680400	1.32588300	-1.96692500

Ts1\*\_H2ax

Zero-point = -3162.925475

Ru	-0.54500500	0.88295500	0.44121600
P	-1.40322400	-1.21785700	-0.26879700
P	1.70891300	0.33711000	-0.09289400
C	1.86427900	-0.83257600	-1.52428500
H	1.52926200	-0.26556100	-2.39530000
H	2.93525700	-1.00733400	-1.63896200
C	-0.43005300	-1.98790400	-1.65654300
C	1.10494100	-2.19286600	-1.49118600
C	1.53511500	-3.00882500	-2.75489700
H	1.14127400	-4.02735900	-2.66472900
H	1.09991000	-2.57822200	-3.66719700
P	3.35284900	-3.14665100	-3.07841600
H	3.41512600	-4.31369500	-3.88046100
H	3.57740000	-2.13131500	-4.04389500
O	4.26605500	-3.10381400	-1.88568400

H	-0.89728600	-2.94896900	-1.88750100
H	-0.60395200	-1.33702700	-2.51559200
C	1.42661800	-3.03578500	-0.24115800
H	1.16073800	-2.51898200	0.68356500
H	0.85945200	-3.97151300	-0.26335300
H	2.48941000	-3.27800800	-0.20116100
C	2.89234100	-0.29012800	1.18233800
C	3.99117000	-1.09714300	0.82816300
C	2.78395200	0.14188100	2.51750000
C	4.93819700	-1.46100500	1.78922000
H	4.12838900	-1.47556600	-0.17685700
C	3.73699900	-0.21734600	3.47091500
H	1.94610900	0.75321900	2.81945100
C	4.81797500	-1.02311800	3.10812400
H	5.76982600	-2.09015600	1.49554200
H	3.63343700	0.12749900	4.49349500
H	5.55746600	-1.30759000	3.84695100
C	2.61282700	1.84868100	-0.66469300
C	2.50986900	2.33006700	-1.98361500
C	3.38951400	2.57681900	0.25928900
C	3.15653700	3.50939600	-2.35929200
H	1.91315400	1.80650000	-2.71617000
C	4.02238500	3.76135000	-0.12089000
H	3.52946100	2.20234000	1.26569100
C	3.90643600	4.23249500	-1.43021400
H	3.07241700	3.86036500	-3.38123100
H	4.62210400	4.30281600	0.60150900
H	4.40621700	5.14689900	-1.72657700
C	-1.76482300	-2.60342700	0.90551300
C	-2.05648200	-3.88434000	0.39395700
C	-1.88434600	-2.39887500	2.29014300
C	-2.41924700	-4.92723500	1.24518100
H	-2.02823900	-4.07274400	-0.67190000
C	-2.25357200	-3.44441600	3.14097700
H	-1.68063500	-1.42706100	2.71304600
C	-2.51332500	-4.71235500	2.62247500
H	-2.63716100	-5.90476200	0.83167700
H	-2.33512600	-3.26571100	4.20695700
H	-2.79455500	-5.52439100	3.28189600
C	-3.09158300	-0.99595400	-0.99238700
C	-3.30386500	-0.65149800	-2.33915100
C	-4.20942000	-1.11875500	-0.14176600
C	-4.59854200	-0.43133600	-2.81709100
H	-2.47054800	-0.53351200	-3.01691300
C	-5.49817300	-0.88484900	-0.62300200
H	-4.07643400	-1.42532500	0.88945400
C	-5.69634100	-0.53971800	-1.96227200
H	-4.74496700	-0.17484000	-3.85986100

H	-6.34681700	-0.99125900	0.04285700
H	-6.69795700	-0.36766500	-2.33760700
C	-0.83564600	1.57702500	2.82230800
C	-0.00295300	2.47242300	2.09207200
C	-0.47564900	3.16411300	0.95515900
C	-1.81420000	2.98850300	0.49366300
C	-2.57222900	1.96022500	1.08998900
C	-2.07500800	1.25588700	2.22216600
H	0.99471600	2.69540500	2.45491500
H	0.18025400	3.86298200	0.44836600
H	-3.55177700	1.70854800	0.70489800
H	-2.71982100	0.52175200	2.69400300
C	-0.41907000	0.97922400	4.13569100
H	0.01126800	-0.02279900	4.00349400
H	0.32913700	1.60224200	4.63182300
H	-1.27772400	0.88633000	4.80595500
C	-2.35138900	3.88744800	-0.60306200
H	-1.56818000	3.94410800	-1.36754600
C	-3.63522600	3.37889000	-1.26832400
H	-4.48179200	3.38377900	-0.57205300
H	-3.89886900	4.03994300	-2.09856300
H	-3.51273500	2.36940600	-1.66783500
C	-2.55537200	5.30601900	-0.01818200
H	-1.63443100	5.71327300	0.40978700
H	-2.88478300	5.98356800	-0.81099200
H	-3.32262200	5.30441900	0.76335600
H	0.42334600	-1.03846300	2.33586000
H	0.15850300	-0.55032700	1.80003500
Cl	-0.65525600	1.34942900	-1.93092600

## 2\_H2ax

Zero-point = -3162.96896

Ru	-0.58438900	0.80391200	-0.25519700
P	-0.79450400	-1.46804000	-0.27967600
P	1.66066600	0.57279600	0.03085200
C	2.42536600	-0.59891200	-1.18128900
H	2.19207500	-0.17234600	-2.16054500
H	3.50743700	-0.53751400	-1.02861800
C	0.47559200	-2.31416400	-1.34908900
C	2.01050400	-2.09918700	-1.16012000
C	2.66586000	-2.77830400	-2.40778000
H	2.53995500	-3.86395300	-2.32835000
H	2.16532500	-2.46404700	-3.33382100
P	4.46752700	-2.44758100	-2.67694000
H	4.81227600	-3.50310700	-3.55901400
H	4.44655600	-1.33955400	-3.56408200
O	5.32532200	-2.27561200	-1.45751200
H	0.25187000	-3.38659000	-1.33585600

H	0.19015700	-1.95514900	-2.34333300
C	2.54521300	-2.81397300	0.09822200
H	2.08334400	-2.44975900	1.01586100
H	2.35190500	-3.88987900	0.02759800
H	3.62585400	-2.67811000	0.17533400
C	2.37611900	0.11948600	1.65767800
C	3.78002300	0.01884000	1.76710700
C	1.58634600	-0.14424200	2.78647000
C	4.36707800	-0.34156600	2.97798900
H	4.41553400	0.22364300	0.91316100
C	2.18188400	-0.50429100	3.99922000
H	0.50792100	-0.09664100	2.72852000
C	3.56929300	-0.60436600	4.09641300
H	5.44533500	-0.41944400	3.04723300
H	1.55773700	-0.71188500	4.86033100
H	4.02972300	-0.88643400	5.03557700
C	2.45781400	2.18811600	-0.33847200
C	2.55948800	2.65872100	-1.66305000
C	2.92952600	2.99865300	0.71328800
C	3.13697100	3.90155200	-1.92432100
H	2.16753300	2.07360700	-2.48513400
C	3.50280700	4.24272600	0.44112200
H	2.86879700	2.65162600	1.73728900
C	3.61011100	4.69501600	-0.87555800
H	3.21675900	4.24900700	-2.94769300
H	3.87120100	4.85211800	1.25804600
H	4.06000700	5.65827100	-1.08400600
C	-0.89170200	-2.33955800	1.33850900
C	-0.35269100	-3.62447000	1.52239200
C	-1.62307200	-1.76283300	2.39552700
C	-0.50575200	-4.29392200	2.73913800
H	0.18549500	-4.11397500	0.72320100
C	-1.77942300	-2.43515300	3.60770900
H	-2.09858100	-0.79651500	2.26850400
C	-1.21202800	-3.69984100	3.78550000
H	-0.07625000	-5.28070200	2.86386700
H	-2.35091800	-1.97734700	4.40688800
H	-1.33053300	-4.22165000	4.72737300
C	-2.37557000	-1.98814500	-1.08377600
C	-2.70032300	-1.52796200	-2.37685200
C	-3.26366800	-2.86452900	-0.42995400
C	-3.88260100	-1.93895300	-2.99429600
H	-2.03937000	-0.84397700	-2.89456700
C	-4.44454300	-3.26768600	-1.05655700
H	-3.03559400	-3.23801400	0.55894700
C	-4.75794900	-2.80665900	-2.33631200
H	-4.11666600	-1.58067100	-3.99014900
H	-5.11514800	-3.94685000	-0.54341400

H	-5.67486500	-3.12339800	-2.81884000
C	-1.36960200	3.89701000	0.76717300
C	-1.49388100	3.25374000	-0.48013900
C	-2.58364400	2.39524700	-0.74647200
C	-3.57380800	2.14389300	0.22403400
C	-3.43135100	2.78613600	1.46849100
C	-2.36060600	3.63830000	1.73022500
H	-0.79810600	3.48842800	-1.28172300
H	-2.70566400	1.99900500	-1.75061700
H	-4.18153300	2.63589000	2.23926800
H	-2.29783800	4.13043600	2.69735500
C	-0.25565700	4.87765500	1.03001200
H	0.71898700	4.46787400	0.75130500
H	-0.40328000	5.79136600	0.44227200
H	-0.22010300	5.16577600	2.08381800
C	-4.79887600	1.31044000	-0.12232500
H	-4.55438500	0.73954500	-1.02629600
C	-5.18448200	0.30162700	0.97235900
H	-5.48519300	0.79915300	1.90062400
H	-6.03257300	-0.30357900	0.63898800
H	-4.36044500	-0.38208700	1.19684300
C	-5.98740900	2.23702700	-0.45949200
H	-5.73955100	2.92772900	-1.27105400
H	-6.85442700	1.64533900	-0.76967600
H	-6.28126000	2.83309500	0.41135900
H	-0.52269700	1.17789000	1.38230900
H	-1.25246700	0.69298700	1.28114500
Cl	-0.27572100	0.90839500	-2.63984400

### 3\_H2ax

Zero-point = -3351.538808

Ru	-0.48779400	0.67659600	0.16037600
P	-0.95086700	-1.41055500	-0.63164800
P	1.69547400	0.08281300	0.40401100
C	2.41171700	-0.73091400	-1.09488800
H	2.29749900	0.00716200	-1.89325200
H	3.47960200	-0.86343100	-0.89365700
C	0.29604600	-2.02136500	-1.87493800
C	1.82521300	-2.09200500	-1.56927500
C	2.49054900	-2.43164000	-2.94366000
H	2.23283700	-3.46074200	-3.21816800
H	2.10258300	-1.78076500	-3.73923600
P	4.33332900	-2.28085300	-3.03081800
H	4.61414300	-3.03264000	-4.20009000
H	4.50967600	-0.95419200	-3.50446000
O	5.11135700	-2.62967700	-1.79619100
H	-0.05149500	-2.99779800	-2.22991700
H	0.13585900	-1.32223900	-2.70217500

C	2.17068400	-3.22800100	-0.58449900
H	1.68076600	-3.10839300	0.38183400
H	1.86127700	-4.19248100	-1.00125100
H	3.25015000	-3.26921000	-0.42464800
C	2.25639200	-0.93262000	1.82379700
C	3.64043700	-1.16055200	1.97724600
C	1.36544900	-1.50858600	2.74140500
C	4.11053000	-1.94961000	3.02484100
H	4.35021600	-0.72022200	1.28611100
C	1.84399700	-2.29701200	3.79207000
H	0.29846700	-1.37228300	2.63324800
C	3.21347800	-2.51895100	3.93445000
H	5.17499900	-2.12104400	3.12965400
H	1.14347300	-2.74032200	4.48991700
H	3.58318000	-3.13259700	4.74706500
C	2.66809800	1.62881500	0.59839600
C	3.05569300	2.40186800	-0.51292400
C	2.98665300	2.08419800	1.89388000
C	3.76497700	3.58991100	-0.32850500
H	2.79412400	2.09721300	-1.51791300
C	3.68793000	3.27870000	2.06846500
H	2.70908300	1.49588700	2.76058800
C	4.08148200	4.03086100	0.95927400
H	4.06868900	4.16690200	-1.19392400
H	3.93598900	3.61309300	3.06899300
H	4.63415600	4.95249900	1.09681700
C	-1.27022000	-2.74670600	0.59385900
C	-0.91746900	-4.08305700	0.33714300
C	-1.98488400	-2.45799400	1.77300600
C	-1.23585500	-5.09188600	1.24959000
H	-0.39689900	-4.34950500	-0.57183400
C	-2.30639800	-3.46782900	2.68058200
H	-2.31757200	-1.44652700	1.97755900
C	-1.92391100	-4.78719800	2.42461900
H	-0.94848400	-6.11465400	1.03718000
H	-2.86167000	-3.22611100	3.57950900
H	-2.17028300	-5.57163900	3.12987500
C	-2.50846400	-1.42460700	-1.62509000
C	-2.65541300	-0.55461200	-2.72541400
C	-3.55788900	-2.30991900	-1.31162400
C	-3.82303300	-0.57642900	-3.48924100
H	-1.86900600	0.14696700	-2.97514800
C	-4.72279900	-2.32219200	-2.08188300
H	-3.46811200	-2.99192700	-0.47718900
C	-4.85948000	-1.45752100	-3.16922500
H	-3.92060900	0.09531300	-4.33426500
H	-5.51936900	-3.01335900	-1.83269700
H	-5.76440500	-1.47183900	-3.76486300



C	-1.29174600	3.29080300	2.00504700
C	-1.41485900	3.05055100	0.62108200
C	-2.51974400	2.33909900	0.10440200
C	-3.53967400	1.85504900	0.94949500
C	-3.40042000	2.09646100	2.32803700
C	-2.30574400	2.79229600	2.84006800
H	-0.71258800	3.50905300	-0.06971000
H	-2.63273900	2.25314900	-0.97299500
H	-4.16915100	1.75417000	3.01407100
H	-2.24557000	2.97248100	3.91040700
C	-0.15594200	4.11867600	2.55193600
H	-0.28655700	5.17261500	2.27968800
H	-0.11224900	4.06234800	3.64278500
H	0.81018300	3.79798900	2.15211700
C	-4.78605300	1.21868700	0.35191400
H	-4.50449500	0.82102000	-0.63032500
C	-5.35387200	0.05597900	1.18102400
H	-5.73048500	0.39022600	2.15357000
H	-6.19372600	-0.40132700	0.65003400
H	-4.60659500	-0.72501000	1.35139900
C	-5.86362100	2.30274400	0.12451400
H	-5.49051500	3.11270000	-0.50943800
H	-6.74286600	1.86829600	-0.36162000
H	-6.18551300	2.74101200	1.07541500
H	-0.49313300	0.47897600	1.83081100
H	-1.26068400	0.14745400	1.55408100
Cl	0.01230800	1.52470200	-2.03637400
C	1.10406000	4.82649500	-2.40219900
O	1.95414800	4.48337100	-3.12762200
O	0.26163100	5.18412700	-1.67319000

Ts2\_H2ax

Zero-point = -3351.528256

Ru	-0.18142900	0.95531000	-0.06785700
P	-0.84744800	-1.20391500	-0.42018900
P	1.97248200	0.25197800	0.22543100
C	2.54782700	-0.91642300	-1.08767600
H	2.41696200	-0.36679000	-2.02490500
H	3.61971800	-1.05840900	-0.91636000
C	0.34057100	-2.19368300	-1.47080900
C	1.87106100	-2.30735700	-1.21374900
C	2.44388900	-2.99274100	-2.49876000
H	2.10851400	-4.03558500	-2.52403300
H	2.05810700	-2.51063000	-3.40739400
P	4.28713800	-2.99709600	-2.67864000
H	4.46896300	-4.02935500	-3.63359800
H	4.51918500	-1.84154500	-3.47013400
O	5.09882900	-3.08482700	-1.41971000

H	-0.09623500	-3.19544500	-1.55449100
H	0.18453000	-1.71757200	-2.44525000
C	2.20004700	-3.21762600	-0.01291000
H	1.76957500	-2.85383600	0.91952800
H	1.81443500	-4.22696100	-0.19493300
H	3.28189200	-3.29655800	0.11228900
C	2.49341700	-0.50651500	1.81318200
C	3.85868600	-0.82538100	1.97682700
C	1.59469500	-0.81207000	2.84648000
C	4.30267600	-1.43565000	3.14779500
H	4.57460700	-0.59498100	1.19617900
C	2.04803200	-1.42132500	4.02048000
H	0.53893100	-0.60344800	2.74263100
C	3.39851800	-1.73414100	4.17227900
H	5.35241000	-1.67869500	3.25931600
H	1.34160000	-1.65356500	4.80858600
H	3.74787300	-2.20829000	5.08150200
C	3.12032500	1.67331800	0.05688600
C	3.51253500	2.14545900	-1.21009200
C	3.57516600	2.34113600	1.20998800
C	4.35634000	3.25269300	-1.31511100
H	3.14835600	1.67327900	-2.11390400
C	4.41202400	3.45195600	1.09503200
H	3.29010400	1.98640600	2.19314800
C	4.80652300	3.90754900	-0.16507500
H	4.65616400	3.60566400	-2.29452800
H	4.76059600	3.95504500	1.98913500
H	5.46091700	4.76646900	-0.25188100
C	-1.27409400	-2.15039300	1.09576400
C	-0.89456500	-3.48903800	1.28723300
C	-2.09174500	-1.53325000	2.06504100
C	-1.28634900	-4.18021800	2.43737000
H	-0.29634800	-4.00223200	0.54811800
C	-2.48298300	-2.22837700	3.20972800
H	-2.45418900	-0.52090000	1.91629000
C	-2.07237700	-3.55087200	3.40301700
H	-0.97835000	-5.21009900	2.57294600
H	-3.11517100	-1.74132100	3.94308300
H	-2.37459900	-4.08908200	4.29328800
C	-2.35662200	-1.44449100	-1.46167500
C	-2.51910200	-0.73836600	-2.66958300
C	-3.29767500	-2.43346300	-1.11722600
C	-3.60124300	-1.01530200	-3.50657900
H	-1.80625900	0.02523200	-2.95522700
C	-4.37235300	-2.70876500	-1.96618800
H	-3.19537300	-2.99115300	-0.19594100
C	-4.52879300	-2.00084700	-3.15890000
H	-3.71553200	-0.46167800	-4.43133500

H	-5.08570700	-3.47660600	-1.69085300
H	-5.36544700	-2.21542000	-3.81300400
C	-2.39287900	3.21781200	1.52395800
C	-2.32083300	2.82496100	0.16589600
C	-3.24154000	1.91213200	-0.36949500
C	-4.26986600	1.35679800	0.41693400
C	-4.30989600	1.72582100	1.76531100
C	-3.38925500	2.63230700	2.30656900
H	-1.63684900	3.33418300	-0.50598500
H	-3.19775900	1.67890000	-1.42896000
H	-5.09061600	1.33262600	2.40919500
H	-3.48033700	2.91808300	3.35157500
C	-1.46225900	4.25475800	2.10613900
H	-1.35564500	5.11420500	1.43742900
H	-1.83671800	4.61874600	3.06616700
H	-0.45555400	3.85463700	2.27056400
C	-5.34399000	0.49174000	-0.23022900
H	-4.87125300	-0.04540300	-1.05905800
C	-5.95334100	-0.55578900	0.71391800
H	-6.54612700	-0.09376300	1.51085900
H	-6.62679900	-1.21273100	0.15542900
H	-5.18439100	-1.18108900	1.17851200
C	-6.44989000	1.38789100	-0.82991800
H	-6.04025400	2.10417300	-1.54876000
H	-7.19824000	0.77893200	-1.34774400
H	-6.96094900	1.95645600	-0.04526900
H	-0.11740600	1.06092100	1.62255200
H	-0.89843900	0.73036000	1.44567400
Cl	0.17801200	1.40399800	-2.37623000
C	1.09847900	4.28897100	-1.08278000
O	1.43155400	4.88232100	-2.02589000
O	0.74789700	3.71667700	-0.11718600

#### 4\_H2ax

Zero-point= -3351.530989

Ru	0.00648300	0.97576800	-0.35977300
P	-0.64854100	-1.20405300	-0.54986600
P	2.09527100	0.34656900	0.25951900
C	2.78839800	-0.92316500	-0.89419800
H	2.76381100	-0.44756600	-1.87885700
H	3.83455100	-1.05378000	-0.59721400
C	0.62381600	-2.26538300	-1.40766900
C	2.12448100	-2.32689500	-0.98499000
C	2.83370500	-3.10077700	-2.14618300
H	2.50907500	-4.14697500	-2.12217700
H	2.53900500	-2.69707800	-3.12428800
P	4.68631300	-3.09366400	-2.13725400
H	4.97319200	-4.21441000	-2.95684600

H	4.99231500	-2.02088000	-3.01538400
O	5.36455300	-3.03879600	-0.79950300
H	0.21456300	-3.28109000	-1.45236600
H	0.56141100	-1.87011400	-2.42794000
C	2.33526300	-3.13375800	0.31269500
H	1.81077600	-2.70186100	1.16463500
H	1.97475500	-4.15932900	0.17696700
H	3.39951000	-3.18731200	0.55140500
C	2.45220200	-0.26224800	1.94909700
C	3.79695500	-0.53128900	2.28324600
C	1.44964700	-0.50603900	2.89980300
C	4.11935300	-1.03270200	3.54241200
H	4.58973600	-0.34775500	1.56687600
C	1.78171100	-1.00633500	4.16217300
H	0.40764900	-0.33752100	2.66316900
C	3.11285800	-1.27022800	4.48415700
H	5.15424700	-1.23907200	3.78691700
H	0.99683400	-1.19404600	4.88506700
H	3.36817900	-1.66038300	5.46196700
C	3.21350900	1.78804800	0.07680900
C	3.69971900	2.17686400	-1.18658900
C	3.53089400	2.56871400	1.20578600
C	4.50135500	3.31308700	-1.30951700
H	3.44189200	1.61507100	-2.07562700
C	4.32631100	3.70749900	1.07101300
H	3.17238200	2.27926900	2.18636400
C	4.81517000	4.07953100	-0.18377700
H	4.87657500	3.59994100	-2.28457700
H	4.57005500	4.29734400	1.94659500
H	5.43690500	4.96086000	-0.28454100
C	-1.19181600	-2.02140000	1.00315900
C	-0.84847100	-3.34394700	1.32956100
C	-2.06349500	-1.31721100	1.85862300
C	-1.32953600	-3.93353100	2.50220000
H	-0.21042400	-3.92340100	0.67751400
C	-2.54239000	-1.91073900	3.02705000
H	-2.40227400	-0.31913300	1.60240200
C	-2.16814100	-3.21707200	3.35654800
H	-1.05034000	-4.95262100	2.74192300
H	-3.21596100	-1.35648100	3.67006300
H	-2.53991100	-3.67648600	4.26450900
C	-2.10718100	-1.47772200	-1.65125000
C	-2.27421700	-0.73965600	-2.83895200
C	-3.03612400	-2.49019000	-1.34015100
C	-3.34715900	-1.01057700	-3.69103400
H	-1.56947100	0.03723800	-3.10445700
C	-4.10085400	-2.75792200	-2.20243500
H	-2.93337100	-3.06741700	-0.43053300

C	-4.26129700	-2.01841100	-3.37651100
H	-3.46315000	-0.43439000	-4.60167700
H	-4.80420900	-3.54387900	-1.95373100
H	-5.09069500	-2.22774000	-4.04151500
C	-3.02156800	3.11954400	1.41936500
C	-3.01546900	2.74374500	0.06306100
C	-3.87790200	1.75301900	-0.41672800
C	-4.78551500	1.09913000	0.43176600
C	-4.77639600	1.46423600	1.78493100
C	-3.90852000	2.44769300	2.26864300
H	-2.36687200	3.26831300	-0.63556300
H	-3.85941400	1.49427100	-1.47222800
H	-5.46529800	0.98945500	2.47739500
H	-3.94360700	2.71705900	3.32157500
C	-2.15595700	4.24735700	1.93091200
H	-1.14216000	4.20333800	1.52158500
H	-2.57605500	5.22004900	1.64742300
H	-2.08380900	4.23139600	3.02194800
C	-5.77836500	0.09413500	-0.13951600
H	-5.33489100	-0.30502800	-1.05985900
C	-6.05650100	-1.09816100	0.78997900
H	-6.59025800	-0.79329600	1.69672900
H	-6.68889900	-1.83170000	0.27988300
H	-5.13194200	-1.59969300	1.09213300
C	-7.09409400	0.80380300	-0.52367600
H	-6.91588000	1.62085100	-1.22943300
H	-7.79228200	0.09920500	-0.98796600
H	-7.58170900	1.22759900	0.36117000
H	-0.12486500	1.12094100	1.33273400
H	-0.93737400	1.11933700	1.04973700
Cl	0.58906200	1.17828600	-2.65523100
C	0.84660400	4.02748100	-1.21576700
O	0.41904900	3.33533300	-0.35921100
O	1.24974900	4.74850000	-2.02794300

## CO2

Zero-point = -188.569347

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16914800
O	0.00000000	0.00000000	-1.16914800

## 1\_CO2eq

Ru	0.11884100	1.02417000	0.30727900
P	-2.08320000	0.49565400	-0.28757800
P	0.74237800	-1.22225300	-0.08623000
C	-0.04620100	-1.95451900	-1.60056300
H	0.34794000	-1.35620600	-2.42552300
H	0.37458500	-2.95806400	-1.69180300

C	-2.26231900	-0.62976900	-1.76161300
C	-1.59662000	-2.03724600	-1.73282800
C	-1.90627000	-2.66610700	-3.13158600
H	-2.97688800	-2.89228700	-3.18792500
H	-1.68415100	-1.95768900	-3.94118000
P	-0.98455800	-4.21856300	-3.54924500
H	-1.82110100	-4.79313800	-4.53916400
H	0.09237500	-3.73807400	-4.33852900
O	-0.58705000	-5.11105900	-2.40700000
H	-3.33928500	-0.74512000	-1.92669000
H	-1.85627700	-0.06328100	-2.60209900
C	-2.24679300	-2.94085200	-0.66484900
H	-2.05441500	-2.59533800	0.34965000
H	-3.33325600	-2.95399700	-0.80245800
H	-1.87634700	-3.96318400	-0.75440400
C	0.55493900	-2.51644400	1.21422100
C	0.54026500	-3.88651900	0.88113900
C	0.52894600	-2.15633400	2.57043200
C	0.47904900	-4.85321700	1.88622400
H	0.55907400	-4.22040600	-0.14916200
C	0.47560500	-3.12628100	3.57413900
H	0.55510100	-1.11092000	2.83935400
C	0.44658900	-4.47886000	3.23190500
H	0.45782800	-5.90111200	1.61199200
H	0.46107300	-2.82709000	4.61638000
H	0.40249900	-5.23586300	4.00565300
C	2.54686000	-1.37401900	-0.46737900
C	3.07503500	-0.87128700	-1.67364700
C	3.42121300	-1.97622800	0.45707300
C	4.43911600	-0.98376400	-1.94705100
H	2.43031000	-0.37793700	-2.38897000
C	4.78648100	-2.07708400	0.17849900
H	3.03801700	-2.38778300	1.38198700
C	5.29885200	-1.58841400	-1.02537200
H	4.82792700	-0.60645000	-2.88604800
H	5.44360500	-2.55788400	0.89403400
H	6.35530600	-1.68326800	-1.24586700
C	-3.23718800	-0.21288500	0.95465100
C	-4.62004200	-0.26001500	0.68593900
C	-2.75666000	-0.78338200	2.14192300
C	-5.49275500	-0.85995500	1.59331700
H	-5.01442100	0.18230400	-0.22205200
C	-3.63411100	-1.38617800	3.04753800
H	-1.69406000	-0.78651100	2.34076000
C	-5.00212000	-1.42311500	2.77565800
H	-6.55435900	-0.88920900	1.37815500
H	-3.24593700	-1.83573500	3.95424000
H	-5.68349300	-1.89116200	3.47590700

C	-2.94915700	2.03654900	-0.81268300
C	-2.76372400	2.57488200	-2.09993000
C	-3.72045200	2.75986600	0.11976100
C	-3.33796000	3.80150600	-2.44140500
H	-2.15274900	2.05960200	-2.82860600
C	-4.28473700	3.98881300	-0.22714500
H	-3.90352700	2.35142800	1.10702700
C	-4.09473700	4.51283200	-1.50804700
H	-3.19202000	4.19947800	-3.43890400
H	-4.88220800	4.52855300	0.49848000
H	-4.53852900	5.46357000	-1.77799900
Cl	0.44914700	1.30782500	-2.09329700
C	0.16046500	1.65597900	2.60247800
C	1.46701900	1.32541500	2.14995000
C	2.08617100	2.01741100	1.07541500
C	1.40512500	3.06299100	0.39922200
C	0.04599600	3.30213700	0.74700100
C	-0.55988500	2.59817800	1.81498100
H	2.03686200	0.56416700	2.67299700
H	3.09479700	1.75019100	0.78505500
H	-0.54285100	4.01795200	0.18951400
H	-1.59025400	2.82233900	2.07058100
C	-0.40000600	1.17319100	3.91476200
H	0.07134400	0.25202900	4.26134800
H	-0.20873400	1.93780900	4.67743300
H	-1.48003900	1.01917200	3.86523600
C	2.13327800	3.86389700	-0.66736200
H	2.58688300	3.13086500	-1.34501300
C	1.22941400	4.78475500	-1.49597800
H	0.80064400	5.58672800	-0.88379700
H	1.82180300	5.26115900	-2.28197300
H	0.41883800	4.23183300	-1.97645900
C	3.27125300	4.67114300	0.00175300
H	3.98123200	4.02747700	0.52785600
H	3.82284100	5.22489400	-0.76352000
H	2.87084900	5.39812000	0.71658800
C	6.48136600	1.15806500	0.53268900
O	5.48525700	1.64783000	0.90818400
O	7.47949400	0.67924800	0.16507300

Ts1\*\_CO2eq

Zero-point = -3350.347832

Ru	-0.76691000	0.41353300	0.17446400
P	-0.47412200	-1.72775400	-0.48572000
P	1.48909000	0.82805800	0.01770100
C	2.35389700	0.00232400	-1.40143400
H	1.96183700	0.53308900	-2.27500200
H	3.40884400	0.27443100	-1.30735400

C	0.75046800	-1.94859600	-1.86864000
C	2.23064900	-1.52589200	-1.65505600
C	2.95317900	-1.83397800	-3.00743500
H	3.02911700	-2.92039100	-3.12836700
H	2.37601700	-1.45468200	-3.86187800
P	4.65793600	-1.13094100	-3.18883000
H	5.19603000	-1.94659700	-4.21594100
H	4.42166500	0.08073400	-3.88857800
O	5.47654700	-0.99548400	-1.93625000
H	0.71077300	-3.01014900	-2.13781900
H	0.33433500	-1.38142900	-2.70626700
C	2.91508500	-2.37391200	-0.56298800
H	2.52654100	-2.16860100	0.43290700
H	2.75526500	-3.43875000	-0.76183800
H	3.98964500	-2.18372400	-0.55897300
C	2.45053200	0.44988900	1.53585700
C	3.81182100	0.09603300	1.50120800
C	1.81990600	0.61593200	2.78258900
C	4.51094800	-0.11155900	2.69244200
H	4.33826800	-0.02262500	0.56161500
C	2.52582600	0.41300700	3.97005200
H	0.77899900	0.92072400	2.81831200
C	3.87209400	0.04261200	3.92519700
H	5.55768100	-0.38839300	2.65331800
H	2.03131800	0.55182000	4.92500000
H	4.42286500	-0.11544300	4.84474800
C	1.95869100	2.59042400	-0.28547800
C	1.75420200	3.18306100	-1.54787400
C	2.52263600	3.36437100	0.74469800
C	2.11202600	4.51397900	-1.76824200
H	1.29328600	2.62224800	-2.35093300
C	2.87349000	4.69679000	0.51655900
H	2.69793700	2.93014000	1.72006800
C	2.67128000	5.27434600	-0.73747900
H	1.94899300	4.95629900	-2.74395000
H	3.31173600	5.27815400	1.31916200
H	2.94842300	6.30684000	-0.91288700
C	-0.00692000	-2.99815600	0.75568500
C	-0.06089300	-4.36694800	0.42472000
C	0.48363000	-2.62140700	2.01527800
C	0.35837500	-5.32916500	1.34353600
H	-0.43938100	-4.68061000	-0.54173700
C	0.90400900	-3.58894800	2.93165900
H	0.57557200	-1.57318200	2.26839700
C	0.83942600	-4.94260200	2.59829500
H	0.31120700	-6.37922300	1.08037100
H	1.29342500	-3.28143100	3.89530700
H	1.16666500	-5.69343700	3.30736900



C	-2.03035000	-2.39581800	-1.21444800
C	-2.43117600	-2.00984700	-2.50852600
C	-2.88516800	-3.22267800	-0.45824500
C	-3.64727500	-2.45129900	-3.03228800
H	-1.81694200	-1.34163000	-3.09792200
C	-4.10422700	-3.65259300	-0.98604200
H	-2.59291800	-3.54938200	0.53234700
C	-4.48718800	-3.27013700	-2.27356000
H	-3.93914400	-2.15045800	-4.03163800
H	-4.74810200	-4.29247900	-0.39407400
H	-5.43101700	-3.60936300	-2.68319400
Cl	-0.98317900	1.13139300	-2.07000100
C	-2.08540400	0.40805900	2.83426600
C	-2.46199600	1.76952200	2.81070400
C	-3.26070600	2.28113800	1.79855100
C	-3.71140800	1.47757400	0.72813700
C	-3.29905600	0.13595100	0.70749600
C	-2.50179100	-0.39727100	1.75316700
H	-2.15371900	2.41787500	3.62680300
H	-3.55108800	3.32704600	1.83311300
H	-3.66274100	-0.53376800	-0.06115300
H	-2.35006600	-1.46997100	1.80717700
C	-1.46577600	-0.18585000	4.07597300
H	-0.72975100	0.48438600	4.52879700
H	-2.24754900	-0.35115800	4.82728000
H	-0.99362300	-1.15031700	3.88239900
C	-4.66443200	2.07105000	-0.30004000
H	-4.24468600	3.04430400	-0.59276800
C	-4.83042900	1.23127800	-1.57259900
H	-5.33255400	0.27957100	-1.36581000
H	-5.45171500	1.77512900	-2.28997400
H	-3.86876800	1.02040000	-2.04673100
C	-6.03728400	2.34333500	0.35738800
H	-5.95374200	2.98801000	1.23718400
H	-6.70390200	2.83453700	-0.35764600
H	-6.50831400	1.40521800	0.67006600
C	-1.14159200	4.07019400	-0.57102500
O	-0.94860800	3.40169800	0.37524200
O	-1.36003700	4.75145800	-1.48965800

2\_CO2eq

Zero-point = -3350.351502

Ru	-0.64444900	0.49898000	0.03942300
P	-0.40850900	-1.71726900	-0.41677000
P	1.59969000	0.83753500	-0.07652600
C	2.51810900	-0.14951900	-1.34587900
H	2.19072700	0.29231200	-2.29336300
H	3.57398900	0.10704000	-1.21925400

C	0.88791400	-2.10693400	-1.69406500
C	2.36419800	-1.69459000	-1.43285900
C	3.16277000	-2.17274500	-2.68939500
H	3.21087800	-3.26736900	-2.68136200
H	2.65407400	-1.88007900	-3.61810200
P	4.89822600	-1.53735100	-2.83153000
H	5.48547500	-2.49338500	-3.69788300
H	4.75228100	-0.42477300	-3.70016000
O	5.62634500	-1.25316600	-1.54807100
H	0.83814800	-3.18818300	-1.86422900
H	0.53849800	-1.61548700	-2.60711300
C	2.94939500	-2.42529500	-0.20667600
H	2.49715900	-2.10164000	0.72942300
H	2.77507100	-3.50250200	-0.29609200
H	4.02567700	-2.25576900	-0.14585300
C	2.44706000	0.61116800	1.53392100
C	3.79666800	0.22868800	1.63834600
C	1.72666300	0.90977600	2.70655900
C	4.39794600	0.12582900	2.89497800
H	4.38683200	0.00642400	0.75686400
C	2.33496000	0.80816000	3.95908300
H	0.69458400	1.24161300	2.63578200
C	3.67103300	0.41040500	4.05365300
H	5.43694900	-0.17311100	2.96481300
H	1.77285500	1.04687600	4.85487100
H	4.14623100	0.33173300	5.02417100
C	2.07969600	2.56082100	-0.53667600
C	1.86480700	3.03796100	-1.84606900
C	2.65270300	3.42347500	0.41616200
C	2.22111900	4.34341800	-2.18748000
H	1.39941700	2.40524800	-2.59131700
C	3.00234400	4.72948800	0.06563900
H	2.83700300	3.07714900	1.42462200
C	2.78938700	5.19194400	-1.23384600
H	2.05139800	4.69662800	-3.19779500
H	3.44843600	5.38019200	0.80846800
H	3.06493200	6.20446600	-1.50304800
C	-0.06945200	-2.86909200	0.97395000
C	-0.13647100	-4.26223600	0.77501600
C	0.31102500	-2.37905300	2.23332600
C	0.16822900	-5.13693500	1.81772100
H	-0.43993700	-4.66156300	-0.18641600
C	0.61545800	-3.25923200	3.27506200
H	0.40560400	-1.31234300	2.39529900
C	0.54314100	-4.63752000	3.06900000
H	0.11242400	-6.20678600	1.65522000
H	0.91865200	-2.86646000	4.23871100
H	0.78005400	-5.32079100	3.87562900

C	-1.94016500	-2.41725100	-1.16642000
C	-2.22747900	-2.23303900	-2.53205600
C	-2.88998500	-3.07023700	-0.35505500
C	-3.42559800	-2.70475200	-3.07136900
H	-1.53777800	-1.70056900	-3.17346100
C	-4.08987100	-3.53085000	-0.89971300
H	-2.68641700	-3.23644700	0.69612900
C	-4.35910200	-3.35231500	-2.25888500
H	-3.62993100	-2.56088900	-4.12580900
H	-4.80767100	-4.03614000	-0.26417600
H	-5.28763800	-3.71687000	-2.68158400
Cl	-0.84894600	0.96349800	-2.27022800
C	-2.38171500	0.97439100	2.82504700
C	-3.02534100	2.21106100	2.64349900
C	-3.81268200	2.45817600	1.52458400
C	-3.99436700	1.49305700	0.51457900
C	-3.32864200	0.26776200	0.66798400
C	-2.53311300	0.00969800	1.80993500
H	-2.93035900	2.97717700	3.40906800
H	-4.31910000	3.41656600	1.43572300
H	-3.49002800	-0.53133600	-0.04511700
H	-2.16533400	-0.99786000	1.98410200
C	-1.66914900	0.66551700	4.11986600
H	-1.03675800	1.49907000	4.44268700
H	-2.39782500	0.49248200	4.92063100
H	-1.05111000	-0.23196700	4.04386900
C	-4.95875800	1.78027100	-0.62963000
H	-4.78503900	2.82208300	-0.93463700
C	-4.75952900	0.89141800	-1.86406100
H	-5.01279200	-0.15392100	-1.65686700
H	-5.41880300	1.22948800	-2.66910200
H	-3.72977600	0.92672700	-2.22945700
C	-6.41522700	1.69055100	-0.12035300
H	-6.59405700	2.35776600	0.72811200
H	-7.11246300	1.96413100	-0.91822000
H	-6.65011200	0.66933900	0.19922300
C	-1.14858500	3.66180300	-0.49670300
O	-0.93349900	2.83224500	0.31340100
O	-1.38085000	4.51016800	-1.25229100

1\_CO2ax

Zero-point = -3350.374885

Ru	1.02449700	-0.25321400	-0.71792600
P	0.44365000	-1.31681100	1.28793700
P	-0.22128200	1.63983100	-0.05876300
C	-0.01980400	2.07922400	1.73305900
H	1.03842800	2.32799900	1.84039000
H	-0.59391900	2.99686500	1.87738000

C	0.47029000	-0.22683300	2.79954900
C	-0.41462300	1.05480200	2.83839800
C	-0.10604900	1.72141000	4.21965300
H	-0.53348400	1.10014100	5.01454900
H	0.97640400	1.77329800	4.39964600
P	-0.73945800	3.44631100	4.45838600
H	-0.77874000	3.54311300	5.87241100
H	0.39882000	4.23860100	4.15685800
O	-1.99340200	3.82904400	3.72412200
H	0.20187300	-0.87256000	3.64292600
H	1.51578700	0.06236700	2.92346000
C	-1.91617100	0.70278800	2.81596000
H	-2.22432200	0.24486100	1.87685900
H	-2.14279400	-0.01107600	3.61500500
H	-2.51866000	1.59928000	2.97209200
C	-2.03321900	1.76793800	-0.37083000
C	-2.80367200	2.75420300	0.27960200
C	-2.65988000	0.94290600	-1.31657000
C	-4.16272300	2.88597200	-0.00696400
H	-2.36973600	3.41175200	1.02282500
C	-4.02082500	1.07793500	-1.60248500
H	-2.08109400	0.18850800	-1.82898600
C	-4.77476700	2.05044800	-0.94528700
H	-4.74225000	3.64174600	0.50942800
H	-4.48575500	0.41904400	-2.32643900
H	-5.83127200	2.15810500	-1.15986900
C	0.39872800	3.13785300	-0.94221300
C	1.63406700	3.72540400	-0.60645000
C	-0.33257900	3.66385900	-2.02484500
C	2.11874200	4.81152200	-1.33751300
H	2.22959200	3.32462800	0.20278400
C	0.16555600	4.74392200	-2.75683200
H	-1.29815500	3.24695400	-2.28357900
C	1.39048800	5.32045200	-2.41556900
H	3.06613100	5.26023900	-1.06172100
H	-0.41215900	5.14235800	-3.58274600
H	1.77044300	6.16424500	-2.97903900
C	-1.13874900	-2.23943100	1.43912600
C	-1.35987400	-3.08155000	2.54787300
C	-2.16429200	-2.07373100	0.49904600
C	-2.58112700	-3.73726600	2.69937200
H	-0.57581800	-3.23604100	3.28078000
C	-3.38696500	-2.73355400	0.65215600
H	-2.01675300	-1.40668300	-0.33735000
C	-3.59615700	-3.56574400	1.75201200
H	-2.74118800	-4.38285800	3.55483600
H	-4.16811100	-2.58757900	-0.08487800
H	-4.54325100	-4.07713100	1.87599000

C	1.69608300	-2.61645700	1.66620100
C	2.93725900	-2.29340500	2.24544800
C	1.46059000	-3.94791800	1.26658400
C	3.91196100	-3.27844800	2.42097100
H	3.16034500	-1.27576700	2.53564500
C	2.44287400	-4.92476000	1.43828900
H	0.50088300	-4.22768200	0.84722200
C	3.67091600	-4.59261600	2.01553300
H	4.86018200	-3.01543500	2.87525100
H	2.24320300	-5.94565800	1.13375200
H	4.43000200	-5.35305400	2.15433100
Cl	2.81246800	0.73748000	0.61339100
C	0.09163700	-1.50351100	-2.51340200
C	0.37889600	-0.17235700	-2.91793100
C	1.69712900	0.35997900	-2.86183200
C	2.77252700	-0.41713200	-2.36705500
C	2.46674100	-1.69885600	-1.81987500
C	1.15419800	-2.21742300	-1.88639600
H	-0.41145100	0.43920900	-3.34068600
H	1.87307200	1.37542700	-3.19737000
H	3.23865000	-2.28305600	-1.33719900
H	0.96121500	-3.20526200	-1.48130300
C	-1.20253900	-2.19761700	-2.84702200
H	-2.03468500	-1.50596400	-2.98644800
H	-1.07181400	-2.73862500	-3.79238000
H	-1.48180400	-2.92745400	-2.08451600
C	4.18618300	0.14027300	-2.41839200
H	4.13734500	1.14156200	-1.97377400
C	5.22070400	-0.67989700	-1.63803600
H	5.36225200	-1.67396300	-2.07798100
H	6.18773100	-0.17078400	-1.67467500
H	4.94048600	-0.79071400	-0.58812400
C	4.61391500	0.28825200	-3.89779200
H	3.93140900	0.92645800	-4.46633700
H	5.61034900	0.73630900	-3.94732300
H	4.66007300	-0.68721500	-4.39376300
C	-5.66850800	-2.81212900	-3.37236700
O	-6.51157300	-3.40673700	-3.91448400
O	-4.81911000	-2.21421300	-2.82579700

Ts1\_CO2ax

Zero-point = -3350.331448

Ru	-0.53968800	0.81805900	-0.04409700
P	-1.18601600	-1.38578100	-0.32666900
P	1.68263600	0.40904700	-0.39937000
C	2.03955400	-1.01532800	-1.52743800
H	1.66943400	-0.69222700	-2.50490200
H	3.12845900	-1.06912300	-1.59378800

C	-0.09159900	-2.43062600	-1.41027500
C	1.45063400	-2.42212800	-1.21449700
C	2.00825300	-3.41840200	-2.28303300
H	1.71003700	-4.43617500	-2.00747400
H	1.57456200	-3.21652300	-3.27176600
P	3.84702900	-3.42058900	-2.51663200
H	4.07604300	-4.71993400	-3.03345700
H	4.01899600	-2.62146600	-3.67588500
O	4.67958900	-3.01351000	-1.33297000
H	-0.47261000	-3.45640300	-1.36788800
H	-0.31530000	-2.06780100	-2.41773700
C	1.84076400	-2.95008400	0.17979900
H	1.45315200	-2.32165500	0.98431700
H	1.43629400	-3.95575100	0.32588100
H	2.92334600	-3.01284200	0.28406300
C	2.82681300	0.22606700	1.03553500
C	3.98682700	-0.57042500	0.97349100
C	2.62325200	1.03336600	2.17234000
C	4.88874200	-0.58118100	2.04084800
H	4.21349900	-1.18952500	0.11395400
C	3.53236100	1.02184800	3.23194000
H	1.75812900	1.67937000	2.22129000
C	4.66461900	0.20645800	3.17088600
H	5.77128900	-1.20645100	1.97806000
H	3.36166000	1.65406800	4.09611600
H	5.37050900	0.19298800	3.99255600
C	2.48301200	1.83067900	-1.28282300
C	2.33518600	2.01117900	-2.67210000
C	3.24539000	2.77040800	-0.56021900
C	2.92857200	3.09935200	-3.31278400
H	1.73789900	1.32584400	-3.25622200
C	3.82497800	3.86361600	-1.20672000
H	3.41175600	2.63709900	0.50041400
C	3.66841500	4.03210400	-2.58320300
H	2.80732000	3.21844800	-4.38304200
H	4.41261200	4.57203700	-0.63460700
H	4.12442700	4.87749500	-3.08423400
C	-1.53159600	-2.33127600	1.21895500
C	-1.26068100	-3.70287700	1.35618000
C	-2.24062300	-1.68101000	2.25144700
C	-1.65110800	-4.39517000	2.50489000
H	-0.75359100	-4.24574000	0.57071400
C	-2.63622800	-2.37763000	3.39468800
H	-2.48874900	-0.63000600	2.15559600
C	-2.33469700	-3.73565600	3.52700600
H	-1.42613500	-5.45110200	2.59542800
H	-3.18568700	-1.86376600	4.17527400
H	-2.63819600	-4.27610800	4.41530400

C	-2.82027100	-1.59311400	-1.19491400
C	-2.92929200	-1.42372800	-2.59045400
C	-3.97670300	-1.94923200	-0.47336700
C	-4.15274500	-1.60451900	-3.23533500
H	-2.07248200	-1.12505000	-3.17692900
C	-5.19912400	-2.12370700	-1.12584400
H	-3.92736100	-2.10839700	0.59442800
C	-5.29218100	-1.95243200	-2.50678800
H	-4.21302300	-1.47123500	-4.30916800
H	-6.07413800	-2.40275500	-0.55063300
H	-6.24034800	-2.09287400	-3.01174400
Cl	-0.79618800	1.04465400	-2.38918100
C	-0.68040800	3.24485400	2.19822900
C	-0.36019600	3.37632500	0.82718900
C	-1.33545400	3.15758000	-0.16296100
C	-2.64391100	2.72089300	0.17125200
C	-2.90441600	2.48458400	1.53085300
C	-1.95349500	2.76774000	2.52176000
H	0.60948300	3.76698600	0.53229800
H	-1.10832800	3.41242200	-1.19181100
H	-3.88741900	2.13866500	1.83416500
H	-2.22265900	2.63200600	3.56596000
C	0.29055100	3.65398100	3.27743700
H	1.27250600	3.90303700	2.86770600
H	-0.07826100	4.54169900	3.80373500
H	0.41464500	2.86641700	4.02782900
C	-3.72224100	2.67766700	-0.90367100
H	-3.24037500	2.31730700	-1.81971100
C	-4.89430000	1.73968500	-0.58654700
H	-5.48102000	2.09159600	0.26981500
H	-5.57358300	1.70054600	-1.44281400
H	-4.56107500	0.71774800	-0.38709200
C	-4.23005600	4.11224500	-1.17477300
H	-3.41471800	4.78535800	-1.45688300
H	-4.95819600	4.10563000	-1.99177000
H	-4.72067900	4.52868100	-0.28804200
C	0.35295200	-0.65941100	3.33074000
O	0.85359700	-1.54473300	3.89391100
O	-0.15477000	0.24542200	2.77690900

## 2\_CO2ax

Zero-point = -3350.349118

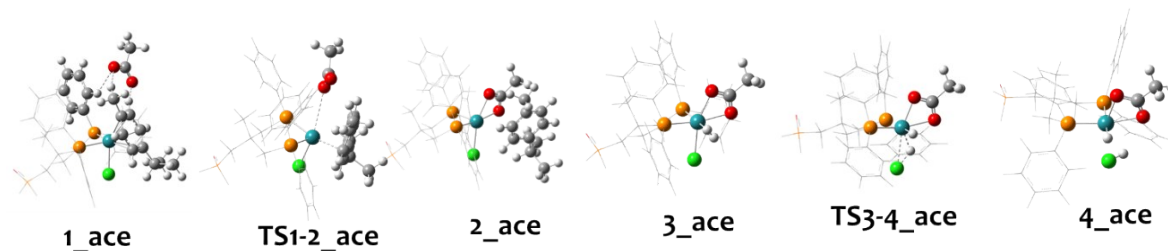
Ru	1.02451600	-0.25317700	-0.71793600
P	0.44371900	-1.31663800	1.28801800
P	-0.22141100	1.63984800	-0.05890600
C	-0.01998900	2.07937800	1.73289100
H	1.03821500	2.32826300	1.84022400
H	-0.59420200	2.99697200	1.87711800

C	0.47029200	-0.22654800	2.79954400
C	-0.41475100	1.05499500	2.83828600
C	-0.10631900	1.72168800	4.21954100
H	-0.53377400	1.10042200	5.01442900
H	0.97611800	1.77363200	4.39961400
P	-0.73980900	3.44657000	4.45819900
H	-0.77901800	3.54346300	5.87221900
H	0.39840500	4.23891200	4.15656800
O	-1.99381600	3.82920700	3.72399300
H	0.20195000	-0.87222100	3.64298500
H	1.51576400	0.06276300	2.92341200
C	-1.91625000	0.70277500	2.81573200
H	-2.22423200	0.24477000	1.87661400
H	-2.14285000	-0.01109400	3.61478000
H	-2.51887800	1.59918700	2.97177400
C	-2.03336500	1.76775400	-0.37096300
C	-2.80392600	2.75399200	0.27938400
C	-2.65993500	0.94258100	-1.31663800
C	-4.16298300	2.88561100	-0.00722300
H	-2.37006700	3.41163800	1.02256800
C	-4.02088400	1.07746400	-1.60260100
H	-2.08105800	0.18819000	-1.82895100
C	-4.77492900	2.04996100	-0.94549900
H	-4.74259400	3.64137400	0.50909000
H	-4.48574600	0.41848000	-2.32651800
H	-5.83143800	2.15750700	-1.16011700
C	0.39842800	3.13790400	-0.94241900
C	1.63371800	3.72558500	-0.60669500
C	-0.33297400	3.66384200	-2.02501700
C	2.11824900	4.81176200	-1.33776000
H	2.22931100	3.32485300	0.20250900
C	0.16501500	4.74397400	-2.75700400
H	-1.29851200	3.24683700	-2.28372700
C	1.38989500	5.32063400	-2.41577700
H	3.06560300	5.26057400	-1.06200200
H	-0.41277400	5.14235700	-3.58289200
H	1.76973200	6.16448100	-2.97924600
C	-1.13858800	-2.23941000	1.43926800
C	-1.35963600	-3.08134900	2.54817000
C	-2.16408500	-2.07411100	0.49907100
C	-2.58077600	-3.73726400	2.69971600
H	-0.57560400	-3.23554700	3.28116500
C	-3.38664400	-2.73413700	0.65222700
H	-2.01664800	-1.40720000	-0.33745300
C	-3.59576500	-3.56613400	1.75224100
H	-2.74077800	-4.38270600	3.55530400
H	-4.16775800	-2.58846500	-0.08490300
H	-4.54277100	-4.07767400	1.87625100



C	1.69625900	-2.61616000	1.66637400
C	2.93746900	-2.29292000	2.24545200
C	1.46081800	-3.94770000	1.26700800
C	3.91225200	-3.27786500	2.42105500
H	3.16051100	-1.27521500	2.53545200
C	2.44318600	-4.92444500	1.43879000
H	0.50108800	-4.22760100	0.84779000
C	3.67125800	-4.59212000	2.01586400
H	4.86049700	-3.01471100	2.87520500
H	2.24355400	-5.94540800	1.13444800
H	4.43040800	-5.35248300	2.15472300
Cl	2.81236500	0.73785100	0.61332200
C	0.09171500	-1.50359600	-2.51335200
C	0.37897000	-0.17245200	-2.91793800
C	1.69718600	0.35991100	-2.86180700
C	2.77258600	-0.41716900	-2.36696800
C	2.46680300	-1.69886700	-1.81973600
C	1.15426100	-2.21744900	-1.88625900
H	-0.41137200	0.43908200	-3.34074600
H	1.87312600	1.37535600	-3.19735600
H	3.23871300	-2.28304200	-1.33703700
H	0.96127800	-3.20526900	-1.48111700
C	-1.20239500	-2.19777100	-2.84708800
H	-2.03465700	-1.50620600	-2.98625000
H	-1.07164700	-2.73847300	-3.79261900
H	-1.48150300	-2.92787500	-2.08478000
C	4.18623000	0.14027100	-2.41826600
H	4.13735400	1.14154900	-1.97362800
C	5.22075700	-0.67988200	-1.63789900
H	5.36234000	-1.67394100	-2.07785100
H	6.18777200	-0.17074500	-1.67450800
H	4.94052500	-0.79072200	-0.58799200
C	4.61399800	0.28829300	-3.89764800
H	3.93148600	0.92648500	-4.46620200
H	5.61041700	0.73639000	-3.94714100
H	4.66020900	-0.68716300	-4.39363800
C	-5.66790300	-2.81302300	-3.37220600
O	-6.51077500	-3.40733600	-3.91494400
O	-4.81870900	-2.21539200	-2.82500500

**S8. Cartesian coordinates (Å) and zero-point corrected energies, (Hartrees) of optimized structures of stationary points for the formation of the active specie Ru<sub>2</sub><sub>ace</sub> H in presence of acetate anion.**



Acetate

Zero-point = -228.454177

C	0.22017600	-0.00001100	-0.01332900
O	0.75203900	-1.13901600	0.00310800
O	0.75268900	1.13868300	0.00311000
C	-1.35462900	0.00032100	-0.00452200
H	-1.71519100	-0.00187000	1.03487800
H	-1.75785400	0.89943800	-0.48695600
H	-1.75806300	-0.89676800	-0.49056400

1\_ace

Zero-point = -3390.403432

Ru	-0.23817400	1.14912500	0.23819100
P	-0.86735800	-0.65593200	-1.16311500
P	1.88227300	0.22026400	0.41119000
C	2.61306300	-0.35183500	-1.20268000
H	2.71188100	0.55538700	-1.80372300
H	3.61721000	-0.71432600	-0.95976100
C	0.43417300	-1.00589700	-2.45300400
C	1.87315600	-1.43854800	-2.03578200
C	2.64010400	-1.58462500	-3.39064500
H	2.25265600	-2.45883700	-3.92693700
H	2.46425300	-0.71001400	-4.03400100
P	4.47123300	-1.75970600	-3.33125300
H	4.74421800	-2.02499200	-4.70124700
H	4.90862500	-0.41151500	-3.23167300
O	5.07886200	-2.70581900	-2.33893600
H	0.02801000	-1.75629800	-3.13756000
H	0.51290600	-0.07003500	-3.00863200
C	1.89147500	-2.81023000	-1.33134600
H	1.34558800	-2.79924400	-0.38860200
H	1.42066100	-3.56666500	-1.96706300
H	2.92024700	-3.12164000	-1.13483300
C	2.24171500	-1.17918700	1.54752400
C	3.56032600	-1.66088600	1.68574300
C	1.20882100	-1.81997900	2.24277300
C	3.82439600	-2.75978100	2.50083600
H	4.37831300	-1.18000900	1.16125800
C	1.47704800	-2.92227700	3.06035400
H	0.19368000	-1.47027800	2.13391200

C	2.78303500	-3.39282900	3.18892300
H	4.83992500	-3.12661200	2.59328500
H	0.66114300	-3.40838500	3.58226100
H	2.99276900	-4.25047500	3.81735200
C	3.09489700	1.50181900	0.96472000
C	3.45079100	2.55942000	0.10523500
C	3.58948600	1.50442200	2.28264600
C	4.29077400	3.58076200	0.55311000
H	3.04249500	2.60581200	-0.89681900
C	4.42280400	2.53468600	2.72548400
H	3.33585700	0.69612200	2.95768800
C	4.77837300	3.57259900	1.86233000
H	4.55946700	4.38545500	-0.12205100
H	4.79776700	2.51940500	3.74254600
H	5.42901600	4.36811200	2.20636200
C	-1.38707400	-2.32220700	-0.57669400
C	-1.48908100	-3.38155100	-1.50512400
C	-1.77621100	-2.55036100	0.74735900
C	-1.91396500	-4.64250100	-1.09548500
H	-1.25670800	-3.22387300	-2.55127100
C	-2.21051300	-3.81780200	1.15430300
H	-1.81897200	-1.75788900	1.48117300
C	-2.26508100	-4.86679400	0.24096700
H	-1.98266200	-5.44663400	-1.81949800
H	-2.53451400	-3.93297600	2.18104100
H	-2.60094500	-5.84846600	0.55511400
C	-2.34326200	-0.16901000	-2.15400500
C	-2.24781000	0.42824300	-3.42208500
C	-3.61314200	-0.33893500	-1.56213200
C	-3.40264500	0.83823800	-4.09500700
H	-1.28320000	0.59366700	-3.88410600
C	-4.75739100	0.08443500	-2.24076400
H	-3.72372600	-0.77522000	-0.57089000
C	-4.65711800	0.66826100	-3.50699300
H	-3.31720700	1.29239300	-5.07596200
H	-5.72563200	-0.04881200	-1.77208000
H	-5.55039800	0.98919000	-4.03072600
C	-0.99174400	1.21107300	2.50221100
C	-0.04925100	2.25557400	2.23478900
C	-0.27887800	3.20725400	1.22541000
C	-1.48610800	3.18047800	0.44347900
C	-2.35356900	2.09360400	0.63224300
C	-2.10090200	1.09987400	1.62821500
H	0.86528500	2.31452900	2.81685400
H	0.46635700	3.97017100	1.02902000
H	-3.22833500	1.97371100	0.00576200
H	-2.84529900	0.29089400	1.73692100
C	-0.88246000	0.35245200	3.73304600

H	0.14977400	0.06426300	3.94857200
H	-1.24003300	0.94772400	4.58401400
H	-1.53625700	-0.52501200	3.65864900
C	-1.75377000	4.30817600	-0.53558400
H	-0.79849900	4.52256300	-1.02826400
C	-2.77970300	3.97041800	-1.62314600
H	-3.78167300	3.82149000	-1.20550000
H	-2.84459700	4.80102400	-2.33291900
H	-2.49791600	3.07209400	-2.17684000
C	-2.17903300	5.56338700	0.26003600
H	-1.43237800	5.84799900	1.00837800
H	-2.31085100	6.40912600	-0.42217800
H	-3.12965800	5.39610300	0.77810300
Cl	0.55774600	2.21966800	-1.83815100
C	-4.25306400	-1.55906800	2.61727500
O	-3.21708900	-1.77964600	3.30419500
O	-4.34286800	-0.78138700	1.61866500
C	-5.52458500	-2.34174900	2.98705500
H	-5.47079200	-2.72337300	4.00951000
H	-6.41314700	-1.71645500	2.86179100
H	-5.62864900	-3.19437600	2.30442800

Ts1\_ace

Zero-point = -3390.382638

Ru	0.52149800	-0.99079400	-0.03475700
P	0.91568800	1.20905200	-0.71705500
P	-1.69678300	-0.57287300	0.01248700
C	-2.35014200	0.34412600	-1.46978900
H	-2.19027400	-0.35563200	-2.29545300
H	-3.43069300	0.43334400	-1.31778800
C	-0.23575900	1.69539000	-2.10914300
C	-1.77351000	1.73412700	-1.85999500
C	-2.38863900	2.12254000	-3.24422300
H	-2.15276600	3.17196400	-3.45625200
H	-1.94332600	1.52372300	-4.05213200
P	-4.20565800	1.92010400	-3.45763600
H	-4.38824100	2.54096600	-4.72376500
H	-4.32592300	0.55060400	-3.81566400
O	-5.12107600	2.37581000	-2.35937800
H	0.08591100	2.68227700	-2.45815400
H	-0.04453700	0.97496800	-2.90626400
C	-2.18073300	2.82435400	-0.84820900
H	-1.82610300	2.61017400	0.15837300
H	-1.75340400	3.78874400	-1.14203500
H	-3.26858100	2.92412200	-0.81830400
C	-2.40105900	0.26277100	1.48611300
C	-3.72925900	0.73866100	1.49619200
C	-1.61932000	0.39327300	2.64331300

C	-4.24931500	1.33919400	2.64173900
H	-4.35821700	0.64884900	0.61769600
C	-2.14668400	1.00064700	3.78842700
H	-0.58298400	0.06843000	2.68235200
C	-3.45869300	1.47164100	3.78965500
H	-5.26801600	1.70954300	2.63586900
H	-1.50434700	1.10832700	4.65450300
H	-3.86746400	1.94615200	4.67462100
C	-2.70256100	-2.12610900	-0.08160900
C	-2.60397500	-2.95491200	-1.21745100
C	-3.51648100	-2.53732200	0.98907100
C	-3.30958600	-4.15750000	-1.27741600
H	-1.95098700	-2.67581700	-2.03640100
C	-4.21540700	-3.74590800	0.92316600
H	-3.61086600	-1.91244600	1.86792600
C	-4.11568300	-4.55724600	-0.20792100
H	-3.22556300	-4.78350000	-2.15882200
H	-4.83966500	-4.04798000	1.75639700
H	-4.66008600	-5.49316500	-0.25640300
C	0.92364900	2.78394000	0.25280900
C	1.42551400	3.93817000	-0.37936100
C	0.37854400	2.89805900	1.53632500
C	1.36802300	5.17741200	0.25955100
H	1.87983900	3.86723700	-1.36147000
C	0.31915300	4.14125100	2.17136600
H	0.02467500	2.02439900	2.05858200
C	0.80926300	5.28308200	1.53556000
H	1.76488000	6.05586200	-0.23676600
H	-0.10443100	4.20645500	3.16686800
H	0.76481600	6.24575800	2.03181400
C	2.57839500	1.27429700	-1.51122600
C	2.77317800	1.14824200	-2.89705900
C	3.69950600	1.41087100	-0.66527100
C	4.06433500	1.17606700	-3.43185700
H	1.93194900	1.01601300	-3.56450300
C	4.98353900	1.43467700	-1.21196600
H	3.54763900	1.46757900	0.41058200
C	5.17018000	1.32274300	-2.59310100
H	4.20172500	1.08147900	-4.50328600
H	5.83997800	1.54113700	-0.55512300
H	6.17012300	1.34454700	-3.01160400
C	0.79579400	-2.53337800	2.34893000
C	0.26556700	-3.14220000	1.17810900
C	1.06163600	-3.32643800	0.03893800
C	2.41084400	-2.86151400	-0.01185500
C	2.86785200	-2.14196100	1.09570500
C	2.08251900	-2.00138100	2.26099700
H	-0.74349800	-3.53974000	1.18900800

H	0.65171400	-3.85749500	-0.81225300
H	3.84944400	-1.68501200	1.08372000
H	2.47859700	-1.45570500	3.10477300
C	0.02439200	-2.48636900	3.64068400
H	-1.05483600	-2.51711300	3.46752600
H	0.28329900	-3.35476000	4.26018200
H	0.27838800	-1.57625500	4.19005200
C	3.27291900	-3.20781500	-1.21594200
H	2.65707200	-3.01557100	-2.10284500
C	4.55138500	-2.37028700	-1.33696000
H	5.24954100	-2.57861200	-0.51738300
H	5.06610600	-2.61959200	-2.27015700
H	4.34315600	-1.29815400	-1.34617700
C	3.61004100	-4.71528200	-1.19354100
H	2.70891700	-5.33564200	-1.15727000
H	4.17043300	-4.99057500	-2.09316100
H	4.22607200	-4.96545100	-0.32225400
Cl	0.37434800	-1.52693600	-2.38880100
C	2.16800200	1.04896900	3.24139000
O	1.19032200	0.60109400	3.89658100
O	2.43886600	0.78194900	2.02758500
C	3.11324700	2.03307500	3.94837800
H	2.98823400	1.99262600	5.03296800
H	4.15508800	1.83128700	3.68142000
H	2.87976200	3.04769900	3.60497400

2\_ace

Zero-point = -3390.45561

Ru	0.65955300	0.43107500	-0.11447400
P	-1.13377500	1.75189900	-0.18024500
P	-0.63392100	-1.44408400	-0.19626300
C	-2.06230700	-1.34986700	-1.39076200
H	-1.55551700	-1.31635500	-2.36151300
H	-2.59594800	-2.30392300	-1.33684600
C	-2.39695400	1.21584500	-1.44354400
C	-3.07997500	-0.17744100	-1.31573700
C	-4.01003900	-0.28293000	-2.56733700
H	-4.84098300	0.42440800	-2.45933200
H	-3.46745900	-0.00386300	-3.48224400
P	-4.74507900	-1.93053700	-2.93338700
H	-5.64218100	-1.58811500	-3.98199600
H	-3.71616400	-2.57950100	-3.66515900
O	-5.32733300	-2.72704600	-1.80170600
H	-3.17231400	1.98925900	-1.47963800
H	-1.84913500	1.25703100	-2.38990300
C	-3.97201100	-0.26514000	-0.06029000
H	-3.39057800	-0.25065600	0.86117100
H	-4.65965000	0.58624100	-0.02508600

H	-4.56701800	-1.18094200	-0.08222700
C	-1.32307200	-2.07846400	1.39342000
C	-2.47950400	-2.87740400	1.46319300
C	-0.60007800	-1.82384900	2.57388800
C	-2.91006000	-3.39177100	2.68774200
H	-3.05314100	-3.10252000	0.57206600
C	-1.03145500	-2.34959900	3.79485900
H	0.29139600	-1.20862900	2.53389300
C	-2.18757900	-3.13015700	3.85474500
H	-3.80764800	-3.99815500	2.72697600
H	-0.46364000	-2.14640800	4.69635100
H	-2.52384300	-3.53420000	4.80280900
C	0.19046300	-2.98161000	-0.84205400
C	0.73966300	-2.98427200	-2.14008600
C	0.30121100	-4.14625100	-0.06034300
C	1.37122300	-4.12461500	-2.63915100
H	0.70041700	-2.08506300	-2.74403400
C	0.94066100	-5.28133400	-0.56524300
H	-0.11450700	-4.17069000	0.93825200
C	1.47476600	-5.27545300	-1.85441200
H	1.78949900	-4.10806100	-3.63948300
H	1.01696400	-6.16983800	0.05139300
H	1.97021200	-6.15773600	-2.24300400
C	-2.13345800	2.08380700	1.33428100
C	-3.28424300	2.89516400	1.25763600
C	-1.78069100	1.52021700	2.56911900
C	-4.07009300	3.11629800	2.38712100
H	-3.55656900	3.36585000	0.31942900
C	-2.57499400	1.74358700	3.69911000
H	-0.88350000	0.92202300	2.64448900
C	-3.71985900	2.53432800	3.61026600
H	-4.95317400	3.74104900	2.31533700
H	-2.29500600	1.29367100	4.64485600
H	-4.33566400	2.70284800	4.48621400
C	-0.71680200	3.46024200	-0.74681900
C	-0.28757600	3.67592800	-2.06988000
C	-0.74673000	4.54878200	0.14322400
C	0.07398600	4.95508600	-2.49366200
H	-0.18847900	2.84023600	-2.75144800
C	-0.37512100	5.82438700	-0.28621300
H	-1.06296600	4.40306300	1.16829100
C	0.02967400	6.03225300	-1.60561300
H	0.40471000	5.10498700	-3.51519500
H	-0.40242100	6.65321500	0.41221800
H	0.31737400	7.02343200	-1.93701600
C	4.03681100	-1.79507600	1.87328300
C	3.24803800	-1.90358200	0.71938400
C	3.47844000	-1.08652500	-0.39113700

C	4.51422000	-0.13426900	-0.39786300
C	5.30380700	-0.03599500	0.75362900
C	5.06670000	-0.84830600	1.86727000
H	2.45251700	-2.64157800	0.67732300
H	2.87149500	-1.21436600	-1.28345700
H	6.12005300	0.68034100	0.79001900
H	5.70216100	-0.74665500	2.74496900
C	3.79527000	-2.69309400	3.06431700
H	4.17798200	-3.70596400	2.88583500
H	4.28996300	-2.31002800	3.96192700
H	2.72596600	-2.78773700	3.28135900
C	4.77910900	0.69853600	-1.64525900
H	3.86674000	0.65365200	-2.25163500
C	5.05073300	2.18108800	-1.34018400
H	5.98361200	2.31864100	-0.78019200
H	5.15007800	2.74353300	-2.27513700
H	4.22923800	2.61365600	-0.76357100
C	5.92744500	0.08297400	-2.47113300
H	5.71614300	-0.95848800	-2.73497400
H	6.08016200	0.64471100	-3.39963200
H	6.86873700	0.10012000	-1.90897100
Cl	0.84816800	0.43979600	-2.55257200
C	1.97925400	1.71540300	1.64592800
O	1.19324900	0.74184300	1.94438100
O	2.03538700	2.09319700	0.43934700
C	2.82247300	2.35593200	2.71437800
H	3.75917100	1.79605000	2.80011900
H	3.05662100	3.38615400	2.44051500
H	2.31022000	2.32118200	3.67827900

3\_ace

Zero-point = -3002.311332

Ru	0.46762500	-1.60690700	0.22206200
P	1.60243800	0.30221300	-0.41755500
P	-1.53176000	-0.49535500	0.13690400
C	-1.72356500	0.63553100	-1.33256500
H	-1.74632100	-0.07538900	-2.16615500
H	-2.72003200	1.08307300	-1.26035200
C	0.76427500	1.18907600	-1.82700100
C	-0.67907300	1.74586300	-1.64565100
C	-1.04919300	2.34901100	-3.03958400
H	-0.43876700	3.24218300	-3.21863200
H	-0.82171300	1.63701200	-3.84602900
P	-2.80556200	2.83072500	-3.30837100
H	-2.70456300	3.49916300	-4.55914500
H	-3.41125800	1.61043400	-3.70684900
O	-3.52164200	3.57593800	-2.21894400
H	1.42137200	2.00697700	-2.14251200



H	0.75740500	0.44493700	-2.62903100
C	-0.71989600	2.89297900	-0.61489100
H	-0.52340900	2.54550700	0.39894000
H	0.04190000	3.64186400	-0.85552900
H	-1.69497700	3.38482200	-0.63236500
C	-2.01495300	0.48655800	1.62119200
C	-2.89371800	1.58488300	1.56144000
C	-1.55074600	0.05635400	2.87779000
C	-3.28307000	2.24282600	2.72995000
H	-3.27755400	1.93735500	0.61157900
C	-1.95000300	0.71435300	4.04368900
H	-0.86953400	-0.78423900	2.93861400
C	-2.81324300	1.80920100	3.97220400
H	-3.95427200	3.09156100	2.66694400
H	-1.58539800	0.36968900	5.00510000
H	-3.12019500	2.32118000	4.87703000
C	-3.04065200	-1.55365500	-0.09222900
C	-3.03340100	-2.55562600	-1.08380700
C	-4.19545000	-1.38634100	0.69273300
C	-4.15685600	-3.35962800	-1.28296500
H	-2.14638100	-2.70912900	-1.68859700
C	-5.31406600	-2.19818000	0.48861000
H	-4.22402700	-0.62621300	1.46190900
C	-5.29912600	-3.18453600	-0.49825000
H	-4.13434600	-4.12622500	-2.04951000
H	-6.19533600	-2.05711900	1.10413800
H	-6.16836100	-3.81357700	-0.65260900
C	1.98434100	1.63823400	0.79245100
C	2.63452500	2.81591200	0.37007800
C	1.61218500	1.51352500	2.13922400
C	2.88613500	3.84742200	1.27260200
H	2.95628300	2.91883500	-0.66028500
C	1.86463500	2.55364100	3.04027100
H	1.13813400	0.60351300	2.47931300
C	2.49522900	3.72029100	2.61005800
H	3.38566400	4.74861900	0.93565300
H	1.56199300	2.44727700	4.07577400
H	2.68657600	4.52629100	3.30908400
C	3.26858400	-0.06316700	-1.12604100
C	3.37971500	-0.74973900	-2.34993100
C	4.44241400	0.27024500	-0.42659400
C	4.63563300	-1.06812300	-2.86771900
H	2.48915500	-1.07666200	-2.87147200
C	5.69522800	-0.05876400	-0.94812400
H	4.38040200	0.79024400	0.52080000
C	5.79583900	-0.72247200	-2.17161100
H	4.70411900	-1.59995500	-3.80991200
H	6.59033200	0.20489500	-0.39605000

H	6.76938500	-0.97622000	-2.57509600
Cl	0.24733400	-2.22161200	-2.15746200
C	2.16993800	-2.32907100	1.99457300
O	2.36632200	-2.64910300	0.78808500
O	1.14306200	-1.60995600	2.28063100
C	3.08691700	-2.79354000	3.09549100
H	3.26086800	-1.98436400	3.80915000
H	2.61178500	-3.61897900	3.63676400
H	4.03173000	-3.14269800	2.67718900
H	-0.12490600	-3.35388800	0.31808700
H	-0.57611300	-2.99661100	0.86499900

Ts3\_ace

Zero-point = -3002.248117

Ru	0.35240908	1.56368040	-0.15059878
P	1.78979180	-0.48724508	0.27525994
P	-1.58339083	0.37492539	0.03446511
C	-1.52862054	-1.08668802	1.20262473
H	-1.41886151	-0.61856418	2.18812521
H	-2.53383476	-1.51682422	1.16852151
C	0.97450110	-1.74661575	1.37998920
C	-0.47418169	-2.22446426	1.06714772
C	-0.78687054	-3.27910923	2.17914787
H	-0.16655393	-4.16790327	2.01310731
H	-0.52779086	-2.88858048	3.17391674
P	-2.53108208	-3.85385350	2.32786001
H	-2.37193825	-4.96417925	3.20087230
H	-3.10476466	-2.90114694	3.20979302
O	-3.31132322	-4.11222280	1.07035627
H	1.61738932	-2.63331573	1.42025589
H	0.99430470	-1.27518318	2.36949389
C	-0.53247305	-2.94721130	-0.29370730
H	-0.36033152	-2.26850320	-1.12870003
H	0.24392787	-3.71914741	-0.33767117
H	-1.50127878	-3.42886346	-0.43595670
C	-2.28615714	-0.28419225	-1.53970360
C	-3.16278913	-1.38609501	-1.58562636
C	-1.97161304	0.38550387	-2.73691031
C	-3.69473219	-1.81260350	-2.80408043
H	-3.42866733	-1.93004043	-0.68659350
C	-2.51277924	-0.04489338	-3.95134704
H	-1.31565353	1.24782291	-2.71273831
C	-3.37084020	-1.14502839	-3.98811881
H	-4.36030010	-2.66781698	-2.82425299
H	-2.26537734	0.48402639	-4.86521392
H	-3.78745751	-1.48000765	-4.93117290
C	-3.03967793	1.25321976	0.76860312
C	-4.29692827	1.27611347	0.14261898

C	-2.87971341	1.91983178	1.99977366
C	-5.36991151	1.94682270	0.73621805
H	-4.44018188	0.77457393	-0.80546927
C	-3.95716327	2.58188538	2.58877978
H	-1.91336923	1.93401658	2.49221694
C	-5.20444958	2.59799423	1.95880295
H	-6.33312040	1.95915277	0.23878188
H	-3.81765628	3.09131931	3.53560641
H	-6.03832477	3.11833762	2.41587944
C	2.30416018	-1.41862890	-1.23226356
C	3.25756282	-2.45036303	-1.17736449
C	1.72948510	-1.08568824	-2.47024676
C	3.60982169	-3.14570573	-2.33461351
H	3.74032742	-2.69353984	-0.23737335
C	2.08374766	-1.78508751	-3.62652437
H	0.99911338	-0.28469901	-2.52444601
C	3.02092648	-2.81724789	-3.55943817
H	4.34745996	-3.93843961	-2.28271607
H	1.62825597	-1.52207000	-4.57442156
H	3.29760186	-3.35911853	-4.45638108
C	3.39598238	-0.20054399	1.12582800
C	3.95826532	-1.09151827	2.05672827
C	4.09692221	0.97517269	0.79821396
C	5.20018486	-0.81922146	2.63515578
H	3.43212183	-1.99186913	2.34895143
C	5.33903004	1.23831660	1.37702931
H	3.65633935	1.69204831	0.11473749
C	5.89418967	0.34270439	2.29360390
H	5.62032151	-1.51202668	3.35552930
H	5.86460914	2.15124259	1.12148805
H	6.85567740	0.55386000	2.74716767
Cl	0.70273674	1.71086334	2.90932992
C	1.26505266	3.26254138	-1.78915106
O	0.10391012	2.71433773	-1.88063765
O	1.99013617	2.94382081	-0.80425610
C	1.70248066	4.26661164	-2.81850609
H	1.52724863	5.27470245	-2.42705502
H	2.77199684	4.16140587	-3.01246463
H	1.13183316	4.14801969	-3.74111363
H	0.32156493	2.16554457	1.44494361
H	-0.52026200	2.77050738	0.35560209

4\_ace

Zero-point = -3002.256073

Ru	0.34730900	1.34506000	-0.72964700
P	1.73393500	-0.29319800	0.37000200
P	-1.61180600	0.44416500	-0.05780500
C	-1.58207600	-0.74311000	1.39448300

H	-1.48910400	-0.09147300	2.27254800
H	-2.57316500	-1.19807700	1.45233600
C	0.90855400	-1.26202100	1.74341200
C	-0.50264400	-1.85905000	1.48003300
C	-0.80464600	-2.73579300	2.73842200
H	-0.16638400	-3.62709700	2.71358600
H	-0.55781600	-2.19295800	3.66303900
P	-2.53604300	-3.31121100	2.97972600
H	-2.35890800	-4.26466000	4.01941500
H	-3.12579700	-2.24039100	3.70311600
O	-3.31603700	-3.77995200	1.78486300
H	1.58270200	-2.07142700	2.04822800
H	0.82860400	-0.56629500	2.58775800
C	-0.50031000	-2.78050200	0.24457500
H	-0.35274800	-2.21503700	-0.67711000
H	0.31224200	-3.51092600	0.31959000
H	-1.44365500	-3.32333800	0.16232700
C	-2.57898700	-0.44151300	-1.36392300
C	-3.38528500	-1.57094100	-1.12905300
C	-2.54784500	0.11008500	-2.65919800
C	-4.13788800	-2.12936300	-2.16599600
H	-3.43122800	-2.04713500	-0.15689900
C	-3.30727300	-0.44941900	-3.68753800
H	-1.91215400	0.96475000	-2.85416700
C	-4.10411300	-1.57018800	-3.44427000
H	-4.74722400	-3.00386700	-1.96770800
H	-3.27084800	-0.01153200	-4.67888400
H	-4.69064400	-2.00665000	-4.24484100
C	-2.93455300	1.59221700	0.57865300
C	-4.14506400	1.09800400	1.10189100
C	-2.74525100	2.98226300	0.52714600
C	-5.12028800	1.96997600	1.58554600
H	-4.34568000	0.03296300	1.10610900
C	-3.72483600	3.85464800	1.01108400
H	-1.84250600	3.37339500	0.07339200
C	-4.90955500	3.35149500	1.54820500
H	-6.04835900	1.57244400	1.98103600
H	-3.56165100	4.92542700	0.95922700
H	-5.66977100	4.02755100	1.92258300
C	2.68096000	-1.61218200	-0.52288500
C	3.76019900	-2.29176600	0.07119000
C	2.28995400	-1.96296400	-1.82717400
C	4.42155100	-3.30879100	-0.61796300
H	4.09515500	-2.01474600	1.06478100
C	2.95585000	-2.98348300	-2.51236000
H	1.47468600	-1.42875300	-2.30126300
C	4.01813900	-3.65891000	-1.91000300
H	5.25354900	-3.82385200	-0.15075000

H	2.64313600	-3.24702600	-3.51661100
H	4.53397300	-4.44885700	-2.44389400
C	3.10905500	0.51935500	1.32828500
C	3.48547400	0.18906800	2.64236500
C	3.77680100	1.59097600	0.68941800
C	4.49673100	0.89933000	3.29742000
H	2.99438900	-0.62129700	3.16662600
C	4.78588900	2.29783900	1.35127300
H	3.50346000	1.85533800	-0.32856600
C	5.14687800	1.95524000	2.65702200
H	4.77241600	0.62750700	4.31029900
H	5.28713300	3.11427700	0.84339000
H	5.92592100	2.50681000	3.17008700
Cl	0.68305600	2.94286800	1.23864900
C	1.56924200	1.34426900	-2.95534500
O	2.02850000	2.07338800	-2.02503000
O	0.55975300	0.59672400	-2.70692700
C	2.15999300	1.37311600	-4.34014100
H	1.97927800	0.42765200	-4.85502600
H	1.68269400	2.17494200	-4.91471700
H	3.23049300	1.58210900	-4.28967200
H	1.96374200	2.72393100	1.37827100
H	-0.54643200	2.50996600	-1.41971500

**S9. Cartesian coordinates (Å) and zero-point corrected energies, (Hartrees) of optimized structures of stationary points for the formation of the active specie Ru<sub>2</sub><sub>ace</sub> H in presence of hexanoate anion.**

Hexanoate

Zero=point = -385.61162

C	-2.48637300	0.05976400	0.03076800
O	-3.47422700	-0.68084400	-0.19239900
O	-2.43856400	1.30411200	0.21744000
C	-1.10002800	-0.69193200	0.13406700
H	-0.99628700	-1.04182900	1.17494100
H	-1.14015600	-1.59611900	-0.48762600
C	0.10308800	0.18282900	-0.22019900
H	-0.04007500	1.13936300	0.29634600
H	0.07614600	0.42208600	-1.29438400
C	1.46977400	-0.42468800	0.12136300
H	1.58963800	-1.39137900	-0.39301400
H	1.50660300	-0.65555700	1.19750100
C	2.65901300	0.47768800	-0.23483600
H	2.54286600	1.44248400	0.27794800
H	2.62972600	0.70541600	-1.30979500
C	4.02226500	-0.12708800	0.11855800
H	4.18046000	-1.07809200	-0.40486400
H	4.85056000	0.54050900	-0.14919700
H	4.09640800	-0.33246700	1.19349600

1\_hex

Zero-point = -3547.553825

Ru	-0.75874900	1.06350200	-0.62928900
P	-0.20694700	0.41457000	1.58183400
P	-2.16162400	-0.78076500	-0.77350500
C	-3.26102800	-1.03780800	0.70679000
H	-3.90138700	-0.15298700	0.73901600
H	-3.88407200	-1.90460400	0.46360700
C	-1.72469300	-0.06066400	2.55706900
C	-2.62034400	-1.25567200	2.10833000
C	-3.78557300	-1.27746000	3.15095600
H	-3.38955200	-1.59994500	4.12108400
H	-4.19984600	-0.26856300	3.29319200
P	-5.24727200	-2.33598800	2.78966600
H	-5.96102500	-2.20691400	4.01260100
H	-6.02821900	-1.50711800	1.93997700
O	-5.02667700	-3.73441300	2.29498700
H	-1.41346900	-0.22596800	3.59269900
H	-2.33816200	0.84172400	2.54460200
C	-1.88173500	-2.60653900	2.19645200
H	-1.02871000	-2.65767000	1.52077700
H	-1.49927400	-2.76105300	3.21031900
H	-2.56331500	-3.42730200	1.96039200
C	-1.52084000	-2.47128200	-1.10839900
C	-2.41736700	-3.54648300	-1.28222300
C	-0.14386600	-2.72540400	-1.13482800
C	-1.93478100	-4.83944700	-1.47477400
H	-3.48794000	-3.37580800	-1.26955100
C	0.33723900	-4.02405200	-1.32854000
H	0.55374900	-1.91537800	-0.98692000
C	-0.55648200	-5.08054700	-1.49768400
H	-2.63288000	-5.65894300	-1.59916800
H	1.40663000	-4.19934200	-1.33650400
H	-0.18593700	-6.08860800	-1.64243400
C	-3.38380300	-0.54277900	-2.14065800
C	-4.40388900	0.42102600	-2.02085100
C	-3.24441700	-1.23342100	-3.35941300
C	-5.26702900	0.67182400	-3.08926600
H	-4.49943600	1.00112700	-1.11131000
C	-4.10702700	-0.97046600	-4.42646300
H	-2.47262600	-1.98536600	-3.47041300
C	-5.12174100	-0.02095500	-4.29371500
H	-6.05037600	1.41339400	-2.97976200
H	-3.98796200	-1.51399500	-5.35685800
H	-5.79299000	0.17786300	-5.12100600
C	1.04162400	-0.86445700	2.02445800
C	1.09476900	-1.35381600	3.34802200

C	2.00669500	-1.29864400	1.10935800
C	2.05465600	-2.29245600	3.71710400
H	0.40225600	-0.99356200	4.09887300
C	2.97512000	-2.23703000	1.48571000
H	2.08101500	-0.88748500	0.11270400
C	2.99186000	-2.74573400	2.78138700
H	2.07944200	-2.66172800	4.73618300
H	3.72041200	-2.51406600	0.75076300
H	3.74133700	-3.47222900	3.07395300
C	0.45741800	1.87026100	2.49686900
C	-0.35600100	2.73721800	3.24564600
C	1.83318600	2.15462000	2.36293800
C	0.19726200	3.86346400	3.86205600
H	-1.41856700	2.55489600	3.34017100
C	2.37078000	3.28828500	2.97516400
H	2.48886500	1.51929600	1.77036500
C	1.55861100	4.14128800	3.72809200
H	-0.43911100	4.52205000	4.44266000
H	3.42840000	3.49581600	2.86008800
H	1.98385300	5.01657100	4.20585900
C	0.79807300	0.69787600	-2.39720300
C	-0.45947100	1.16626500	-2.89746300
C	-1.00625400	2.38950100	-2.47132900
C	-0.30451800	3.22922900	-1.53727400
C	0.87343700	2.71983000	-0.96967600
C	1.40879000	1.45590500	-1.36834900
H	-1.00913000	0.56453700	-3.61467100
H	-1.97468500	2.70233900	-2.84588000
H	1.39210800	3.26898200	-0.19409400
H	2.35446200	1.13737900	-0.89699500
C	1.50434500	-0.47298100	-3.02561100
H	0.81843400	-1.28678100	-3.27505200
H	1.95324800	-0.12407900	-3.96526200
H	2.32535900	-0.82362400	-2.38943500
C	-0.86704900	4.60032100	-1.21256900
H	-1.95194300	4.47513700	-1.11999400
C	-0.34832700	5.20075300	0.09893800
H	0.72200600	5.42929200	0.04696200
H	-0.87097200	6.14096300	0.30072300
H	-0.51877900	4.52935400	0.94348300
C	-0.59015000	5.54364600	-2.40537000
H	-0.99926600	5.15198800	-3.34228100
H	-1.04776400	6.52068800	-2.22087300
H	0.48584300	5.69548200	-2.54404600
Cl	-2.66063400	2.24437400	0.40875800
C	4.55342600	0.08679100	-0.41706900
O	4.04551800	-0.84043700	-1.10881900
O	3.93737700	1.08242900	0.06975900

C	6.05742100	-0.01306100	-0.08154500
H	6.45377900	1.00371100	0.02080700
H	6.12889800	-0.46395300	0.92045100
C	6.87918700	-0.83632700	-1.07582800
H	6.39196300	-1.80958700	-1.20373800
H	6.83931500	-0.35540300	-2.06316900
C	8.34336300	-1.02301900	-0.66035000
H	8.81796000	-0.03950600	-0.52632000
H	8.38413200	-1.51047900	0.32548400
C	9.16660200	-1.84469300	-1.66084600
H	8.69405500	-2.82754200	-1.79491300
H	9.12978800	-1.35688500	-2.64471500
C	10.62773300	-2.03319600	-1.23962000
H	11.18791400	-2.62247400	-1.97400100
H	11.13610800	-1.06789100	-1.13105800
H	10.69841900	-2.55033000	-0.27540400

Ts1\_hex

Zero-point = -3547.532945

Ru	-0.63009000	1.05895900	-0.52071400
P	-0.01291300	0.42273000	1.63963700
P	-1.91783800	-0.78680800	-0.69092400
C	-2.98555800	-1.13374600	0.79367300
H	-3.67440700	-0.28412900	0.81805900
H	-3.57029900	-2.02507900	0.54406300
C	-1.50830000	-0.08380500	2.64340800
C	-2.35109300	-1.31757600	2.20094900
C	-3.52191300	-1.38830400	3.23509100
H	-3.12097000	-1.70574300	4.20480900
H	-3.97353300	-0.39653400	3.38345800
P	-4.93953600	-2.49566800	2.84422600
H	-5.65902100	-2.43769100	4.06927400
H	-5.75615500	-1.67622200	2.01969100
O	-4.66121000	-3.86803000	2.30473100
H	-1.16240700	-0.24774400	3.66937400
H	-2.16520500	0.78773000	2.64296000
C	-1.56164900	-2.63857100	2.30215900
H	-0.74723000	-2.69237400	1.58193100
H	-1.11783800	-2.73595100	3.29840900
H	-2.22708400	-3.48944600	2.13639000
C	-1.11435500	-2.37640500	-1.13087900
C	-1.81042400	-3.60076400	-1.04729700
C	0.20615300	-2.37193100	-1.60334800
C	-1.18445500	-4.78895400	-1.42133700
H	-2.83289800	-3.63504600	-0.68848300
C	0.82976400	-3.56869200	-1.97325500
H	0.79552300	-1.46129000	-1.66335700
C	0.13678200	-4.77499600	-1.88447100



H	-1.72515100	-5.72527800	-1.34466000
H	1.85984600	-3.52915900	-2.30736600
H	0.61944500	-5.70382900	-2.16678400
C	-3.21217500	-0.61890300	-2.00579800
C	-4.18993600	0.39084300	-1.89895600
C	-3.20447000	-1.43694300	-3.14975100
C	-5.13664300	0.56652100	-2.90919100
H	-4.18892300	1.05768700	-1.04430900
C	-4.15286700	-1.25061300	-4.15936400
H	-2.46607000	-2.22231400	-3.24845700
C	-5.12048900	-0.25184500	-4.04208900
H	-5.88421300	1.34593300	-2.81190700
H	-4.13438000	-1.89054100	-5.03420600
H	-5.85538400	-0.11091700	-4.82613600
C	1.20163100	-0.84885600	2.21340100
C	1.53765600	-0.86052000	3.58121600
C	1.72760900	-1.84105900	1.37893900
C	2.37044900	-1.85395900	4.09754400
H	1.16685700	-0.08294700	4.23994100
C	2.55806700	-2.83652400	1.90034300
H	1.52023800	-1.83115400	0.32163700
C	2.87872600	-2.84872400	3.25868900
H	2.62597000	-1.84574100	5.15116700
H	2.95649700	-3.59419900	1.23557400
H	3.52577700	-3.62025700	3.65996400
C	0.59683500	1.91846600	2.52832300
C	-0.22526200	2.71685900	3.34147000
C	1.94478600	2.28789500	2.33385900
C	0.29369200	3.85528900	3.96468600
H	-1.26872900	2.46963200	3.48555000
C	2.44972300	3.42859300	2.95994500
H	2.56889300	1.69036800	1.67287400
C	1.63037100	4.21134900	3.77896600
H	-0.34950300	4.46143800	4.59289400
H	3.48717300	3.70496900	2.80653600
H	2.02960000	5.09464400	4.26464900
C	0.55058000	1.09923400	-3.12461000
C	-0.78888300	1.54539900	-2.95375300
C	-1.07380100	2.70135700	-2.21352500
C	-0.04315300	3.43946400	-1.55659600
C	1.24742200	2.90661200	-1.61981700
C	1.54045300	1.77233400	-2.40808200
H	-1.59560400	1.03204000	-3.46569200
H	-2.09612400	3.05753700	-2.16172300
H	2.05719200	3.36898000	-1.06937200
H	2.55464000	1.40318200	-2.44948500
C	0.90034500	-0.02770000	-4.05941000
H	0.06235000	-0.71782900	-4.19034200

H	1.15295500	0.37471100	-5.04892800
H	1.76400600	-0.57521500	-3.67359600
C	-0.38528500	4.76003500	-0.88440100
H	-1.30745600	4.58832700	-0.31620000
C	0.68430500	5.26570800	0.09077200
H	1.61047400	5.53606700	-0.43038300
H	0.32361800	6.16735200	0.59559900
H	0.92554700	4.52659800	0.85785800
C	-0.68678300	5.82507100	-1.96209100
H	-1.48350300	5.50553100	-2.64131100
H	-1.00383600	6.76097100	-1.49017300
H	0.20446000	6.03554200	-2.56423700
Cl	-2.46065500	2.24739900	0.51972000
C	3.35891200	-0.25819100	-0.71927900
O	2.97342200	-0.99877200	-1.66303800
O	2.64325600	0.58829400	-0.09709000
C	4.81919000	-0.39413800	-0.23960300
H	5.18139600	0.60095600	0.04664500
H	4.78581100	-0.97718300	0.69260300
C	5.76473200	-1.06094800	-1.24047300
H	5.32988500	-2.02021300	-1.54327900
H	5.80817900	-0.45651300	-2.15711200
C	7.18441100	-1.26855500	-0.69932500
H	7.60840400	-0.30057600	-0.39311600
H	7.14097400	-1.87789200	0.21582300
C	8.13288300	-1.93644400	-1.70336500
H	7.71124400	-2.90406500	-2.00848100
H	8.17872000	-1.32717900	-2.61659400
C	9.54943300	-2.14526200	-1.15800400
H	10.20100000	-2.62283600	-1.89790900
H	10.01011700	-1.19103100	-0.87662700
H	9.54029800	-2.78042800	-0.26443600

2\_hex

Zero-point = -3547.604958

Ru	-0.21206900	0.24879700	-0.38392500
P	0.28883000	-1.91447600	-0.58147700
P	1.94295800	0.76644800	0.14810200
C	3.22877900	-0.12317100	-0.86807600
H	3.07724400	0.30409700	-1.86541400
H	4.20990300	0.21211600	-0.51747400
C	1.86601500	-2.22221500	-1.52719900
C	3.21679400	-1.67343400	-0.98076700
C	4.27549800	-2.07359800	-2.05858800
H	4.41190200	-3.16155400	-2.04297700
H	3.92622800	-1.80805100	-3.06695600
P	5.94741400	-1.31620900	-1.91911300
H	6.64727200	-2.04534500	-2.91923700

H	5.78223900	-0.06498400	-2.56907800
O	6.60090500	-1.25611600	-0.56877900
H	1.95549000	-3.30446500	-1.67333000
H	1.67131800	-1.77384100	-2.50614700
C	3.61785200	-2.35281800	0.34486600
H	2.95550400	-2.07982600	1.16590400
H	3.57470000	-3.44187500	0.23972900
H	4.63979600	-2.07856000	0.61640300
C	2.45448800	0.58512500	1.91154000
C	3.79121300	0.39034700	2.30612800
C	1.46847600	0.74192400	2.90358300
C	4.12745100	0.33603900	3.66017400
H	4.57647800	0.27688800	1.56829500
C	1.81329800	0.69578900	4.25719600
H	0.43486400	0.88989100	2.61259200
C	3.14077500	0.48945600	4.63759800
H	5.16004200	0.17654600	3.94867500
H	1.04320700	0.81959900	5.01088700
H	3.40688500	0.44973500	5.68772300
C	2.47339400	2.51942700	-0.17742000
C	2.40001400	3.03714500	-1.48637600
C	2.93185000	3.35822000	0.85498500
C	2.78428900	4.35288900	-1.74974800
H	2.01281900	2.42030500	-2.28924600
C	3.30832900	4.67621700	0.58380300
H	3.00077800	2.98372100	1.86775600
C	3.23831000	5.17646800	-0.71694100
H	2.71997400	4.73487400	-2.76259600
H	3.65897400	5.30834200	1.39186300
H	3.53140700	6.19928200	-0.92392400
C	0.43925600	-3.00479700	0.89949300
C	0.78785000	-4.36225100	0.74332300
C	0.23419200	-2.50062700	2.19203500
C	0.94682400	-5.18430900	1.85738300
H	0.91926600	-4.77952400	-0.24891900
C	0.39770200	-3.33014800	3.30693500
H	-0.06429700	-1.46971800	2.32027500
C	0.75832800	-4.66695100	3.14356900
H	1.21616700	-6.22598600	1.72444200
H	0.24504600	-2.92392500	4.30038600
H	0.88810100	-5.30659100	4.00897600
C	-0.96260300	-2.82039500	-1.59491900
C	-1.08904400	-2.54270900	-2.96883600
C	-1.85616500	-3.72997100	-1.00091800
C	-2.06880900	-3.18173900	-3.72961000
H	-0.45812000	-1.79416900	-3.43192000
C	-2.83961300	-4.35877600	-1.76724500
H	-1.78198200	-3.95139600	0.05625600

C	-2.94500300	-4.09121700	-3.13308000
H	-2.15496100	-2.95606800	-4.78653700
H	-3.52115200	-5.05732000	-1.29487700
H	-3.70887200	-4.58071500	-3.72632800
C	-1.83429000	3.80660900	1.69983800
C	-0.86267100	3.53695000	0.72602500
C	-1.22328800	3.26386000	-0.59715400
C	-2.57039100	3.26058900	-1.00282900
C	-3.53583800	3.53641900	-0.02788500
C	-3.17410400	3.80079500	1.29677400
H	0.18948900	3.55495300	0.99450800
H	-0.44683300	3.09130500	-1.33701400
H	-4.58832100	3.55076200	-0.29802300
H	-3.95125400	4.01533600	2.02789300
C	-1.43868100	4.12341200	3.12329600
H	-1.08137400	5.15668800	3.21859700
H	-2.28253800	4.00512300	3.80970100
H	-0.62917000	3.47054600	3.46613900
C	-2.93152100	3.02110600	-2.46274200
H	-2.04468400	2.58662100	-2.93861300
C	-4.08165700	2.01583800	-2.64328700
H	-5.02459100	2.39852400	-2.23421400
H	-4.24678800	1.82151500	-3.70891100
H	-3.84687700	1.06874700	-2.15096400
C	-3.24407300	4.35579400	-3.16974000
H	-2.40763600	5.05753400	-3.08636000
H	-3.44531300	4.19147400	-4.23439700
H	-4.12693800	4.83618100	-2.73150400
Cl	0.25643900	0.64347500	-2.75414900
C	-2.42936600	-0.04849500	0.84011700
O	-1.31258100	0.11950500	1.45785500
O	-2.40679800	-0.12549500	-0.42285300
C	-3.71346300	-0.13690600	1.63047100
H	-3.99253900	0.89286200	1.89091700
H	-3.48693400	-0.64053800	2.57755400
C	-4.86161800	-0.82857000	0.88730200
H	-5.05091700	-0.29535900	-0.05064400
H	-4.55052700	-1.84092100	0.59966400
C	-6.14761000	-0.89747900	1.71947400
H	-5.94861000	-1.42754500	2.66253000
H	-6.45378700	0.11980100	2.00432000
C	-7.30698200	-1.58674900	0.98882200
H	-7.50545100	-1.05682700	0.04754800
H	-7.00076000	-2.60269900	0.70453500
C	-8.59210100	-1.65350800	1.82007000
H	-8.94243900	-0.65046700	2.08966200
H	-9.39919900	-2.15042300	1.27164800
H	-8.43338400	-2.20792000	2.75233400

3\_hex

Zero-point = -3159.460209

Ru	0.50500900	-0.21315800	-1.19323300
P	0.08310400	1.75834700	-0.06233500
P	-1.37490300	-1.17048200	-0.30397400
C	-2.86566200	-0.05183600	-0.26389600
H	-3.07956800	0.08004800	-1.33053000
H	-3.68875700	-0.63423400	0.16245700
C	-1.70614400	2.26894300	-0.17154900
C	-2.81535000	1.34703700	0.41613600
C	-4.15657500	2.07461400	0.07606800
H	-4.22899300	2.99265800	0.67136300
H	-4.18081700	2.37428100	-0.98159700
P	-5.71564700	1.13226200	0.34197300
H	-6.67915700	2.15566100	0.12803000
H	-5.84530600	0.38886300	-0.86022000
O	-5.86856900	0.33737200	1.60681000
H	-1.79651100	3.26294200	0.28022500
H	-1.87322300	2.37972000	-1.24712300
C	-2.71559800	1.24619400	1.95230000
H	-1.82774200	0.70308900	2.27476800
H	-2.66197900	2.24759800	2.39214500
H	-3.59774400	0.74576000	2.35777200
C	-1.22872600	-1.91059900	1.37898600
C	-2.32590900	-2.06128900	2.24816400
C	0.02110200	-2.42665600	1.76812200
C	-2.16906200	-2.69847300	3.48080200
H	-3.30453400	-1.68410100	1.97659000
C	0.16957500	-3.06974600	2.99940800
H	0.87602400	-2.31286400	1.11192600
C	-0.92266700	-3.20408400	3.85848000
H	-3.02177200	-2.80008100	4.14216400
H	1.13864400	-3.46434900	3.28451700
H	-0.80585800	-3.70048400	4.81503500
C	-2.08917700	-2.59676000	-1.25524400
C	-2.24478300	-2.48217100	-2.65159400
C	-2.48469700	-3.79043200	-0.62560400
C	-2.78796100	-3.53484300	-3.38994700
H	-1.93256200	-1.57428200	-3.15602200
C	-3.02429400	-4.84012500	-1.37324600
H	-2.37202600	-3.90345000	0.44437800
C	-3.17839700	-4.71592400	-2.75452900
H	-2.90018000	-3.43051300	-4.46339800
H	-3.32211500	-5.75428000	-0.87221200
H	-3.59596700	-5.53314700	-3.33148300
C	0.49921200	1.94443700	1.72275000
C	0.19033900	3.13902300	2.40500000

C	1.10304000	0.89450700	2.43046000
C	0.46412700	3.26745500	3.76532500
H	-0.25030500	3.97216100	1.86877900
C	1.37277200	1.02787200	3.79680500
H	1.36791600	-0.01561600	1.91069700
C	1.05115100	2.20800900	4.46591300
H	0.22107200	4.19046200	4.27933500
H	1.82996200	0.20402200	4.33296200
H	1.25777600	2.30789900	5.52526500
C	0.94575100	3.20877900	-0.81267600
C	0.57884100	3.66218600	-2.09389400
C	2.02169300	3.83199200	-0.15522100
C	1.25757200	4.72822900	-2.68515900
H	-0.20116200	3.15415900	-2.64663800
C	2.70059400	4.89332900	-0.75723200
H	2.32674900	3.49412900	0.82696300
C	2.31725700	5.34816800	-2.01963600
H	0.96497200	5.06340200	-3.67374900
H	3.52838200	5.36232100	-0.23730300
H	2.84520000	6.17265500	-2.48489800
Cl	-0.81075800	0.64503900	-3.09642600
C	3.03026700	-0.21448100	-0.75629700
O	2.57456700	0.43666900	-1.73981300
O	2.19727700	-0.82434800	0.01169700
C	4.51127200	-0.28302400	-0.46689800
H	4.69807500	0.31456500	0.43606100
H	5.03762200	0.20198000	-1.29401200
H	0.90454400	-1.42742700	-2.52666000
H	0.76597000	-1.90335600	-1.90655000
C	5.01971300	-1.71706300	-0.24466200
H	4.44049800	-2.17769400	0.56385500
H	4.82288900	-2.31312100	-1.14596800
C	6.51558700	-1.77305700	0.08650100
H	6.71116700	-1.17386900	0.98771200
H	7.08781500	-1.29805300	-0.72307100
C	7.03627100	-3.19949300	0.30423600
H	6.46267000	-3.67388700	1.11217100
H	6.84061600	-3.79651700	-0.59676500
C	8.53050700	-3.25255300	0.63796900
H	8.75242600	-2.69313100	1.55406100
H	8.87125700	-4.28238100	0.78690400
H	9.13216100	-2.81668700	-0.16778400

Ts3\_hex

Zero-point = -3159.401489

Ru	0.52972100	-0.61523800	-0.83269600
P	0.37642400	1.73904500	-0.17225900
P	-1.65793900	-1.08970600	-0.27570900

C	-2.85312900	0.34521500	-0.31652300
H	-2.99415000	0.52855400	-1.38884900
H	-3.80380300	-0.03911900	0.06085900
C	-1.35187100	2.44357500	-0.29537900
C	-2.53136400	1.69564700	0.38656300
C	-3.76702200	2.63443600	0.18998400
H	-3.64357500	3.52152700	0.82223800
H	-3.83001500	2.98863000	-0.84930800
P	-5.42737400	1.92640600	0.55746700
H	-6.22569000	3.10187600	0.58651300
H	-5.81771200	1.37142500	-0.68997300
O	-5.56926300	1.00510500	1.73605100
H	-1.32905600	3.46831800	0.09307900
H	-1.55204500	2.50476200	-1.37208800
C	-2.29125200	1.54763200	1.90205200
H	-1.48222300	0.85025300	2.12115900
H	-2.01227500	2.51556300	2.33172600
H	-3.19279300	1.19596300	2.40638100
C	-1.89181600	-1.89617700	1.36511900
C	-3.02618600	-1.69839300	2.17532000
C	-0.91816900	-2.82750800	1.77314700
C	-3.17322800	-2.41295400	3.36670200
H	-3.79803100	-0.98668000	1.90714500
C	-1.07515700	-3.53888700	2.96370700
H	-0.03574900	-2.97772700	1.16430900
C	-2.20128900	-3.33332300	3.76315200
H	-4.04986400	-2.24500600	3.98177500
H	-0.31581200	-4.25191100	3.26466500
H	-2.32080400	-3.88525800	4.68847200
C	-2.59412400	-2.26490900	-1.36444400
C	-3.93361900	-2.59100500	-1.07568000
C	-1.98106300	-2.85237200	-2.48179200
C	-4.64341000	-3.46598000	-1.89738900
H	-4.41882300	-2.18959000	-0.19345700
C	-2.69630200	-3.73004400	-3.30176600
H	-0.94444200	-2.62829700	-2.69599600
C	-4.02723600	-4.03405500	-3.01612900
H	-5.67208700	-3.71157600	-1.65885900
H	-2.20779500	-4.17566200	-4.16094500
H	-4.57975100	-4.71568900	-3.65269100
C	0.95371400	2.33976600	1.48123000
C	1.12518400	3.70969400	1.75222000
C	1.20940100	1.40629300	2.50090300
C	1.52372100	4.13529800	3.01970000
H	0.96757400	4.44090400	0.96694900
C	1.60980100	1.83859700	3.76874900
H	1.10407700	0.34746500	2.29594900
C	1.76330100	3.20047200	4.03153600

H	1.65399600	5.19360000	3.21644800
H	1.80131500	1.10887300	4.54759400
H	2.07422500	3.53361500	5.01513300
C	1.28881400	2.90046900	-1.29281400
C	0.76569400	4.10831600	-1.78770300
C	2.59765600	2.53208300	-1.66437000
C	1.53120200	4.92708600	-2.62305500
H	-0.24038600	4.41919800	-1.53605100
C	3.35855400	3.35529700	-2.49521200
H	3.00677300	1.58913900	-1.31827800
C	2.82861400	4.55498100	-2.97639900
H	1.11000500	5.85308200	-2.99848500
H	4.36183900	3.05318000	-2.77388200
H	3.41892300	5.18998200	-3.62685100
Cl	-0.27832000	0.08642400	-3.26967000
C	2.76091300	-1.10849900	0.26859700
O	2.76108700	-0.61784600	-0.90061100
O	1.62480200	-1.28540300	0.83341400
C	4.03633300	-1.44951900	0.99842200
H	3.78375200	-2.11306700	1.83164700
H	4.41545000	-0.51687400	1.44064500
H	0.89041000	0.07472300	-2.41688400
H	0.63929600	-2.14024100	-1.34639600
C	5.11066600	-2.06884400	0.09251900
H	4.72374100	-3.00125000	-0.33865400
H	5.29411500	-1.39462500	-0.75134700
C	6.42181000	-2.35055200	0.83535200
H	6.22551200	-3.01654200	1.68808200
H	6.80591500	-1.41392400	1.26521300
C	7.50092200	-2.97738000	-0.05669800
H	7.69581500	-2.31202000	-0.90858000
H	7.11619600	-3.91266100	-0.48523900
C	8.81146300	-3.25605700	0.68606100
H	8.65397900	-3.94626300	1.52288400
H	9.55988800	-3.70301000	0.02353100
H	9.23897400	-2.33376700	1.09604000

4\_hex

Zero-point = -3159.405261

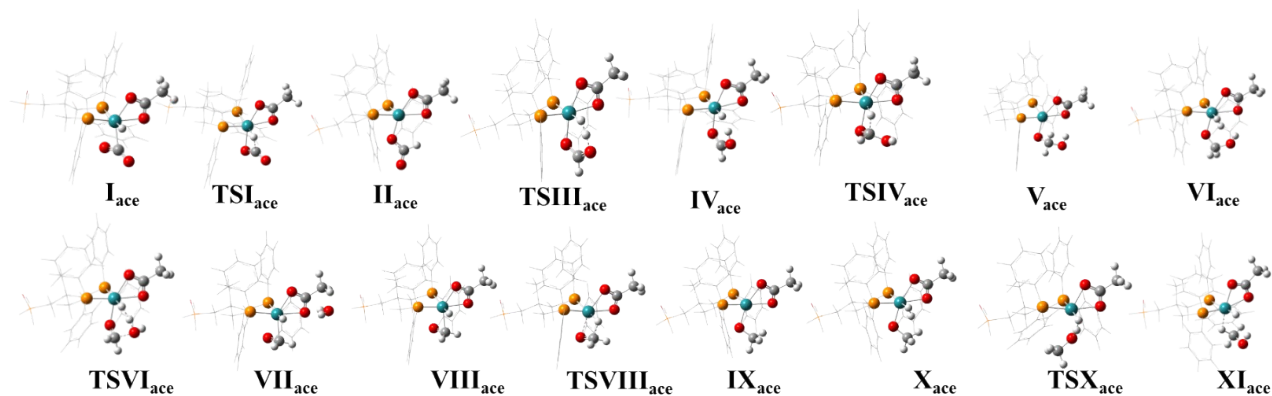
Ru	-0.15245200	-0.58267400	1.11780300
P	-0.71265200	1.43104000	-0.08361000
P	1.97494200	-0.68985200	0.36832800
C	2.72677300	0.86351700	-0.36759500
H	2.98280000	1.47761300	0.50511200
H	3.67347700	0.57104700	-0.82668100
C	0.73793800	2.45880900	-0.67056900
C	1.91906200	1.73205400	-1.37345700
C	2.84733500	2.88224100	-1.88186000



H	2.35576400	3.39384600	-2.71795400
H	3.00463300	3.63567900	-1.09567400
P	4.54051700	2.42664700	-2.44093800
H	4.95121100	3.63669100	-3.06425500
H	5.29468000	2.48173500	-1.23841000
O	4.72292700	1.17558800	-3.25163300
H	0.35873800	3.24346800	-1.33624000
H	1.13153700	2.95180800	0.22678700
C	1.43512500	0.93085400	-2.59789300
H	0.82417700	0.07647600	-2.30155800
H	0.82413200	1.56652900	-3.24758100
H	2.28073600	0.55831400	-3.17880700
C	2.32022600	-2.01142800	-0.88062900
C	3.25150800	-1.89185800	-1.92905500
C	1.64627900	-3.23606600	-0.71028800
C	3.49787500	-2.97196100	-2.78121100
H	3.78306400	-0.96673300	-2.11763600
C	1.90287900	-4.31183400	-1.56124000
H	0.91076200	-3.32879700	0.07902600
C	2.82886700	-4.18314700	-2.59867700
H	4.21310600	-2.85859900	-3.58803300
H	1.37447800	-5.24742600	-1.41532000
H	3.02452600	-5.01821100	-3.26187200
C	3.32251400	-1.06959600	1.59808100
C	4.68139800	-1.04746500	1.22889100
C	2.99332500	-1.40670300	2.92053800
C	5.67801000	-1.32468100	2.16444200
H	4.96741200	-0.84401800	0.20351500
C	3.99388900	-1.68602300	3.85629300
H	1.94902700	-1.48225600	3.19937900
C	5.33701400	-1.63785000	3.48351900
H	6.71914200	-1.30717200	1.86194200
H	3.71945300	-1.94790800	4.87216100
H	6.11306200	-1.85513900	4.20855200
C	-1.84453800	1.47414700	-1.55097700
C	-2.47530300	2.65759900	-1.97635800
C	-2.06448600	0.28795700	-2.27367100
C	-3.29455700	2.65661400	-3.10592900
H	-2.34091900	3.57588100	-1.41531800
C	-2.88664300	0.29300700	-3.40465300
H	-1.60055400	-0.63332600	-1.94117500
C	-3.49960900	1.47476100	-3.82387100
H	-3.77682100	3.57473100	-3.42259700
H	-3.04608200	-0.62766000	-3.95486200
H	-4.13768600	1.47607700	-4.70022400
C	-1.55816900	2.66532400	1.02544200
C	-1.24934500	4.03528700	1.09698300
C	-2.54562100	2.15431800	1.90089200

C	-1.90476000	4.87027100	2.00780000
H	-0.49656700	4.46291700	0.44642900
C	-3.19547400	2.99487600	2.81032400
H	-2.80254900	1.09947600	1.85276800
C	-2.87527600	4.35395400	2.86753400
H	-1.65237400	5.92415500	2.04582800
H	-3.95082200	2.58446500	3.47123900
H	-3.37655300	5.00307300	3.57586100
Cl	0.29070600	0.79531900	3.22736600
C	-2.25422300	-1.87828500	0.51453600
O	-2.30918600	-1.08074500	1.50001900
O	-1.16490800	-1.94456300	-0.15635600
C	-3.42904100	-2.74907200	0.13519700
H	-3.21310200	-3.21389900	-0.83187500
H	-3.48603700	-3.55831700	0.87660100
H	-0.75078100	1.57543600	3.10702500
H	0.20318600	-1.89548700	2.00192200
C	-4.76261200	-1.98644000	0.10298600
H	-4.91213800	-1.49859400	1.07287200
H	-4.69865500	-1.18379300	-0.64360100
C	-5.95863900	-2.89095300	-0.21603100
H	-6.01585900	-3.69594100	0.53103600
H	-5.79626200	-3.38746200	-1.18369200
C	-7.29540600	-2.13936000	-0.25242300
H	-7.45627800	-1.64333500	0.71440400
H	-7.23730500	-1.33553200	-0.99883700
C	-8.49001200	-3.04528000	-0.56757100
H	-8.59464200	-3.83829800	0.18183400
H	-9.42794600	-2.48040700	-0.58636000
H	-8.37388900	-3.52917000	-1.54424200

**S10. Cartesian coordinates (Å) and zero-point corrected energies, (Hartrees) of optimized structures of stationary points for the methanol formation in presence of acetate anion.**



Ru-H<sub>ace</sub>

Zero-point = -2541.448112

Ru	0.32857000	-1.16685600	1.10116600
P	1.76001100	0.00546800	-0.44284000
P	-1.60950800	-0.50528500	0.15794200
C	-1.55739600	0.36375800	-1.50514200
H	-1.46387200	-0.45042100	-2.23426000
H	-2.54980400	0.79529400	-1.66029300
C	0.93429300	0.73947900	-1.96020100
C	-0.45544800	1.42196200	-1.79155300
C	-0.74642400	2.08106500	-3.17777300
H	-0.07925200	2.94113900	-3.31018900
H	-0.52923300	1.38106100	-3.99826500
P	-2.46128000	2.66583700	-3.49984100
H	-2.26853500	3.42160700	-4.68830600
H	-3.09577300	1.50820400	-4.02415100
O	-3.20852700	3.35818700	-2.39594800
H	1.63120600	1.45462100	-2.41261200
H	0.81624700	-0.09055100	-2.66695900
C	-0.41727500	2.53497000	-0.72614200
H	-0.27761700	2.12200000	0.27496500
H	0.41309600	3.22140200	-0.92240400
H	-1.34557200	3.10953700	-0.73060900
C	-2.69197200	0.55176700	1.21506600
C	-3.46268600	1.62993800	0.74202800
C	-2.76589600	0.21134500	2.58017900
C	-4.29174400	2.34038700	1.61600500
H	-3.42104600	1.95351100	-0.29117000
C	-3.60039100	0.92114600	3.44308500
H	-2.15363400	-0.60079200	2.95428700
C	-4.36631000	1.98671200	2.96344800
H	-4.87265100	3.17281100	1.23556600
H	-3.64636700	0.64563800	4.49075200
H	-5.01069600	2.54082700	3.63655400
C	-2.76298100	-1.86738400	-0.33554900
C	-2.26710900	-3.17946200	-0.40566900
C	-4.10006600	-1.62487600	-0.69482000
C	-3.08234800	-4.22514000	-0.84547300
H	-1.25080200	-3.38428100	-0.08086900
C	-4.91459600	-2.67210100	-1.12880500
H	-4.51005900	-0.62429800	-0.61107000
C	-4.40593900	-3.97156700	-1.21074600
H	-2.68865600	-5.23440500	-0.88922800
H	-5.94706600	-2.47600200	-1.39544900
H	-5.04190100	-4.78308000	-1.54543100
C	2.89561000	1.37888300	0.07276100
C	4.08377000	1.66954500	-0.62163100
C	2.54770500	2.16804400	1.18417400

C	4.89461500	2.73337000	-0.22256700
H	4.38404200	1.05326900	-1.46144600
C	3.36245100	3.23338100	1.57785100
H	1.64837400	1.93762700	1.74305600
C	4.53429100	3.51943800	0.87526600
H	5.80979000	2.94466600	-0.76439600
H	3.08062100	3.83600000	2.43425800
H	5.16675800	4.34393400	1.18393700
C	2.95370700	-1.17895800	-1.21963500
C	3.32036800	-1.17841600	-2.57779400
C	3.51839000	-2.15198500	-0.36827100
C	4.22225400	-2.12504100	-3.07174700
H	2.90959400	-0.44176600	-3.25783600
C	4.42234600	-3.09171200	-0.86685200
H	3.24594000	-2.16454200	0.68242400
C	4.77387800	-3.08288900	-2.21886400
H	4.49349400	-2.11205400	-4.12156200
H	4.84692100	-3.83257500	-0.19875200
H	5.47129900	-3.81716900	-2.60523400
C	1.53202200	-0.48431300	3.20749000
O	1.97167300	-1.49333200	2.58472200
O	0.52079400	0.13716500	2.71297900
C	2.17911700	0.02633800	4.46572900
H	2.95898300	0.74759700	4.19670200
H	1.44536700	0.53052600	5.09783500
H	2.64533000	-0.79960300	5.00605400
H	-0.59889800	-2.08065600	2.07681200

lace

Zero-point = - 2730.036774

Ru	0.28083400	-1.40346700	0.62971900
P	1.79790500	0.31203800	-0.40683100
P	-1.66638600	-0.35589200	0.03963200
C	-1.55553400	0.80347400	-1.42239900
H	-1.44385100	0.14030400	-2.28774600
H	-2.54773000	1.25481400	-1.50652700
C	0.94907300	1.30034400	-1.75046400
C	-0.46072700	1.90583100	-1.49035000
C	-0.74825300	2.78989700	-2.74771300
H	-0.09514800	3.67006400	-2.71954800
H	-0.50859600	2.24505300	-3.67273100
P	-2.47100200	3.39728300	-2.98654300
H	-2.27338100	4.36468900	-4.00878800
H	-3.07481400	2.34728300	-3.72771100
O	-3.24488800	3.85730100	-1.78444700
H	1.62451700	2.11360900	-2.03999400
H	0.88102300	0.61409400	-2.60296900
C	-0.45826900	2.82252400	-0.25220700

H	-0.28798900	2.25988400	0.66714500
H	0.34259800	3.56491000	-0.33501800
H	-1.40947200	3.34916600	-0.15589700
C	-2.49702300	0.61081800	1.36824100
C	-3.37723800	1.67756100	1.09830300
C	-2.28473000	0.22379700	2.70443600
C	-4.02168700	2.33921400	2.14487100
H	-3.55745200	2.02177300	0.08701100
C	-2.93940500	0.88811400	3.74499300
H	-1.59571300	-0.58100900	2.92437300
C	-3.80714700	1.94537300	3.46825400
H	-4.68764900	3.16445900	1.92118600
H	-2.76573300	0.57837500	4.76936600
H	-4.31109600	2.46251600	4.27679600
C	-3.03284100	-1.43974700	-0.57628800
C	-2.83908800	-2.21295800	-1.73860700
C	-4.25877300	-1.53360400	0.10319100
C	-3.85158200	-3.05086400	-2.20659600
H	-1.88922200	-2.18536500	-2.25907800
C	-5.26686900	-2.37683500	-0.37044700
H	-4.42692300	-0.94971900	0.99873200
C	-5.06796500	-3.13458900	-1.52495400
H	-3.68441000	-3.64592600	-3.09719700
H	-6.20681500	-2.43911700	0.16599900
H	-5.85115600	-3.78977000	-1.88826600
C	2.66499700	1.60205500	0.59082400
C	3.73020900	2.35395700	0.06238200
C	2.24068300	1.85263600	1.90803700
C	4.34218700	3.34662400	0.82814500
H	4.09582900	2.14727600	-0.93727900
C	2.85782800	2.84886700	2.67009100
H	1.44045300	1.26017100	2.33622800
C	3.90436100	3.59885200	2.13173300
H	5.16417400	3.91775600	0.41154100
H	2.51965500	3.03496200	3.68333800
H	4.38255100	4.37000100	2.72468100
C	3.18880100	-0.44294300	-1.35798200
C	3.63542400	0.03664600	-2.60325500
C	3.83747600	-1.55623200	-0.78974400
C	4.70784900	-0.57531800	-3.25687700
H	3.15160800	0.88216800	-3.07644400
C	4.90962000	-2.16138500	-1.44754700
H	3.48936500	-1.95515400	0.15605500
C	5.34793400	-1.67354700	-2.68030100
H	5.03872200	-0.19508100	-4.21686200
H	5.39286200	-3.02207200	-0.99949900
H	6.17645500	-2.14979300	-3.19164300
C	1.66652900	-1.62327000	2.75777400

O	2.00915600	-2.30640200	1.75092700
O	0.64209700	-0.85576200	2.64778300
C	2.44212600	-1.65677400	4.04605100
H	3.07580800	-0.76476600	4.10453900
H	1.75963900	-1.64078000	4.89911100
H	3.07463600	-2.54461400	4.08278700
H	-0.74414300	-2.39551200	1.34770100
C	0.13003600	-3.18825900	-0.45806800
O	0.30828200	-2.33222000	-1.35587500
O	0.03021800	-4.35980500	-0.25289500

TSIace

Zero-point = -2730.032798

Ru	0.32891400	-1.28963800	0.65928500
P	1.74156200	0.31782000	-0.43282300
P	-1.62854000	-0.31293500	-0.00505800
C	-1.56525600	0.92452700	-1.40442600
H	-1.47528400	0.31226700	-2.30934000
H	-2.55956600	1.37698100	-1.44096600
C	0.92319600	1.39765900	-1.72548100
C	-0.46810100	2.02146800	-1.42618100
C	-0.75027900	2.97609100	-2.63056700
H	-0.08963100	3.84793700	-2.55621700
H	-0.51924000	2.48186600	-3.58575800
P	-2.46990900	3.60631100	-2.82564800
H	-2.27424700	4.62218500	-3.80009400
H	-3.08592000	2.59789300	-3.61319800
O	-3.23129300	4.01042000	-1.59582400
H	1.62685700	2.20079400	-1.97240200
H	0.82735200	0.76308000	-2.61424500
C	-0.44907900	2.86573500	-0.13775100
H	-0.29660500	2.24467800	0.74670900
H	0.36667700	3.59528100	-0.17456400
H	-1.38989500	3.40539600	-0.01377100
C	-2.54991300	0.54024300	1.34721200
C	-3.41244900	1.63259700	1.13035900
C	-2.41884300	0.02906500	2.65253500
C	-4.12090200	2.19383700	2.19512000
H	-3.53265900	2.07642500	0.14964700
C	-3.13689000	0.59094900	3.71021500
H	-1.73958600	-0.79304600	2.83668800
C	-3.98854300	1.67361700	3.48443900
H	-4.77227800	3.04033800	2.01115900
H	-3.02372000	0.18449600	4.70888600
H	-4.54165900	2.11259100	4.30692800
C	-2.92473900	-1.42568300	-0.71822600
C	-2.61512400	-2.19462600	-1.85817200
C	-4.20732600	-1.53386300	-0.15581900

C	-3.57024800	-3.04204500	-2.42019300
H	-1.61922400	-2.15805700	-2.28360200
C	-5.15797400	-2.38694500	-0.72248300
H	-4.46390200	-0.95298100	0.72057400
C	-4.84395700	-3.13994100	-1.85431000
H	-3.31479100	-3.63389000	-3.29182200
H	-6.14319500	-2.46063900	-0.27627500
H	-5.58261700	-3.80309500	-2.28941700
C	2.77983100	1.53587200	0.50058700
C	3.96222900	2.06578300	-0.04850100
C	2.36957700	1.96747200	1.77510300
C	4.70460500	3.01616000	0.65370100
H	4.31271700	1.72042900	-1.01424000
C	3.11780200	2.91980600	2.47302500
H	1.48041600	1.54310500	2.22498300
C	4.28250700	3.44790400	1.91395800
H	5.61549700	3.41359300	0.22030900
H	2.78889200	3.24468700	3.45388700
H	4.86236800	4.18454500	2.45811700
C	3.01145500	-0.55139400	-1.45656900
C	3.42198100	-0.11070000	-2.72870800
C	3.60433200	-1.71076500	-0.91945300
C	4.39851600	-0.81004600	-3.44252200
H	2.98813500	0.77649700	-3.17326100
C	4.58028100	-2.40354900	-1.63778200
H	3.29495000	-2.06938500	0.05500600
C	4.97891200	-1.95735700	-2.89939100
H	4.70258900	-0.45776600	-4.42184700
H	5.02093500	-3.29773300	-1.21196700
H	5.73268100	-2.50118400	-3.45691800
C	1.68015300	-1.26611600	2.81961300
O	2.04017200	-2.03908300	1.87898400
O	0.65917400	-0.51693400	2.63148900
C	2.45016100	-1.18790600	4.10942200
H	3.16262200	-0.35779200	4.04490300
H	1.77490400	-0.99185800	4.94515900
H	3.00455400	-2.11291000	4.27516600
H	-0.67807400	-2.44756500	1.27807400
C	-0.04957800	-3.42894300	0.13108700
O	0.25711000	-2.81054500	-0.90696800
O	-0.19978300	-4.52192100	0.58595100

llace

Zero-point = -2730.054588

Ru	0.52627200	-1.22631200	0.68342000
P	1.54031300	0.40732900	-0.40399300
P	-1.52011600	-0.36670300	0.23690000
C	-1.74372700	0.25643100	-1.49788800

H	-1.64583100	-0.65345500	-2.09993600
H	-2.77469200	0.60875500	-1.59754100
C	0.71329900	0.82449200	-2.02198000
C	-0.75868700	1.32952600	-2.04121400
C	-1.08969800	1.55396400	-3.55130300
H	-0.52855300	2.42131800	-3.91884200
H	-0.77594200	0.68898800	-4.15336500
P	-2.85917300	1.82440600	-3.98426000
H	-2.74196300	2.21113200	-5.34703100
H	-3.35486800	0.50164500	-4.12340000
O	-3.68048300	2.72752800	-3.10963300
H	1.35035200	1.55269100	-2.53670300
H	0.76353700	-0.11369800	-2.58218600
C	-0.90579300	2.68313600	-1.31703400
H	-0.72029200	2.60046700	-0.24584100
H	-0.18457900	3.40389100	-1.71687700
H	-1.90932500	3.08792400	-1.46488400
C	-2.24120800	0.90576100	1.35354500
C	-3.26472500	1.78430100	0.95108600
C	-1.79557200	0.94215900	2.68804400
C	-3.81732900	2.68630100	1.86217800
H	-3.63184500	1.78155800	-0.06846300
C	-2.35888700	1.84263500	3.59565700
H	-1.01057700	0.26711500	3.01006300
C	-3.36676900	2.71690500	3.18444900
H	-4.59880300	3.36315200	1.53680200
H	-2.00926800	1.85863900	4.62202400
H	-3.80031400	3.41767600	3.88869900
C	-2.79298100	-1.70844900	0.30750000
C	-2.62927600	-2.84878700	-0.50700300
C	-3.89876000	-1.64203700	1.17362300
C	-3.56085000	-3.88677100	-0.45830900
H	-1.76497100	-2.92545800	-1.15657900
C	-4.82272900	-2.68858100	1.21822000
H	-4.04078300	-0.77568600	1.80655300
C	-4.65782600	-3.81016100	0.40355800
H	-3.42253100	-4.75703700	-1.08989800
H	-5.67174100	-2.62381000	1.88928700
H	-5.37706000	-4.62022500	0.44191900
C	1.87499100	2.02310800	0.40788300
C	2.50915000	3.06158400	-0.30264500
C	1.49542200	2.23813600	1.74137100
C	2.73649700	4.29455800	0.30634100
H	2.83820700	2.90089500	-1.32350500
C	1.72634300	3.47803100	2.34643200
H	1.03530500	1.43413900	2.30064600
C	2.33955600	4.50638800	1.63113400
H	3.22367700	5.08827500	-0.24843000



H	1.42389300	3.63541800	3.37544100
H	2.51400000	5.46743900	2.10096200
C	3.21917000	-0.11459900	-0.96135500
C	3.37022100	-1.02046500	-2.02861000
C	4.36455400	0.30869500	-0.26228300
C	4.63808900	-1.47599300	-2.39279500
H	2.50656000	-1.39732300	-2.56139200
C	5.62872000	-0.15485400	-0.62952900
H	4.26827500	1.00303100	0.56359500
C	5.76894900	-1.04518600	-1.69593100
H	4.73628300	-2.17724100	-3.21332400
H	6.50227600	0.18007700	-0.08177300
H	6.75133800	-1.40573800	-1.97800100
C	1.92827400	-1.65679600	2.76883200
O	2.20572600	-2.26792400	1.69053200
O	0.97865400	-0.79359100	2.76131600
C	2.71223400	-1.90744500	4.02932000
H	3.54769100	-1.19963600	4.07379500
H	2.08447200	-1.74955200	4.90844300
H	3.12182700	-2.91885600	4.02447500
H	1.65865400	-3.61836000	-0.51063000
C	1.03725400	-3.29609100	-1.37254300
O	0.34865000	-2.19349800	-1.16251300
O	1.01231100	-3.92692200	-2.41680500

Ilace at T=160°C

Zero-point = -2730.054587

Ru	-0.52622700	-1.22658900	-0.68281700
P	-1.54032600	0.40752000	0.40385000
P	1.52013200	-0.36677400	-0.23658300
C	1.74373500	0.25728900	1.49785900
H	1.64596800	-0.65231900	2.10034900
H	2.77466200	0.60979200	1.59728200
C	-0.71334300	0.82536900	2.02168000
C	0.75858300	1.33056200	2.04067200
C	1.08951600	1.55578900	3.55065600
H	0.52823100	2.42323000	3.91777100
H	0.77585800	0.69104200	4.15309800
P	2.85895000	1.82667400	3.98356500
H	2.74161700	2.21440400	5.34603700
H	3.35472200	0.50405300	4.12372700
O	3.68028600	2.72919800	3.10834600
H	-1.35047500	1.55365100	2.53619800
H	-0.76339800	-0.11265800	2.58216300
C	0.90556400	2.68381300	1.31581700
H	0.72029200	2.60052100	0.24463000
H	0.18412200	3.40463600	1.71512300
H	1.90898100	3.08888300	1.46366600

C	2.24118500	0.90507700	-1.35391100
C	3.26450800	1.78401500	-0.95186300
C	1.79568100	0.94057800	-2.68848100
C	3.81707100	2.68554100	-1.86344600
H	3.63152500	1.78192400	0.06772900
C	2.35896000	1.84058000	-3.59657700
H	1.01083400	0.26520300	-3.01017900
C	3.36664800	2.71526900	-3.18578300
H	4.59840600	3.36270900	-1.53839700
H	2.00945900	1.85589700	-4.62299400
H	3.80016100	3.41567500	-3.89041300
C	2.79303500	-1.70852400	-0.30659800
C	2.62938100	-2.84857800	0.50831100
C	3.89889600	-1.64230900	-1.17262900
C	3.56106200	-3.88648500	0.46005800
H	1.76505200	-2.92508100	1.15786800
C	4.82296800	-2.68877900	-1.21678300
H	4.04091000	-0.77616000	-1.80584100
C	4.65809200	-3.81009100	-0.40175500
H	3.42278100	-4.75652800	1.09196300
H	5.67203600	-2.62415600	-1.88779500
H	5.37740300	-4.62010200	-0.43976900
C	-1.87512700	2.02298200	-0.40856000
C	-2.51004600	3.06134800	0.30144600
C	-1.49484500	2.23793800	-1.74185300
C	-2.73748900	4.29413900	-0.30786600
H	-2.83960200	2.90069900	1.32215400
C	-1.72587800	3.47765100	-2.34724900
H	-1.03409400	1.43404000	-2.30073000
C	-2.33987400	4.50589700	-1.63246800
H	-3.22525900	5.08777400	0.24649800
H	-1.42289000	3.63498300	-3.37610600
H	-2.51440500	5.46680300	-2.10255400
C	-3.21920900	-0.11427900	0.96128400
C	-3.37031000	-1.01982000	2.02881100
C	-4.36455200	0.30868500	0.26193300
C	-4.63817500	-1.47539100	2.39295500
H	-2.50668700	-1.39645400	2.56181300
C	-5.62870900	-0.15488300	0.62916100
H	-4.26823000	1.00282100	-0.56411400
C	-5.76898200	-1.04491300	1.69581700
H	-4.73640300	-2.17640400	3.21368000
H	-6.50223900	0.17980900	0.08122000
H	-6.75137500	-1.40546200	1.97787500
C	-1.92791500	-1.65800200	-2.76818000
O	-2.20535900	-2.26895700	-1.68976000
O	-0.97852800	-0.79454700	-2.76083900
C	-2.71170000	-1.90920500	-4.02865300

H	-3.54809600	-1.20248400	-4.07274100
H	-2.08425100	-1.75023400	-4.90780200
H	-3.12001000	-2.92113900	-4.02407900
H	-1.65835000	-3.61823200	0.51138100
C	-1.03707800	-3.29595500	1.37337600
O	-0.34847400	-2.19332000	1.16327500
O	-1.01224100	-3.92666900	2.41768800

Illace

Zero-point = -2731.233745

Ru	0.45678200	-1.38865000	0.57563800
P	1.60849000	0.33890700	-0.43878100
P	-1.54672700	-0.35702400	0.23078500
C	-1.71448400	0.47358600	-1.43137500
H	-1.69626800	-0.36943500	-2.13084700
H	-2.72057900	0.90205800	-1.47037400
C	0.75980300	0.94234200	-1.98661500
C	-0.67767900	1.53177200	-1.89869200
C	-1.03891200	1.93063400	-3.36603100
H	-0.43331600	2.79529200	-3.66253600
H	-0.79710900	1.11611500	-4.06449400
P	-2.79683800	2.35274700	-3.71579900
H	-2.68697700	2.85492100	-5.04142800
H	-3.38218200	1.08253500	-3.96142000
O	-3.53719000	3.22127900	-2.74049500
H	1.41912100	1.67416400	-2.46626600
H	0.73711500	0.05604300	-2.62842500
C	-0.72396800	2.81170100	-1.03965900
H	-0.51946400	2.61011800	0.01171500
H	0.02961700	3.52644700	-1.38636400
H	-1.70498300	3.28567000	-1.11616200
C	-2.11763200	0.87643200	1.47404900
C	-3.09411100	1.85007300	1.18771400
C	-1.60511300	0.78849700	2.78096300
C	-3.53363100	2.72180300	2.18491900
H	-3.51187400	1.94271600	0.19201800
C	-2.05639700	1.65978900	3.77648900
H	-0.85256000	0.04376900	3.01230900
C	-3.01694400	2.62794600	3.48034500
H	-4.27898200	3.47238200	1.94853800
H	-1.65558900	1.57896700	4.78087800
H	-3.36327100	3.30570500	4.25222900
C	-3.00837900	-1.49008400	0.13439600
C	-3.01836900	-2.50387500	-0.84340000
C	-4.08999600	-1.39936600	1.02617600
C	-4.08682900	-3.39588800	-0.92920200
H	-2.17919700	-2.60524600	-1.52009900
C	-5.15580100	-2.29903600	0.93796900

H	-4.10306400	-0.62786500	1.78498600
C	-5.15861300	-3.29591400	-0.03820000
H	-4.07602100	-4.17466000	-1.68326300
H	-5.98296300	-2.21723300	1.63397900
H	-5.98595300	-3.99312500	-0.10232800
C	2.06160600	1.87739700	0.46424300
C	2.70432400	2.94116100	-0.20075600
C	1.75206600	2.01426600	1.82641100
C	3.01110100	4.11823600	0.47989000
H	2.97689700	2.84343500	-1.24580200
C	2.06124300	3.19864800	2.50365100
H	1.28525000	1.19107400	2.35100900
C	2.68424800	4.25104300	1.83367600
H	3.50417900	4.93031300	-0.04226900
H	1.81102200	3.29420800	3.55414100
H	2.91934200	5.16904500	2.35986200
C	3.23225000	-0.21920100	-1.12070900
C	3.25549700	-1.18714900	-2.14318200
C	4.45209400	0.24241800	-0.59748000
C	4.46965900	-1.65931300	-2.64137100
H	2.32501100	-1.59680000	-2.51539300
C	5.66423700	-0.24025900	-1.09644900
H	4.45787300	0.97886600	0.19590000
C	5.67709300	-1.18647700	-2.12174100
H	4.47177000	-2.40677200	-3.42680600
H	6.59676500	0.12447100	-0.68072200
H	6.61900500	-1.55955700	-2.50699400
C	2.12706700	-1.73542500	2.48411400
O	2.34746100	-2.27301700	1.36148400
O	1.09891000	-0.97495700	2.61086000
C	3.01710100	-1.99904400	3.67022000
H	3.11331900	-1.09957400	4.28275200
H	2.56475800	-2.78160700	4.28936700
H	3.99736100	-2.34278500	3.33698500
H	0.37672400	-3.79808300	-2.57117000
C	0.30529300	-3.46866200	-1.51425500
O	0.30933700	-2.17308500	-1.40150200
O	0.21732200	-4.30061600	-0.61402600
H	-0.18950500	-3.11822700	0.88397100
H	-0.47122800	-2.67133300	1.49413500

TSIIIace

Zero-point = -2731.22774

Ru	0.40060500	-1.38489400	0.56307600
P	1.67202000	0.32484500	-0.42636800
P	-1.56472800	-0.32636600	0.15541800
C	-1.64430900	0.68227000	-1.41873400
H	-1.61484300	-0.06332800	-2.22090200

H	-2.63982100	1.13434000	-1.44727200
C	0.84270900	1.13443400	-1.89594900
C	-0.56961700	1.76260400	-1.71570300
C	-0.90467000	2.40404600	-3.10106500
H	-0.26895500	3.28483400	-3.25036700
H	-0.67970500	1.70648300	-3.92164200
P	-2.64374300	2.93161200	-3.39554600
H	-2.49780700	3.64074200	-4.61956500
H	-3.25870600	1.73680300	-3.85641100
O	-3.38002500	3.64901800	-2.30193000
H	1.52502900	1.89431100	-2.29282000
H	0.77612600	0.34466400	-2.65238500
C	-0.56982900	2.88825900	-0.66234800
H	-0.37161200	2.50949100	0.34043200
H	0.20927900	3.62225600	-0.89308900
H	-1.53467000	3.39997900	-0.65044700
C	-2.24318900	0.78678900	1.46087100
C	-3.24543200	1.74203500	1.20232300
C	-1.76887800	0.63470200	2.77612700
C	-3.74983200	2.53136200	2.23633900
H	-3.63077400	1.89082000	0.20049900
C	-2.28528000	1.42423500	3.80817700
H	-0.99373900	-0.09301300	2.98349000
C	-3.27246200	2.37338000	3.54073600
H	-4.51305200	3.27022500	2.02082600
H	-1.91250000	1.29495400	4.81832000
H	-3.66851500	2.98829500	4.34092300
C	-3.01321100	-1.44215000	-0.16044500
C	-3.08465200	-2.19283100	-1.34976400
C	-4.01916700	-1.61749400	0.80496700
C	-4.13645200	-3.08343200	-1.56838500
H	-2.30871000	-2.09730200	-2.10050900
C	-5.06676000	-2.51451000	0.58459000
H	-3.98457500	-1.05163700	1.72737700
C	-5.13091200	-3.24717800	-0.60149200
H	-4.17638500	-3.65251400	-2.49062100
H	-5.83369400	-2.63698400	1.34100500
H	-5.94598000	-3.94116500	-0.77074800
C	2.30594900	1.77474300	0.52560000
C	3.07546300	2.77726400	-0.09757400
C	1.98694700	1.91102100	1.88636400
C	3.50121400	3.89348500	0.62139900
H	3.35484700	2.67645800	-1.14074100
C	2.41669900	3.03313300	2.60280000
H	1.41507300	1.13445800	2.37878000
C	3.16798100	4.02549300	1.97356600
H	4.09229200	4.65836900	0.13034600
H	2.15997000	3.12832200	3.65190700

H	3.49668200	4.89574000	2.53004000
C	3.21586200	-0.31416000	-1.22343900
C	3.12812400	-1.13154000	-2.36666900
C	4.48150900	-0.08998500	-0.65383800
C	4.27633100	-1.68386400	-2.93523600
H	2.15997700	-1.36683400	-2.79118800
C	5.62675100	-0.65219900	-1.22208900
H	4.57331500	0.52578200	0.23205900
C	5.52950500	-1.44455100	-2.36662000
H	4.19077300	-2.30884000	-3.81735900
H	6.59405900	-0.46950900	-0.76770000
H	6.41978300	-1.87818000	-2.80724300
C	1.95625400	-1.79631700	2.54039000
O	2.20666000	-2.35203900	1.43119500
O	0.96820600	-0.98179400	2.60974900
C	2.76697100	-2.10140300	3.77270400
H	2.23578800	-2.84792100	4.37360100
H	3.74064700	-2.50728400	3.49413600
H	2.88709300	-1.20306000	4.38277900
H	0.13669500	-4.11595600	-2.29776800
C	0.08292500	-3.56160500	-1.35194200
O	0.29106300	-2.31833500	-1.38634900
O	-0.19469400	-4.23388200	-0.31035000
H	-0.29507300	-3.39970500	0.55988300
H	-0.48711800	-2.66006800	1.29197300

IVace

Zero-point = -2731.226816

Ru	0.31030000	-1.25907300	0.71049500
P	1.72969900	0.31438200	-0.39220200
P	-1.61443400	-0.28428100	0.02882300
C	-1.55973300	0.88555300	-1.43110000
H	-1.46393000	0.24024700	-2.31111300
H	-2.55110900	1.34135100	-1.49305900
C	0.93640200	1.33713000	-1.74709600
C	-0.45911900	1.97656000	-1.49781500
C	-0.72409300	2.86729100	-2.75411200
H	-0.06786500	3.74479500	-2.71395300
H	-0.47435600	2.32568000	-3.67873000
P	-2.43999100	3.47892700	-3.01952600
H	-2.22640600	4.42121600	-4.06274100
H	-3.04148200	2.41605100	-3.74520100
O	-3.22665300	3.97149000	-1.83934200
H	1.64270000	2.12888900	-2.02264500
H	0.85080100	0.66243200	-2.60758700
C	-0.46209700	2.88820500	-0.25596300
H	-0.31454100	2.31676900	0.66175200
H	0.34794700	3.62216400	-0.32105100

H	-1.40994800	3.42437100	-0.17363400
C	-2.56689000	0.63198000	1.32045200
C	-3.47836200	1.66582500	1.03121600
C	-2.39595100	0.23399100	2.65990000
C	-4.19673400	2.28105000	2.05842300
H	-3.62677300	2.02422800	0.02003300
C	-3.12488700	0.84863200	3.68103300
H	-1.67614200	-0.53957600	2.89427500
C	-4.02587500	1.87218800	3.38319200
H	-4.88519300	3.08320900	1.81873700
H	-2.98050800	0.53019700	4.70744500
H	-4.58672600	2.35306100	4.17664700
C	-2.90414900	-1.44949100	-0.62802000
C	-2.69196200	-2.11341100	-1.85256000
C	-4.07026900	-1.74076000	0.09913000
C	-3.62364900	-3.03355700	-2.33556100
H	-1.78935500	-1.92569600	-2.42343400
C	-4.99723800	-2.66701800	-0.38521400
H	-4.25369300	-1.24258800	1.04268000
C	-4.77932500	-3.31381200	-1.60245100
H	-3.44641900	-3.53254800	-3.28212200
H	-5.89174500	-2.87856400	0.18971300
H	-5.50166800	-4.02979500	-1.97703000
C	2.67360400	1.60684500	0.54511600
C	3.79269700	2.25071900	-0.01511400
C	2.24672700	1.98311000	1.83067200
C	4.45550400	3.25788500	0.68694900
H	4.15776200	1.95031500	-0.99088900
C	2.91484800	2.99309900	2.52924000
H	1.40691300	1.47179500	2.28515700
C	4.01557400	3.63402400	1.95939600
H	5.31816200	3.74389000	0.24486900
H	2.57380100	3.27451400	3.51944400
H	4.53308300	4.41578200	2.50371400
C	3.10323800	-0.49589200	-1.33625300
C	3.51509100	-0.11513400	-2.62575800
C	3.77412800	-1.56038000	-0.70147200
C	4.56957900	-0.77729800	-3.26198100
H	3.02123800	0.69619000	-3.14605200
C	4.82896500	-2.21419300	-1.33954400
H	3.45619900	-1.87856700	0.28533500
C	5.22937300	-1.82626200	-2.62084600
H	4.87327200	-0.47081600	-4.25691700
H	5.33383900	-3.03136900	-0.83629600
H	6.04649300	-2.33865700	-3.11569200
C	1.61165000	-1.36313800	2.90439400
O	1.98217100	-2.10031700	1.93958000
O	0.64066400	-0.55293900	2.71872400

C	2.26748300	-1.45976000	4.25694000
H	2.24903700	-0.49089300	4.76008200
H	1.71222000	-2.17560000	4.87360100
H	3.29372700	-1.81740200	4.15601900
H	0.36409300	-4.34641500	-1.83020300
C	0.20314200	-3.67975300	-0.97772800
O	0.43575100	-2.46382600	-1.08758100
O	-0.23045600	-4.26344800	0.09411200
H	-0.66401600	-2.38795700	1.47601400
H	-0.38956200	-3.48994800	0.78589900

TSIVace

Zero-point = -2731.196094

Ru	0.39630500	-1.44119000	0.41472100
P	1.65197200	0.38200700	-0.40142500
P	-1.56011300	-0.32955100	0.15598200
C	-1.67754400	0.70490900	-1.39647800
H	-1.65455500	-0.03254500	-2.20586000
H	-2.67426100	1.15647200	-1.40000600
C	0.81008000	1.18550900	-1.86536300
C	-0.61250500	1.79387300	-1.69769300
C	-0.94959800	2.41478600	-3.09176600
H	-0.32090200	3.29888800	-3.25147300
H	-0.71578000	1.70743600	-3.90128000
P	-2.69001500	2.92638200	-3.40055900
H	-2.54613100	3.59397600	-4.64812800
H	-3.30297900	1.71561700	-3.82052900
O	-3.42634700	3.67943800	-2.33143300
H	1.48156800	1.94861000	-2.27476200
H	0.76713000	0.38044700	-2.60874000
C	-0.63749200	2.92812200	-0.65393700
H	-0.41768300	2.56435200	0.35026100
H	0.11450500	3.68545100	-0.89794200
H	-1.61737400	3.41066600	-0.63823800
C	-2.14372400	0.77300500	1.51173400
C	-3.18926900	1.69882700	1.32788600
C	-1.55092200	0.65354700	2.78073600
C	-3.61936100	2.49507100	2.38905400
H	-3.66691800	1.81165500	0.36150300
C	-1.99277600	1.45112200	3.84138600
H	-0.74819700	-0.05827900	2.93063000
C	-3.02202500	2.37271100	3.64754200
H	-4.41774100	3.21116300	2.23205600
H	-1.52914400	1.34939400	4.81643300
H	-3.35943700	2.99363800	4.46964800
C	-3.05110000	-1.40486400	-0.10284600
C	-3.23499300	-2.09605600	-1.31769000
C	-3.97655800	-1.61449400	0.93521000



C	-4.32118400	-2.95747300	-1.48844000
H	-2.51601500	-1.98289700	-2.12059700
C	-5.05689000	-2.48197400	0.76086600
H	-3.85516800	-1.09388600	1.87700200
C	-5.23537600	-3.15226100	-0.45092500
H	-4.44907000	-3.47794800	-2.43116900
H	-5.76170200	-2.62815300	1.57162000
H	-6.07792600	-3.82068200	-0.58544900
C	2.23517500	1.80345700	0.62062100
C	2.79518000	2.96333500	0.04861900
C	2.11836700	1.72800100	2.01909500
C	3.22013600	4.01905800	0.85532100
H	2.90516100	3.04289400	-1.02702900
C	2.54516200	2.78979500	2.82287300
H	1.69379900	0.83790600	2.46804200
C	3.09344800	3.93492400	2.24524100
H	3.64722600	4.90628300	0.40149600
H	2.44424400	2.71968800	3.90017900
H	3.42022400	4.75820500	2.87004500
C	3.20108500	-0.21360300	-1.22042200
C	3.10364600	-1.36317300	-2.03080400
C	4.45392000	0.39924100	-1.05654700
C	4.23222200	-1.86196100	-2.68150300
H	2.15566600	-1.88476900	-2.11674900
C	5.58083200	-0.11184500	-1.70654000
H	4.55541900	1.26674500	-0.41742800
C	5.47216100	-1.23698000	-2.52449900
H	4.14408900	-2.75087500	-3.29611100
H	6.54271200	0.36916300	-1.56749200
H	6.34866600	-1.63231000	-3.02530000
C	2.01902000	-2.00951400	2.32059900
O	1.01976000	-1.22086800	2.48435600
O	2.22422500	-2.50199000	1.17550800
C	2.93579100	-2.30116400	3.48181500
H	2.35159900	-2.51021100	4.38189700
H	3.58736800	-3.14403800	3.24803800
H	3.55437300	-1.41971600	3.68368500
C	-0.29907600	-3.31782000	-0.70273600
O	0.59433100	-4.36195300	-0.67583000
O	0.01639000	-2.34534400	-1.49738400
H	-1.35230900	-3.62717900	-0.66739300
H	0.32860500	-4.98759600	0.01296600
H	-0.42599900	-2.85871500	0.80429500

Vace

Zero-point = -2731.211841

Ru	0.51695100	-1.32010100	0.38936100
P	1.54526000	0.50440600	-0.41631800

P	-1.52827200	-0.38456000	0.15589700
C	-1.77644800	0.63448300	-1.38570400
H	-1.72939100	-0.10489100	-2.19276100
H	-2.80176900	1.01571200	-1.35987200
C	0.66225400	1.26835800	-1.87353400
C	-0.79305500	1.78930900	-1.71013800
C	-1.17909600	2.36952200	-3.10816100
H	-0.61178500	3.29125100	-3.28411500
H	-0.90712800	1.66881100	-3.91128900
P	-2.95436900	2.76028400	-3.39905400
H	-2.87235800	3.42962700	-4.65089800
H	-3.48875500	1.50818300	-3.80345900
O	-3.72367900	3.46749300	-2.32162900
H	1.29358800	2.07432700	-2.26437000
H	0.67446000	0.47038500	-2.62529900
C	-0.88413600	2.93228600	-0.67917900
H	-0.64473200	2.59454100	0.32960000
H	-0.17716700	3.72903600	-0.93257100
H	-1.89006400	3.35792900	-0.67065800
C	-2.18144100	0.64256500	1.53910200
C	-3.26124800	1.53272200	1.38238500
C	-1.60336600	0.48749300	2.81187100
C	-3.73931300	2.25923900	2.47336800
H	-3.72921600	1.67351300	0.41503800
C	-2.09322400	1.21303800	3.90191200
H	-0.77373600	-0.19771000	2.94323600
C	-3.15692500	2.10064300	3.73437000
H	-4.56441300	2.94877800	2.33712300
H	-1.64108700	1.08259700	4.87887400
H	-3.53226800	2.66654800	4.57934900
C	-2.89600800	-1.61165500	-0.08435100
C	-2.92672900	-2.39567400	-1.25615400
C	-3.88570600	-1.81497200	0.89224700
C	-3.93264200	-3.34416400	-1.44547200
H	-2.14084700	-2.28720500	-1.99501200
C	-4.88508000	-2.77222300	0.69888200
H	-3.88059800	-1.22249500	1.79834300
C	-4.91454900	-3.53452900	-0.46960300
H	-3.94422500	-3.93947500	-2.35173300
H	-5.64191100	-2.91663100	1.46155700
H	-5.69300800	-4.27395500	-0.61803900
C	2.02105000	1.93752000	0.64187200
C	2.53851200	3.12771100	0.09237600
C	1.86914300	1.84321100	2.03489700
C	2.88200400	4.19816300	0.91780200
H	2.68205400	3.21747700	-0.97857300
C	2.21426000	2.92031500	2.85751000
H	1.48946400	0.92528200	2.46642500

C	2.71628200	4.09746700	2.30274500
H	3.27723300	5.10915200	0.48276700
H	2.08729900	2.83587800	3.93090100
H	2.97947800	4.93242100	2.94182700
C	3.13704300	0.01882400	-1.22030300
C	3.10174800	-1.04924000	-2.14037600
C	4.36633300	0.63335900	-0.93252700
C	4.27267900	-1.46836800	-2.77232000
H	2.16887200	-1.57686000	-2.31762100
C	5.53492200	0.20226900	-1.56674800
H	4.41540000	1.44225200	-0.21487100
C	5.49039600	-0.84286500	-2.49019300
H	4.23455600	-2.29451500	-3.47361600
H	6.47855300	0.68316900	-1.33428900
H	6.39910200	-1.17566100	-2.97879500
C	2.16673100	-1.99161800	2.25692800
O	1.16502500	-1.24195400	2.50798100
O	2.38177000	-2.35313300	1.05407400
C	3.10429000	-2.40992700	3.35957300
H	2.60874300	-2.34912100	4.32980100
H	3.47002100	-3.42284100	3.17876100
H	3.96941500	-1.73740200	3.36432800
C	0.10669000	-3.47134600	-0.72270100
O	1.21021700	-4.33074900	-0.69415400
O	0.25220800	-2.31341700	-1.42140000
H	-0.75731500	-4.07154700	-1.04247100
H	1.94984100	-3.82926700	-0.31191000
H	-0.17799800	-3.21222700	0.39331500

Vlacc

Zero-point = -2732.383916

Ru	0.49005600	-1.30352400	0.62649500
P	1.54102800	0.43753100	-0.45421100
P	-1.55736500	-0.40147500	0.25472800
C	-1.77765600	0.38052600	-1.42247900
H	-1.70476000	-0.47836400	-2.09821900
H	-2.80839400	0.74539100	-1.46643700
C	0.65577900	0.96210500	-2.00631000
C	-0.80547200	1.48587800	-1.91429200
C	-1.19875300	1.84332400	-3.38372200
H	-0.64264500	2.73440300	-3.69858000
H	-0.91959000	1.03174200	-4.07149600
P	-2.97917400	2.16448700	-3.72364300
H	-2.90832900	2.64771600	-5.05913900
H	-3.49816800	0.86086800	-3.94126900
O	-3.75733900	3.01042400	-2.75764800
H	1.27798700	1.70839500	-2.51257000
H	0.66343500	0.05372300	-2.61637400

C	-0.90843600	2.77337600	-1.07216900
H	-0.68505100	2.59554300	-0.02009200
H	-0.19448800	3.52052400	-1.43442600
H	-1.91274600	3.19662200	-1.14470300
C	-2.20890100	0.81369200	1.47629900
C	-3.24365500	1.72105600	1.17718900
C	-1.68459000	0.78390100	2.78134900
C	-3.73139900	2.58288900	2.16090200
H	-3.66784700	1.77194600	0.18104100
C	-2.18279700	1.64509800	3.76283000
H	-0.88464100	0.09238900	3.02051900
C	-3.20342500	2.54589400	3.45453600
H	-4.52179400	3.28256800	1.91475000
H	-1.77139900	1.61004400	4.76560600
H	-3.58642800	3.21632800	4.21544400
C	-2.93326000	-1.63489600	0.16696800
C	-2.80305800	-2.69966200	-0.74615800
C	-4.07690200	-1.56840600	0.97835700
C	-3.80090100	-3.66864700	-0.84768800
H	-1.90674500	-2.76476100	-1.35207400
C	-5.07060000	-2.54650200	0.87519100
H	-4.19437600	-0.75687300	1.68503900
C	-4.93699800	-3.59460400	-0.03634400
H	-3.68720100	-4.48499800	-1.55226200
H	-5.94856900	-2.48560800	1.50836800
H	-5.70961200	-4.35110600	-0.11216000
C	1.95130500	2.01493300	0.40176600
C	2.54990500	3.08247100	-0.29720100
C	1.64891500	2.17755600	1.76294400
C	2.82109100	4.28739000	0.34921600
H	2.81551200	2.96647400	-1.34221600
C	1.92240000	3.38947100	2.40593600
H	1.21513200	1.35309100	2.31355000
C	2.50209900	4.44471100	1.70222700
H	3.28028200	5.10217700	-0.19902700
H	1.67845200	3.50430800	3.45599600
H	2.70937800	5.38412400	2.20167500
C	3.17582600	-0.08752700	-1.13567500
C	3.21759500	-1.07452000	-2.13967000
C	4.38543600	0.41673500	-0.62895600
C	4.44152700	-1.52598000	-2.63414000
H	2.29032100	-1.50964600	-2.49142800
C	5.60722600	-0.04559300	-1.12424300
H	4.37580500	1.17012100	0.14856200
C	5.63924600	-1.01277400	-2.12961100
H	4.45901500	-2.28626400	-3.40719800
H	6.53230700	0.35191700	-0.72200400
H	6.58873900	-1.36882200	-2.51261600

C	2.22459800	-1.53110700	2.52798900
O	1.16429100	-0.82952600	2.66721200
O	2.46090200	-2.07431500	1.40580100
C	3.15555200	-1.73537200	3.69579200
H	2.84004100	-2.62567900	4.25130400
H	4.17495600	-1.89878200	3.34161100
H	3.11647900	-0.87967800	4.37270400
C	0.63047100	-3.46376900	-1.47477900
O	1.25985600	-4.09233400	-0.35921200
O	0.39389200	-2.10868800	-1.33114300
H	1.24761100	-3.61944300	-2.38205100
H	2.04576400	-3.57345800	-0.12422200
H	-0.29813300	-4.05165900	-1.59802200
H	-0.43661500	-2.59411200	1.57178900
H	0.00069800	-3.03862700	1.07530800

TSVIace

Zero-point = -2732.362378

Ru	0.38199300	-1.43553300	0.34133200
P	1.67232500	0.40499800	-0.37246200
P	-1.55059700	-0.30558600	0.12561600
C	-1.63920300	0.84056800	-1.34524800
H	-1.58910300	0.16395600	-2.20638400
H	-2.63287200	1.29970500	-1.33914500
C	0.85375100	1.35798700	-1.75768300
C	-0.56982000	1.94963700	-1.54046600
C	-0.89166600	2.69500100	-2.87641900
H	-0.25725600	3.58640700	-2.94930200
H	-0.65043500	2.06228400	-3.74375100
P	-2.62279000	3.24206800	-3.16901900
H	-2.45532600	3.99497600	-4.36429500
H	-3.23629200	2.06870400	-3.68743800
O	-3.37410500	3.92072800	-2.06227700
H	1.52830400	2.15999400	-2.07734500
H	0.81081900	0.63663200	-2.58172100
C	-0.60504200	2.98423500	-0.39829300
H	-0.39650000	2.52922700	0.57038000
H	0.14984300	3.75979900	-0.56372900
H	-1.58570200	3.46346800	-0.34820900
C	-2.18511100	0.68258100	1.54989200
C	-3.28690300	1.54957700	1.43060700
C	-1.57683800	0.51549800	2.80547900
C	-3.75439800	2.24999900	2.54210900
H	-3.78161500	1.68646600	0.47560500
C	-2.05662000	1.21455200	3.91767700
H	-0.73695100	-0.16235200	2.90556900
C	-3.13968000	2.08426100	3.78732600
H	-4.59703000	2.92362400	2.43640600

H	-1.58219200	1.07650700	4.88314900
H	-3.50732400	2.62935600	4.64929600
C	-3.04349100	-1.36772500	-0.19636000
C	-3.78455500	-1.36214000	-1.38913900
C	-3.42555700	-2.26035000	0.82550500
C	-4.87166000	-2.22782400	-1.55840000
H	-3.53058000	-0.68715000	-2.19587500
C	-4.51071000	-3.11708700	0.65605100
H	-2.85921900	-2.28636500	1.74999500
C	-5.23696300	-3.10584400	-0.53962600
H	-5.43142700	-2.20829200	-2.48693000
H	-4.78950700	-3.79510400	1.45483400
H	-6.07939400	-3.77485000	-0.67175100
C	2.24330300	1.73250900	0.77842700
C	2.87594600	2.90113700	0.30917200
C	2.03493300	1.58498200	2.15949800
C	3.27343800	3.89966700	1.19780500
H	3.06970000	3.02629900	-0.75035800
C	2.43530200	2.58944500	3.04698800
H	1.56889700	0.68109000	2.53107400
C	3.04910800	3.74727500	2.56990800
H	3.75696300	4.79466500	0.82255700
H	2.26346600	2.46383800	4.11018900
H	3.35447000	4.52646900	3.25886300
C	3.25094200	-0.08239100	-1.21448000
C	3.17615100	-0.96438700	-2.31192100
C	4.51668500	0.33375500	-0.76911800
C	4.33687100	-1.38791600	-2.95947700
H	2.21031900	-1.34758200	-2.62178900
C	5.67602800	-0.10303900	-1.41659600
H	4.59996400	0.99908200	0.08050700
C	5.59035800	-0.95691000	-2.51639500
H	4.26332000	-2.06427400	-3.80433900
H	6.64488900	0.22696500	-1.05838900
H	6.49102700	-1.29129900	-3.01858500
C	1.99326500	-2.27344700	2.15472000
O	1.06801700	-1.43178500	2.41337500
O	2.16007600	-2.65782400	0.95485700
C	2.84414400	-2.82543100	3.27032400
H	2.32909000	-3.68016800	3.72336300
H	3.80502300	-3.16684000	2.88158300
H	2.99241900	-2.07198500	4.04687900
C	-0.34871300	-3.16951300	-1.91730100
O	0.16654000	-4.27531400	-0.74994200
O	0.25666600	-2.03911800	-1.72807400
H	1.13995300	-4.19879900	-0.73183600
H	-1.41535100	-3.24864800	-1.66735100
H	-0.11300200	-3.61532100	0.09723800

H -0.51984500 -2.79142800 0.85311100

TSVlace at T=160°

Zero-point = -2732.362378

Ru	0.38199300	-1.43553300	0.34133200
P	1.67232500	0.40499800	-0.37246200
P	-1.55059700	-0.30558600	0.12561600
C	-1.63920300	0.84056800	-1.34524800
H	-1.58910300	0.16395600	-2.20638400
H	-2.63287200	1.29970500	-1.33914500
C	0.85375100	1.35798700	-1.75768300
C	-0.56982000	1.94963700	-1.54046600
C	-0.89166600	2.69500100	-2.87641900
H	-0.25725600	3.58640700	-2.94930200
H	-0.65043500	2.06228400	-3.74375100
P	-2.62279000	3.24206800	-3.16901900
H	-2.45532600	3.99497600	-4.36429500
H	-3.23629200	2.06870400	-3.68743800
O	-3.37410500	3.92072800	-2.06227700
H	1.52830400	2.15999400	-2.07734500
H	0.81081900	0.63663200	-2.58172100
C	-0.60504200	2.98423500	-0.39829300
H	-0.39650000	2.52922700	0.57038000
H	0.14984300	3.75979900	-0.56372900
H	-1.58570200	3.46346800	-0.34820900
C	-2.18511100	0.68258100	1.54989200
C	-3.28690300	1.54957700	1.43060700
C	-1.57683800	0.51549800	2.80547900
C	-3.75439800	2.24999900	2.54210900
H	-3.78161500	1.68646600	0.47560500
C	-2.05662000	1.21455200	3.91767700
H	-0.73695100	-0.16235200	2.90556900
C	-3.13968000	2.08426100	3.78732600
H	-4.59703000	2.92362400	2.43640600
H	-1.58219200	1.07650700	4.88314900
H	-3.50732400	2.62935600	4.64929600
C	-3.04349100	-1.36772500	-0.19636000
C	-3.78455500	-1.36214000	-1.38913900
C	-3.42555700	-2.26035000	0.82550500
C	-4.87166000	-2.22782400	-1.55840000
H	-3.53058000	-0.68715000	-2.19587500
C	-4.51071000	-3.11708700	0.65605100
H	-2.85921900	-2.28636500	1.74999500
C	-5.23696300	-3.10584400	-0.53962600
H	-5.43142700	-2.20829200	-2.48693000
H	-4.78950700	-3.79510400	1.45483400
H	-6.07939400	-3.77485000	-0.67175100
C	2.24330300	1.73250900	0.77842700

C	2.87594600	2.90113700	0.30917200
C	2.03493300	1.58498200	2.15949800
C	3.27343800	3.89966700	1.19780500
H	3.06970000	3.02629900	-0.75035800
C	2.43530200	2.58944500	3.04698800
H	1.56889700	0.68109000	2.53107400
C	3.04910800	3.74727500	2.56990800
H	3.75696300	4.79466500	0.82255700
H	2.26346600	2.46383800	4.11018900
H	3.35447000	4.52646900	3.25886300
C	3.25094200	-0.08239100	-1.21448000
C	3.17615100	-0.96438700	-2.31192100
C	4.51668500	0.33375500	-0.76911800
C	4.33687100	-1.38791600	-2.95947700
H	2.21031900	-1.34758200	-2.62178900
C	5.67602800	-0.10303900	-1.41659600
H	4.59996400	0.99908200	0.08050700
C	5.59035800	-0.95691000	-2.51639500
H	4.26332000	-2.06427400	-3.80433900
H	6.64488900	0.22696600	-1.05838900
H	6.49102700	-1.29129800	-3.01858500
C	1.99326500	-2.27344700	2.15472000
O	1.06801700	-1.43178500	2.41337500
O	2.16007600	-2.65782400	0.95485700
C	2.84414400	-2.82543100	3.27032400
H	2.32909000	-3.68016800	3.72336300
H	3.80502300	-3.16684000	2.88158300
H	2.99241900	-2.07198500	4.04687900
C	-0.34871300	-3.16951300	-1.91730100
O	0.16654000	-4.27531400	-0.74994200
O	0.25666600	-2.03911800	-1.72807400
H	-0.08062800	-3.71328800	-2.83359300
H	1.13995300	-4.19879900	-0.73183600
H	-1.41535100	-3.24864800	-1.66735100
H	-0.11300200	-3.61532100	0.09723800
H	-0.51984500	-2.79142800	0.85311100

Vllace

Zero-point = -2732.386666

Ru	0.35768300	-1.50183700	0.33276500
P	1.53460500	0.53084400	-0.47161300
P	-1.69581600	-0.54891900	0.12077600
C	-1.87040100	0.63083900	-1.31967400
H	-1.79630200	-0.01877500	-2.19689200
H	-2.90019200	0.99712100	-1.27671500
C	0.55450000	1.37401800	-1.81943500
C	-0.90394500	1.83185100	-1.51449100
C	-1.35509000	2.59441900	-2.80303400



H	-0.80987900	3.54363400	-2.86502600
H	-1.10126400	2.02126500	-3.70694000
P	-3.14670200	2.98458000	-2.97589600
H	-3.11780200	3.86122000	-4.09490200
H	-3.66778400	1.80756500	-3.57590100
O	-3.89864600	3.47565300	-1.77277600
H	1.13160900	2.23528600	-2.17415700
H	0.53319800	0.64566700	-2.63720500
C	-0.96401500	2.82213900	-0.33486900
H	-0.68866400	2.35059300	0.60908600
H	-0.26886700	3.65194000	-0.49891500
H	-1.97149800	3.23081200	-0.23177400
C	-2.37856600	0.34259500	1.57812000
C	-3.44498400	1.25731100	1.47437300
C	-1.83887800	0.06184900	2.84624500
C	-3.94943900	1.88099700	2.61576400
H	-3.87931400	1.50233300	0.51201700
C	-2.35479900	0.68689600	3.98552400
H	-1.01485600	-0.63584900	2.93489100
C	-3.40692200	1.59641700	3.87250700
H	-4.76351700	2.59025800	2.52125300
H	-1.93164800	0.46057000	4.95792200
H	-3.80322500	2.08320900	4.75633400
C	-3.07536400	-1.70663500	-0.30975600
C	-3.10296800	-2.32651500	-1.57510000
C	-4.07398400	-2.03175000	0.62347000
C	-4.11078000	-3.23718200	-1.89580400
H	-2.32155700	-2.11633200	-2.29656500
C	-5.07744900	-2.94713100	0.29748200
H	-4.07011500	-1.56781100	1.60174500
C	-5.10132400	-3.54902600	-0.96157300
H	-4.11841100	-3.70613000	-2.87353000
H	-5.84158300	-3.18565600	1.02855900
H	-5.88292100	-4.25678000	-1.21243500
C	2.04511900	1.91487300	0.63091100
C	2.61159500	3.09756800	0.11459800
C	1.84127000	1.80842900	2.01693500
C	2.95557900	4.14806800	0.96462900
H	2.79410100	3.19291300	-0.95024100
C	2.18744100	2.86592200	2.86442200
H	1.41765100	0.89928500	2.42602200
C	2.74043000	4.03485900	2.34207400
H	3.39025300	5.05296500	0.55532600
H	2.02093000	2.77248400	3.93155200
H	3.00523500	4.85396100	3.00063900
C	3.09760700	0.11864400	-1.36907600
C	3.03535300	-0.78851600	-2.44704800
C	4.35476600	0.59502500	-0.95716100

C	4.19982600	-1.18228700	-3.10692800
H	2.08084500	-1.22096300	-2.72623300
C	5.51897200	0.18795400	-1.61869400
H	4.42885300	1.27932500	-0.12192900
C	5.44422900	-0.69586400	-2.69742500
H	4.13631800	-1.88476200	-3.93032500
H	6.48093100	0.56405300	-1.28831700
H	6.34778400	-1.01247100	-3.20495100
C	2.11037100	-1.95638800	2.14703300
O	1.04900100	-1.26914100	2.35659600
O	2.29132000	-2.42575400	0.98043700
C	3.10527100	-2.20201800	3.24625100
H	2.93522200	-3.20032100	3.66486300
H	4.11400900	-2.17620600	2.82509500
H	2.98978600	-1.46576000	4.04349400
C	0.06748600	-3.03893300	-1.07660000
O	0.14562500	-1.91690400	-1.75741600
H	0.95605300	-3.68181900	-1.02404200
H	-0.89704000	-3.55120700	-1.03323600
H	-0.41440300	-2.71627200	1.03604300
O	5.13898700	-2.42058900	0.60615700
H	5.21178100	-1.65977600	0.01469600
H	4.19120200	-2.63301900	0.57406100

#### Villace

Zero-point = -2655.976526

Ru	0.32165700	-1.59724900	0.44994400
P	1.74380600	0.24505500	-0.42208000
P	-1.60983800	-0.44271100	0.11880300
C	-1.61318100	0.67959800	-1.37707200
H	-1.58148000	-0.01480300	-2.22208000
H	-2.59873200	1.15400200	-1.38782000
C	0.88993100	1.13420400	-1.82720000
C	-0.51691500	1.75996800	-1.58748500
C	-0.84602900	2.51061900	-2.91921200
H	-0.19811600	3.39125300	-3.00197300
H	-0.63159900	1.87432500	-3.79055300
P	-2.57743400	3.08536200	-3.16809100
H	-2.42021000	3.89654900	-4.32544000
H	-3.20966200	1.94459600	-3.73029200
O	-3.30450800	3.71620200	-2.01589300
H	1.56700300	1.91148000	-2.19902100
H	0.81113500	0.37866100	-2.61632400
C	-0.50078300	2.80058600	-0.45053700
H	-0.30199900	2.34278200	0.51909800
H	0.28396000	3.54354100	-0.62628800
H	-1.46044600	3.31882400	-0.39366800
C	-2.24186000	0.58628500	1.50788200

C	-3.20313600	1.59961900	1.32382500
C	-1.77196200	0.31717100	2.80592300
C	-3.67318500	2.32966300	2.41579700
H	-3.58055800	1.83896700	0.33639500
C	-2.25330700	1.04951000	3.89540700
H	-1.02713900	-0.45518400	2.95572300
C	-3.20084500	2.05546900	3.70280700
H	-4.40511000	3.11355700	2.25906500
H	-1.88443900	0.83142400	4.89154900
H	-3.56981000	2.62533400	4.54801800
C	-3.09280000	-1.46546300	-0.31214700
C	-3.13927200	-2.14696100	-1.54494100
C	-4.15814200	-1.62716700	0.58920500
C	-4.22962600	-2.95688100	-1.86580400
H	-2.31003500	-2.06373500	-2.23833400
C	-5.24461700	-2.44258800	0.26352600
H	-4.14106000	-1.11383300	1.54227100
C	-5.28585300	-3.10584200	-0.96380500
H	-4.25079700	-3.47497500	-2.81823800
H	-6.05941200	-2.55500600	0.96981300
H	-6.13167900	-3.73543100	-1.21486300
C	2.37403400	1.61561800	0.63715800
C	3.06472800	2.71562200	0.09029100
C	2.13644800	1.58450000	2.02161800
C	3.49803100	3.75872600	0.90818300
H	3.27356600	2.75152200	-0.97327600
C	2.57213000	2.63427500	2.83686700
H	1.61407800	0.73910600	2.45344000
C	3.24903300	3.72117200	2.28400000
H	4.02778900	4.59955400	0.47481100
H	2.37693900	2.60016800	3.90281000
H	3.58261200	4.53518200	2.91726700
C	3.26875100	-0.35793900	-1.27499500
C	3.12556100	-1.30939900	-2.30596200
C	4.56209200	0.03625900	-0.89260700
C	4.24964200	-1.82252700	-2.95280500
H	2.13691900	-1.67448900	-2.56136500
C	5.68320800	-0.48938100	-1.54072300
H	4.69691900	0.75096100	-0.09115100
C	5.53121300	-1.41229400	-2.57575000
H	4.12409500	-2.55458500	-3.74294400
H	6.67436000	-0.17585900	-1.23242600
H	6.40281700	-1.81724100	-3.07709800
C	1.93510400	-2.16416400	2.34609700
O	0.95995200	-1.33695400	2.48569800
O	2.12042900	-2.69123100	1.21450900
C	2.81000000	-2.48794900	3.52834200
H	2.23389200	-3.06764800	4.25718400

H	3.67680100	-3.06812300	3.21009100
H	3.13312100	-1.56624600	4.02025500
C	-0.08079400	-3.16827900	-0.89224600
O	0.12593000	-2.09815700	-1.62640200
H	0.73966200	-3.88833500	-0.77452700
H	-1.09182500	-3.58255600	-0.85551800
H	-0.60245900	-2.68144400	1.18329600

TSVlllace

Zero-point = -2655.971654

Ru	0.39461000	-1.57073700	0.34536000
P	1.67516900	0.29571400	-0.41135000
P	-1.56352300	-0.43587300	0.12981300
C	-1.66331500	0.70043200	-1.35131800
H	-1.65658100	0.01263500	-2.20376000
H	-2.65552800	1.16062400	-1.31998100
C	0.82341300	1.18715900	-1.81664800
C	-0.59052900	1.79625300	-1.59167400
C	-0.93799800	2.51223600	-2.93680200
H	-0.30300900	3.39962700	-3.04499100
H	-0.72168900	1.85878400	-3.79494500
P	-2.67839000	3.05807000	-3.18438500
H	-2.54504700	3.81857500	-4.37869200
H	-3.30645600	1.88743600	-3.68663800
O	-3.39426900	3.73258500	-2.05050400
H	1.49699200	1.96930900	-2.18467300
H	0.76367400	0.43016900	-2.60747000
C	-0.58833000	2.85965900	-0.47550600
H	-0.36982900	2.42675600	0.50120200
H	0.17663200	3.61722900	-0.67466600
H	-1.55881400	3.35785800	-0.42118600
C	-2.13309400	0.57681100	1.55889300
C	-3.13181600	1.56281400	1.43725600
C	-1.57509700	0.32191600	2.82413700
C	-3.55069500	2.28259400	2.55639400
H	-3.58062900	1.78412900	0.47582300
C	-2.00510700	1.04351600	3.94208600
H	-0.80481800	-0.43315200	2.92669600
C	-2.98886700	2.02412700	3.81041200
H	-4.31289900	3.04548100	2.44737900
H	-1.56831500	0.83658000	4.91283800
H	-3.31777800	2.58579800	4.67735600
C	-3.06336800	-1.46565100	-0.22755600
C	-3.15780600	-2.15786400	-1.45237300
C	-4.09373700	-1.61938800	0.71535500
C	-4.26204400	-2.96679800	-1.72535400
H	-2.34931300	-2.08902300	-2.17182100
C	-5.19369300	-2.43479600	0.43748300
H	-4.04032800	-1.09794900	1.66258900

C	-5.28389000	-3.10588300	-0.78290400
H	-4.32008300	-3.49287600	-2.67188400
H	-5.98103900	-2.54020600	1.17531900
H	-6.14046100	-3.73461200	-0.99707500
C	2.29156200	1.65185300	0.67381400
C	2.90370500	2.80868000	0.15128500
C	2.13664100	1.53656200	2.06566500
C	3.34186200	3.82444200	1.00079700
H	3.04464000	2.91502600	-0.91855300
C	2.57662900	2.55901900	2.91230000
H	1.67608600	0.64589200	2.47622000
C	3.17600600	3.70232500	2.38395000
H	3.80974100	4.71010200	0.58589200
H	2.44606900	2.45954900	3.98400700
H	3.51291100	4.49504700	3.04198100
C	3.19777400	-0.28512400	-1.28460700
C	3.04968700	-1.33579600	-2.21348300
C	4.47890000	0.23661500	-1.04488900
C	4.15876400	-1.82363500	-2.90442900
H	2.07456500	-1.79241700	-2.35702700
C	5.58593300	-0.26466500	-1.73586800
H	4.61680100	1.02680100	-0.31819600
C	5.42851500	-1.28815800	-2.67074000
H	4.03266700	-2.63395000	-3.61400600
H	6.57016600	0.14533200	-1.53842800
H	6.28924600	-1.67467800	-3.20456900
C	2.05330100	-2.24499200	2.17988500
O	1.07986900	-1.44521900	2.41447700
O	2.21856700	-2.67376700	1.00003400
C	2.96195400	-2.67109400	3.30434700
H	3.84723700	-3.17034900	2.90871000
H	3.25291100	-1.80345100	3.90254000
H	2.42394700	-3.36169000	3.96261900
C	-0.22545300	-3.32940500	-0.76544700
O	0.03023900	-2.34503300	-1.61352700
H	0.55461500	-4.08735600	-0.61509600
H	-1.24805100	-3.72575000	-0.75944100
H	-0.46398900	-2.91864000	0.78432800

IXace

Zero-point = -2655.987554

Ru	0.51240800	-1.43191100	0.21917700
P	1.55901100	0.41848000	-0.35177800
P	-1.49643200	-0.42713500	0.09619400
C	-1.73518600	0.67154600	-1.38394900
H	-1.66687200	-0.03574600	-2.21819500
H	-2.75845500	1.05901100	-1.36065800
C	0.72930700	1.30797500	-1.76717400

C	-0.72882400	1.83126200	-1.62214200
C	-1.06595100	2.47772400	-3.00348700
H	-0.48097000	3.39728600	-3.12527200
H	-0.78359000	1.80645400	-3.82766400
P	-2.82672600	2.90771700	-3.32199400
H	-2.70399500	3.62087500	-4.54625100
H	-3.37175100	1.68086300	-3.78442400
O	-3.61091600	3.58991300	-2.23874100
H	1.38063400	2.13473900	-2.07267900
H	0.75264000	0.55743400	-2.56369500
C	-0.83812700	2.92976500	-0.54542200
H	-0.63596000	2.54641700	0.45503200
H	-0.11133800	3.72501800	-0.74243900
H	-1.83607200	3.37377300	-0.55208100
C	-2.15383700	0.49733900	1.54699300
C	-3.16779800	1.46852300	1.44509200
C	-1.66152700	0.15600800	2.82016300
C	-3.66622800	2.09057300	2.59127200
H	-3.56859100	1.75334900	0.47930600
C	-2.16997500	0.77807100	3.96329500
H	-0.88273300	-0.59324800	2.90877800
C	-3.16919900	1.74655800	3.85120000
H	-4.44091700	2.84293900	2.49783300
H	-1.78376900	0.50463400	4.93902000
H	-3.55976700	2.23131800	4.73869000
C	-2.82704000	-1.68313000	-0.18958200
C	-2.66448200	-2.59317500	-1.25448900
C	-3.96979100	-1.77847100	0.62280800
C	-3.63524800	-3.56434200	-1.50343300
H	-1.76453400	-2.53039700	-1.85867400
C	-4.93320700	-2.75798000	0.36908500
H	-4.10908600	-1.08977900	1.44613800
C	-4.77028800	-3.64981600	-0.69268900
H	-3.50087800	-4.25856300	-2.32575400
H	-5.81115100	-2.82142600	1.00211400
H	-5.52048200	-4.40851800	-0.88464800
C	1.94954800	1.71736300	0.89334700
C	2.49633800	2.95695700	0.50606500
C	1.71575900	1.47040500	2.25532600
C	2.78023600	3.93266500	1.46053800
H	2.71156000	3.15520900	-0.53805400
C	2.00235400	2.45377200	3.20800700
H	1.32486600	0.50800600	2.56164200
C	2.52758500	3.68423300	2.81378700
H	3.19826100	4.88402600	1.15153800
H	1.81267200	2.25390600	4.25653100
H	2.74476200	4.44609500	3.55361800
C	3.21235500	0.05973700	-1.09201700

C	3.27014900	-0.69633400	-2.27885900
C	4.41185400	0.46347300	-0.48159200
C	4.50112700	-1.01522800	-2.85139400
H	2.34828200	-1.05739000	-2.71975900
C	5.64131100	0.13195600	-1.05635000
H	4.38749000	1.03730700	0.43610900
C	5.68920800	-0.60143000	-2.24291000
H	4.53296700	-1.59755400	-3.76557600
H	6.55992300	0.44826900	-0.57505700
H	6.64500900	-0.85611700	-2.68639500
C	1.93572000	-2.53082900	2.05291100
O	1.02496700	-1.68001800	2.34824700
O	2.18037000	-2.77781100	0.83090300
C	2.67710700	-3.25449800	3.14842400
H	3.66984600	-3.54722400	2.80218600
H	2.74934900	-2.62832000	4.03996000
H	2.12510600	-4.16297400	3.41432000
C	0.81085300	-3.13440900	-2.09019400
O	0.31244100	-1.84932100	-1.80292500
H	1.86581200	-3.26195200	-1.79917900
H	0.73951200	-3.31637200	-3.17590800
H	0.23894700	-3.94285300	-1.59624300

Xace

Zero-point = -2657.161168

Ru	0.46322100	-1.44702300	0.52754400
P	1.58079100	0.32098000	-0.43761000
P	-1.55251900	-0.44708600	0.21417400
C	-1.74304600	0.45293600	-1.40447200
H	-1.68761400	-0.36102900	-2.13552000
H	-2.76276100	0.84933000	-1.42888300
C	0.70850400	0.99310500	-1.94067400
C	-0.73342800	1.56000000	-1.80842000
C	-1.10922100	2.04371200	-3.24588500
H	-0.52219000	2.93703200	-3.49049400
H	-0.85566600	1.27872000	-3.99431600
P	-2.87629700	2.45020500	-3.56210300
H	-2.78379000	3.03068800	-4.85706100
H	-3.43843700	1.18547400	-3.87922700
O	-3.62989100	3.24669800	-2.53641100
H	1.35739900	1.75181400	-2.39181700
H	0.68136500	0.13262600	-2.61573000
C	-0.79420900	2.78060200	-0.86851600
H	-0.57532400	2.51399100	0.16570200
H	-0.05697200	3.53054200	-1.17397400
H	-1.78440100	3.24036600	-0.90385500
C	-2.17919500	0.69407200	1.51642700
C	-3.19342600	1.64316400	1.28419300

C	-1.65059200	0.56463100	2.81370000
C	-3.65962600	2.44558500	2.32701100
H	-3.61618000	1.77343000	0.29455700
C	-2.12661900	1.36713200	3.85398800
H	-0.86321100	-0.15747400	3.00016100
C	-3.12901400	2.30807100	3.61274300
H	-4.43434700	3.17839000	2.13284000
H	-1.71167200	1.25607400	4.84971100
H	-3.49483100	2.93299900	4.41947300
C	-2.94916100	-1.64763300	0.03210800
C	-2.79082500	-2.69514700	-0.89839300
C	-4.13346600	-1.57121100	0.78164300
C	-3.80501900	-3.63630200	-1.07555000
H	-1.86149700	-2.75834400	-1.45751600
C	-5.14250500	-2.52226500	0.60130400
H	-4.27008900	-0.77401600	1.50134200
C	-4.98251600	-3.55266300	-0.32601500
H	-3.67381200	-4.43838400	-1.79369000
H	-6.05240300	-2.45448200	1.18701600
H	-5.76746800	-4.28788300	-0.46222000
C	2.04995600	1.81260800	0.53415400
C	2.67697200	2.91175000	-0.08645300
C	1.76777600	1.87657500	1.90791100
C	2.99472900	4.05258600	0.64887500
H	2.92877400	2.86965900	-1.14042200
C	2.08861400	3.02450700	2.64030200
H	1.31571600	1.02402700	2.39825800
C	2.69521600	4.11292800	2.01408300
H	3.47535700	4.89265900	0.16039000
H	1.86094700	3.06346100	3.69957700
H	2.93900300	5.00276600	2.58305600
C	3.19196800	-0.19952400	-1.17304800
C	3.19411700	-1.08461900	-2.26775800
C	4.42089300	0.20920400	-0.62780900
C	4.39852700	-1.52741700	-2.81447700
H	2.25141900	-1.44980400	-2.65516200
C	5.62300500	-0.24462800	-1.17562700
H	4.44106700	0.88290000	0.21953700
C	5.61576800	-1.10803700	-2.27205400
H	4.38551400	-2.20920400	-3.65760800
H	6.56355000	0.07856500	-0.74376800
H	6.55027000	-1.45708700	-2.69622900
C	2.19653200	-1.91551600	2.38683200
O	1.19027800	-1.15596700	2.60681100
O	2.35912700	-2.40687000	1.22958200
C	3.15236500	-2.24039100	3.50803800
H	2.69598100	-2.98895700	4.16503800
H	4.08409300	-2.64345300	3.10892700



H	3.34849400	-1.34828800	4.10792600
C	0.73226800	-3.39304200	-1.62784800
O	0.26705400	-2.08235700	-1.46078200
H	1.74974400	-3.54889400	-1.23301200
H	0.75353000	-3.64451700	-2.70248300
H	0.07812600	-4.14507100	-1.13784000
H	-0.21196700	-3.13476300	0.85525300
H	-0.50168100	-2.69701100	1.45776800

TSXace

Zero-point = -2657.131395

Ru	0.43057400	-1.60397500	0.09726300
P	1.67228900	0.32036400	-0.33973900
P	-1.52483400	-0.43690000	0.07031500
C	-1.66384600	0.89390000	-1.23289000
H	-1.70976700	0.34483500	-2.18046800
H	-2.62962800	1.38913700	-1.09441700
C	0.84346500	1.40574300	-1.61670600
C	-0.57109900	1.99281600	-1.34214400
C	-0.88964500	2.85902200	-2.60410200
H	-0.25037400	3.74983000	-2.59619500
H	-0.65315100	2.30708800	-3.52604900
P	-2.61881200	3.44024800	-2.83965600
H	-2.45055100	4.30329700	-3.95733900
H	-3.23900700	2.32421600	-3.46553100
O	-3.36196300	4.01163000	-1.66883400
H	1.52648400	2.22484900	-1.86819600
H	0.79870100	0.76459000	-2.50537400
C	-0.58951600	2.92168800	-0.11142500
H	-0.38087600	2.38145600	0.81238300
H	0.16963800	3.70378200	-0.21219800
H	-1.56608200	3.40215500	-0.01426900
C	-2.07167500	0.40212700	1.62634400
C	-3.19269300	1.25393800	1.64228800
C	-1.39800300	0.13851000	2.82978700
C	-3.60976600	1.84923000	2.83172400
H	-3.74814300	1.45438900	0.73333700
C	-1.82727500	0.73287300	4.02114000
H	-0.55058900	-0.53432500	2.83384300
C	-2.92583200	1.59181300	4.02405100
H	-4.46839700	2.51077100	2.82807300
H	-1.30030000	0.51976200	4.94473800
H	-3.25389200	2.05483800	4.94769000
C	-3.06616200	-1.41711700	-0.26651100
C	-4.02597500	-1.08608600	-1.23729900
C	-3.28467800	-2.55516000	0.53409800
C	-5.16713400	-1.87678400	-1.40866200
H	-3.89862100	-0.21652400	-1.86905200

C	-4.42562200	-3.33735400	0.36449000
H	-2.54986200	-2.83090400	1.28281400
C	-5.36989500	-3.00192800	-0.61049500
H	-5.89569200	-1.60780100	-2.16525900
H	-4.57631600	-4.20970500	0.99028200
H	-6.25474800	-3.61309900	-0.74489400
C	2.24959000	1.50786800	0.95114700
C	2.78840700	2.76885800	0.62428000
C	2.16556300	1.14164200	2.30501200
C	3.22301200	3.63784100	1.62513900
H	2.87441400	3.07461200	-0.41212900
C	2.60214500	2.01661000	3.30451100
H	1.75706600	0.17398600	2.56771500
C	3.12854900	3.26374400	2.96888000
H	3.63287100	4.60537100	1.35802200
H	2.52630500	1.72103300	4.34494800
H	3.46319500	3.94187100	3.74540400
C	3.23035100	-0.09765500	-1.24665300
C	3.15269200	-1.10072200	-2.23452100
C	4.46880000	0.51401600	-0.99179600
C	4.28744100	-1.45396000	-2.96594600
H	2.21833900	-1.63222800	-2.39214500
C	5.60038500	0.14994500	-1.72645400
H	4.55624300	1.26345300	-0.21603900
C	5.51150800	-0.82747700	-2.71853000
H	4.21687500	-2.23313400	-3.71685600
H	6.55095500	0.62779500	-1.51686000
H	6.39203600	-1.10921200	-3.28481700
C	2.00130000	-2.58614600	1.85581400
O	1.01915400	-1.82443600	2.17936100
O	2.23523100	-2.78332400	0.62907400
C	2.82551700	-3.24520900	2.93041100
H	2.25918100	-4.08123400	3.35510600
H	3.75805600	-3.62542200	2.51150300
H	3.03127700	-2.53884600	3.73869600
C	-0.70167100	-2.23842000	-2.88346600
O	0.29131900	-2.45268300	-1.90666500
H	-0.60598400	-3.00218100	-3.66856300
H	-0.58212900	-1.25445800	-3.36644100
H	-1.72210500	-2.29684600	-2.48084500
H	-0.17822200	-3.06814500	-0.81952600
H	-0.40140900	-3.18834900	0.12292600

Xlace

Zero-point =

Ru	-0.36236800	1.40039400	0.60817300
P	-1.72811400	-0.30303300	-0.42552700
P	1.61511400	0.44868600	0.03444000

C	1.61710200	-0.81509700	-1.35260100
H	1.58302500	-0.20062800	-2.26150600
H	2.60751100	-1.27830800	-1.33898000
C	-0.87149800	-1.28892000	-1.76425400
C	0.51987000	-1.91042700	-1.45274600
C	0.84690900	-2.80950800	-2.68836600
H	0.18270800	-3.68198800	-2.68089900
H	0.65642600	-2.27109600	-3.62867200
P	2.57105300	-3.43780600	-2.83891100
H	2.41856800	-4.39258000	-3.88102300
H	3.23045400	-2.39003600	-3.53432700
O	3.26976400	-3.92246700	-1.60067200
H	-1.55113600	-2.08696400	-2.08589000
H	-0.75442300	-0.59989700	-2.61003600
C	0.46245300	-2.81717800	-0.20770800
H	0.32383700	-2.23810900	0.70635100
H	-0.37724600	-3.51519400	-0.28740200
H	1.38121200	-3.39754100	-0.10824100
C	2.48796000	-0.38170900	1.43616500
C	3.21225700	-1.58343600	1.32182900
C	2.47582000	0.28543800	2.67649300
C	3.90219700	-2.10014500	2.42261600
H	3.24749200	-2.13953600	0.39274800
C	3.17112200	-0.23405900	3.76862900
H	1.90664400	1.20089800	2.77878900
C	3.88503600	-1.42826600	3.64544000
H	4.45079300	-3.02913300	2.31661500
H	3.15059500	0.29285800	4.71605700
H	4.42206200	-1.83255800	4.49599300
C	2.99571000	1.49430100	-0.64202700
C	2.74362500	2.78416000	-1.13555500
C	4.30590300	0.98324000	-0.72186700
C	3.77289700	3.53694500	-1.71034000
H	1.75787100	3.22379800	-1.05258300
C	5.32896100	1.73818500	-1.29552600
H	4.53368800	0.00665700	-0.31056100
C	5.06391400	3.01605300	-1.79611000
H	3.56022100	4.53372300	-2.08044600
H	6.33342200	1.33265000	-1.34312900
H	5.86103900	3.60297300	-2.23811300
C	-2.60876400	-1.62379200	0.53061400
C	-3.64764400	-2.37737300	-0.04670400
C	-2.21949900	-1.90077100	1.85242900
C	-4.27011200	-3.39457800	0.67711900
H	-3.98102500	-2.15631800	-1.05490200
C	-2.84828100	-2.92029100	2.57347300
H	-1.43255400	-1.31418100	2.31151700
C	-3.86966500	-3.66960700	1.98826200

H	-5.07025000	-3.96774600	0.22219500
H	-2.53728900	-3.12642300	3.59162000
H	-4.35593300	-4.45930900	2.54954100
C	-3.15572400	0.40773900	-1.37182300
C	-3.44528000	0.13522400	-2.71977800
C	-3.99361700	1.30048800	-0.66986800
C	-4.54018500	0.73757600	-3.34919800
H	-2.82727600	-0.54633400	-3.29070000
C	-5.08684500	1.89296800	-1.30077000
H	-3.77076400	1.53950600	0.36512500
C	-5.36284200	1.61478100	-2.64300800
H	-4.74762200	0.51695900	-4.39044500
H	-5.71901900	2.57745800	-0.74629500
H	-6.20978100	2.08081100	-3.13311300
C	-1.60056100	1.47919200	2.82755400
O	-0.58641000	0.72752500	2.61800100
O	-2.05251600	2.17108000	1.86447700
C	-2.20878500	1.55830600	4.20234400
H	-1.76289500	2.40180600	4.74135400
H	-3.28412100	1.73378100	4.12992300
H	-2.00775900	0.64496700	4.76508900
C	-0.90876600	3.14974500	-1.12103500
O	-0.18430600	4.31068900	-0.81602400
H	-1.08323800	3.13131600	-2.20193600
H	-1.87325300	3.07816500	-0.61833700
H	-0.24401200	2.19365200	-1.03667100
H	0.54587400	2.59505600	1.26103800
H	0.01526900	4.25207400	0.13223100

**S11. Cartesian coordinates (Å) and zero-point corrected energies, (Hartrees) of optimized structures of stationary points for the methanol formation in presence of hexanoate anion.**

Ru-H<sub>hex</sub>

Zero-point = -2698.594221

Ru	-0.12625500	-0.95830000	1.01537900
P	-1.06038000	1.11911900	0.22202700
P	1.99508400	-0.48641000	0.40825700
C	2.42803100	1.27103400	-0.08634300
H	2.54523400	1.79801200	0.86865100
H	3.42477700	1.23054600	-0.53379700
C	0.16980500	2.47028000	-0.21017400
C	1.46056600	2.08344500	-0.99048200
C	2.13818100	3.44623300	-1.34354900
H	1.54486600	3.94966600	-2.11612100
H	2.15505700	4.11428900	-0.46962700
P	3.88022200	3.40032500	-1.93556100
H	4.04065400	4.73283600	-2.40395100
H	4.62516000	3.45434000	-0.72740900

O	4.29066000	2.31533000	-2.88992300
H	-0.36457900	3.24628700	-0.77068400
H	0.47455500	2.91241100	0.74626700
C	1.13360500	1.35332000	-2.30764200
H	0.71567500	0.36229200	-2.12064900
H	0.39664400	1.92122300	-2.88495900
H	2.03059200	1.23439800	-2.91849100
C	2.71454700	-1.54969700	-0.91689800
C	3.59234700	-1.09263500	-1.91739000
C	2.38061000	-2.91773800	-0.87874600
C	4.12607800	-1.98865600	-2.84904400
H	3.85932600	-0.04653500	-2.00935000
C	2.92262300	-3.80515600	-1.80812500
H	1.68530300	-3.26949200	-0.12579900
C	3.79728800	-3.34345300	-2.79498300
H	4.79506400	-1.61810000	-3.61731800
H	2.65616100	-4.85525800	-1.76471800
H	4.21388100	-4.03367300	-3.51979500
C	3.25175700	-0.64876500	1.75948100
C	2.80799500	-0.71350500	3.09048500
C	4.63351800	-0.64913900	1.50205600
C	3.72401700	-0.75717300	4.14419600
H	1.74249100	-0.76675000	3.29626600
C	5.54720700	-0.69881300	2.55629500
H	4.99366400	-0.63586700	0.47912000
C	5.09468700	-0.74661100	3.87793900
H	3.36780000	-0.81318500	5.16669900
H	6.61090700	-0.70765400	2.34652500
H	5.80676100	-0.78787200	4.69419000
C	-2.23628800	1.22285000	-1.20879500
C	-3.14481800	2.28654400	-1.35638200
C	-2.19750600	0.21951600	-2.19358900
C	-3.98043500	2.35367700	-2.47268700
H	-3.21136500	3.05159500	-0.59096500
C	-3.03413700	0.29356200	-3.31123900
H	-1.52420600	-0.62109400	-2.07287800
C	-3.92335400	1.36012300	-3.45469800
H	-4.67773300	3.17784600	-2.57440700
H	-2.99271200	-0.48530200	-4.06455400
H	-4.57334300	1.41458600	-4.32045100
C	-2.03725800	1.94927600	1.55955800
C	-2.02579100	3.33088200	1.82479800
C	-2.83865700	1.11396300	2.36570200
C	-2.79281500	3.86218600	2.86542200
H	-1.42216100	4.00101800	1.22448900
C	-3.60650600	1.65143900	3.40028100
H	-2.85388900	0.04542900	2.17615400
C	-3.58387900	3.02496000	3.65427000

H	-2.77179400	4.92916100	3.05777500
H	-4.21711400	0.99515900	4.01028000
H	-4.17618800	3.43950900	4.46184800
C	-1.87206900	-2.54159400	0.11514400
O	-2.10366200	-1.98793200	1.22817700
O	-0.81028800	-2.18898500	-0.52172700
C	-2.72766900	-3.65242200	-0.45229500
H	-2.79293500	-3.51264600	-1.53791400
H	-2.13457300	-4.56588400	-0.30900800
H	0.49874600	-2.30916500	1.67397000
C	-4.11658600	-3.82696300	0.18711400
H	-4.38505600	-4.88841600	0.12797300
H	-4.04321700	-3.58247000	1.25262900
C	-5.24774700	-3.01207200	-0.46170900
H	-6.19636500	-3.31313500	0.00465900
H	-5.33207800	-3.29808100	-1.52113100
C	-5.10990600	-1.48777200	-0.36481700
H	-4.19869700	-1.15918500	-0.87584900
H	-4.98883600	-1.20041100	0.68723200
C	-6.30740900	-0.74633700	-0.96837400
H	-6.17326800	0.33772500	-0.90428700
H	-6.43620500	-0.99951400	-2.02736700
H	-7.23954000	-1.00496800	-0.45168600

lhex

Zero-point = -2887.186152

Ru	-0.39708300	-0.74655300	0.71573500
P	-0.48620100	1.71891000	0.23905300
P	1.81231900	-0.99442900	0.17133000
C	2.85517700	0.55172800	0.29730600
H	2.95538100	0.72450400	1.37499700
H	3.84591400	0.25948100	-0.06090800
C	1.19964100	2.52384600	0.34620200
C	2.41227000	1.87769900	-0.38425400
C	3.57237700	2.91244700	-0.21455000
H	3.35498900	3.79344500	-0.82985500
H	3.63823600	3.25975400	0.82706300
P	5.27684400	2.35788500	-0.63997000
H	5.96660600	3.60048800	-0.65175200
H	5.74297300	1.80702700	0.58301400
O	5.46930200	1.48581000	-1.84745000
H	1.09701400	3.55635700	-0.00714400
H	1.42134800	2.56699100	1.41919200
C	2.13577700	1.71374900	-1.89104600
H	1.34640900	0.98475200	-2.08097900
H	1.80936900	2.66753100	-2.31908400
H	3.03371200	1.38746600	-2.41887600

C	2.15976700	-1.68327600	-1.50027700
C	3.37056400	-1.45180400	-2.18308800
C	1.19568100	-2.52316600	-2.08795500
C	3.60149800	-2.04471400	-3.42544900
H	4.13454700	-0.79950500	-1.77742200
C	1.43868900	-3.11718900	-3.32928000
H	0.25446300	-2.69228700	-1.58172200
C	2.63919600	-2.87939200	-3.99972700
H	4.53353900	-1.84832100	-3.94247400
H	0.68613700	-3.76171300	-3.76940600
H	2.82446100	-3.33754400	-4.96456800
C	2.81834400	-2.09078200	1.26996100
C	2.95847800	-1.76960300	2.63509300
C	3.43132700	-3.25670000	0.78190000
C	3.69901700	-2.59420500	3.48233900
H	2.46518800	-0.89497200	3.04200600
C	4.16937500	-4.07852000	1.63722900
H	3.33419200	-3.52218400	-0.26270700
C	4.30708300	-3.74978400	2.98614200
H	3.79069900	-2.33838900	4.53180100
H	4.63538000	-4.97547800	1.24548100
H	4.87826600	-4.39082500	3.64755800
C	-1.19279200	2.40397000	-1.32297000
C	-1.49928800	3.77006100	-1.46089300
C	-1.41736800	1.54075500	-2.41023800
C	-1.99959800	4.26306900	-2.66620400
H	-1.36949700	4.44224100	-0.61997500
C	-1.91898800	2.04097700	-3.61531400
H	-1.21195800	0.48153700	-2.30606300
C	-2.20623900	3.40026200	-3.74683100
H	-2.23507100	5.31715000	-2.76049900
H	-2.08572900	1.36613400	-4.44740100
H	-2.59636400	3.78606500	-4.68165400
C	-1.40414700	2.66732200	1.53064700
C	-0.98048200	3.91024900	2.03635800
C	-2.59875400	2.10819300	2.02412600
C	-1.73658900	4.57945800	3.00184400
H	-0.05971900	4.36346200	1.69054800
C	-3.35014800	2.78344100	2.98742200
H	-2.92549400	1.13873200	1.66592700
C	-2.92299300	4.01907100	3.47786500
H	-1.39528500	5.53544900	3.38292600
H	-4.26325700	2.33516600	3.36213000
H	-3.50528800	4.53761300	4.23071300
C	-2.62555500	-1.25396800	-0.41866600
O	-2.64464500	-0.85440400	0.78115700
O	-1.48255600	-1.37271200	-0.99454400
C	-3.88823100	-1.55173700	-1.19049400

H	-4.17927600	-0.61920000	-1.69606700
H	-3.63843500	-2.26613100	-1.98224300
H	-0.28533900	-2.32811700	0.90970800
C	-0.37575400	-1.20984500	2.75682400
O	0.24417100	-0.12084200	2.71819300
O	-0.82412400	-2.03440000	3.49442300
C	-5.04319600	-2.05971200	-0.31819400
H	-5.22878200	-1.33591000	0.48296200
H	-4.73758800	-2.98982100	0.17766100
C	-6.32875600	-2.29889500	-1.11855300
H	-6.63055700	-1.36377900	-1.61280600
H	-6.13051500	-3.01768300	-1.92694000
C	-7.49042200	-2.81397900	-0.25934000
H	-7.68745700	-2.09609500	0.54822600
H	-7.18809900	-3.74777600	0.23347400
C	-8.77518900	-3.05024000	-1.05957400
H	-9.58390700	-3.41739300	-0.41922600
H	-9.12190900	-2.12569100	-1.53556800
H	-8.61790300	-3.79000000	-1.85301200

Ts1\_hex

Zero-point = -2887.182099

Ru	-0.24378700	-0.70516700	0.87428800
P	-0.62736500	1.56814400	0.19526400
P	1.93152100	-0.75158600	0.17196200
C	2.78431300	0.87756100	-0.16161300
H	3.03040300	1.26743100	0.83300600
H	3.73673900	0.61889600	-0.63134300
C	0.89921800	2.59832200	-0.14307000
C	2.06135800	1.98533400	-0.97228500
C	3.06313400	3.16309600	-1.19745400
H	2.62499400	3.87187800	-1.91004100
H	3.23503400	3.71647000	-0.26245600
P	4.74571400	2.73596300	-1.81322400
H	5.23885700	4.02276500	-2.16079800
H	5.46568200	2.49057600	-0.61405700
O	4.87748700	1.67320600	-2.86617200
H	0.56755500	3.52403100	-0.62703400
H	1.29091300	2.86841500	0.84456400
C	1.57939600	1.49412800	-2.35064300
H	0.90500700	0.64078200	-2.25964700
H	1.03548200	2.29153300	-2.86773600
H	2.42447100	1.19275800	-2.97252400
C	2.22236300	-1.76224000	-1.34423600
C	3.26631800	-1.51188100	-2.25625500
C	1.38506200	-2.87319200	-1.56109800
C	3.46079400	-2.35355000	-3.35370300
H	3.92542400	-0.65932000	-2.14659400



C	1.59129200	-3.71439500	-2.65650100
H	0.56350900	-3.06127500	-0.88232500
C	2.62832300	-3.45678800	-3.55465200
H	4.26288000	-2.13958700	-4.05054000
H	0.93662700	-4.56519000	-2.80789900
H	2.78457100	-4.10723800	-4.40766200
C	3.18149300	-1.44623000	1.34817000
C	3.32818700	-0.85575400	2.61964700
C	3.98694100	-2.54804000	1.01594100
C	4.26286200	-1.35463200	3.52730400
H	2.68895200	-0.03137100	2.91284900
C	4.91890900	-3.04410500	1.93134800
H	3.88852700	-3.01625600	0.04516100
C	5.06082900	-2.44936900	3.18544900
H	4.35834300	-0.89541800	4.50470000
H	5.53245100	-3.89587600	1.66069100
H	5.78256300	-2.83847600	3.89426000
C	-1.73255500	2.02106200	-1.22008600
C	-2.36215700	3.27784300	-1.28761300
C	-1.93103700	1.10368800	-2.26761600
C	-3.15608000	3.61317700	-2.38500400
H	-2.24887000	3.98457900	-0.47355700
C	-2.72841500	1.44573900	-3.36390400
H	-1.47984900	0.12060300	-2.21231700
C	-3.33837800	2.69956200	-3.42679200
H	-3.63796500	4.58366500	-2.42317500
H	-2.87305900	0.72912400	-4.16467800
H	-3.95799900	2.96160000	-4.27672500
C	-1.38790200	2.52039500	1.58517300
C	-1.03982800	3.84638100	1.90395400
C	-2.37867600	1.87878400	2.35385900
C	-1.66613800	4.51153400	2.96112500
H	-0.28209700	4.37128200	1.33548400
C	-3.00086500	2.54999200	3.40777200
H	-2.65318800	0.85524900	2.12834100
C	-2.64681500	3.86524400	3.71513500
H	-1.38529900	5.53256900	3.19410100
H	-3.75606700	2.03835400	3.99348100
H	-3.12777900	4.38127200	4.53803100
C	-2.43791700	-1.57991800	-0.08611600
O	-2.43471100	-1.07191700	1.07879500
O	-1.33886500	-1.58608200	-0.74362300
C	-3.69119000	-2.17435000	-0.67958600
H	-3.48610300	-2.43813400	-1.72195800
H	-3.88796500	-3.10795500	-0.13756500
H	0.10802000	-2.21410800	1.45671200
C	-0.05816100	-1.54508600	2.93658800
O	0.29937800	-0.35086500	2.96075200

O	-0.35467200	-2.46963600	3.63069000
C	-4.90558600	-1.23392100	-0.57491200
H	-4.66701900	-0.29880100	-1.09581500
H	-5.05976300	-0.97409900	0.47857700
C	-6.19859200	-1.82016400	-1.16312200
H	-6.95912500	-1.02778100	-1.18019100
H	-6.03052500	-2.09814600	-2.21391900
C	-6.76645100	-3.02744400	-0.40338300
H	-6.04151800	-3.85137300	-0.40950900
H	-6.90627700	-2.75417100	0.65140900
C	-8.09418600	-3.52549700	-0.98407800
H	-7.97846300	-3.83525000	-2.02919300
H	-8.47950200	-4.38393100	-0.42423800
H	-8.85812400	-2.73992500	-0.95654400

llhex

Zero-point = -2887.203337

Ru	0.26572800	-0.71158800	-0.88033700
P	0.52278100	1.33391500	-0.08755600
P	-1.84190300	-0.85647600	-0.06415500
C	-2.87124600	0.67185000	-0.29536900
H	-2.95589300	0.74712300	-1.38496200
H	-3.87039500	0.46626200	0.10018300
C	-0.97296700	2.41175900	-0.36341600
C	-2.34351200	2.02315000	0.26373500
C	-3.33060000	3.14317300	-0.19615600
H	-3.08091800	4.07831800	0.31906000
H	-3.23135400	3.33346900	-1.27460100
P	-5.12566400	2.83269100	0.07420400
H	-5.66472300	4.11142900	-0.23359400
H	-5.49647200	2.10050300	-1.08385200
O	-5.55943500	2.22983600	1.37944800
H	-0.70777400	3.42717900	-0.04768800
H	-1.08134200	2.42129600	-1.45188900
C	-2.28989300	2.04131700	1.80481600
H	-1.64336900	1.25950600	2.20422500
H	-1.89545100	3.00066600	2.15635800
H	-3.29041100	1.91084800	2.22281000
C	-2.11620400	-1.42443900	1.66441800
C	-3.29372500	-1.14483700	2.38327700
C	-1.13123200	-2.23682700	2.25657300
C	-3.47168700	-1.65663600	3.66990700
H	-4.07235100	-0.52364900	1.95645300
C	-1.32023100	-2.75143500	3.54165700
H	-0.22187000	-2.46184400	1.71068200
C	-2.48720200	-2.46032300	4.25065100
H	-4.37929600	-1.42634800	4.21573100
H	-0.55538100	-3.37899100	3.98562800

H	-2.63086300	-2.85709600	5.24912600
C	-2.81230200	-2.09655100	-1.03668600
C	-2.91105000	-1.94104300	-2.43544000
C	-3.42424300	-3.20717400	-0.42909200
C	-3.61712200	-2.87241700	-3.19807500
H	-2.41879800	-1.10514400	-2.91891300
C	-4.12451700	-4.13624100	-1.20204900
H	-3.35876500	-3.34357200	0.64256300
C	-4.22403700	-3.97126100	-2.58468800
H	-3.68497500	-2.74020900	-4.27200700
H	-4.59307300	-4.98718600	-0.72069400
H	-4.76798300	-4.69510100	-3.18063800
C	1.02138400	1.62005700	1.65927200
C	1.16289600	2.93095700	2.15616000
C	1.26268500	0.53394700	2.51411800
C	1.51724100	3.14488100	3.48714200
H	1.01193500	3.78122500	1.50000500
C	1.61808300	0.75574400	3.84879500
H	1.18454000	-0.47436100	2.12923700
C	1.73979900	2.05635600	4.33746400
H	1.62210000	4.15689900	3.86122300
H	1.79664000	-0.09057000	4.50230100
H	2.01141800	2.22563100	5.37301900
C	1.82424100	2.24190100	-1.02755700
C	1.57915100	2.68517100	-2.34126600
C	3.11015000	2.41106700	-0.48218500
C	2.59351400	3.29555500	-3.08028700
H	0.61306000	2.53303900	-2.80527300
C	4.12071300	3.01836200	-1.22917900
H	3.31932600	2.07301600	0.52539800
C	3.86479500	3.46396000	-2.52744900
H	2.38949400	3.62657900	-4.09197100
H	5.10653700	3.14275100	-0.79547800
H	4.65150300	3.93350600	-3.10652700
C	2.49157300	-1.88330000	-0.46430400
O	2.32033500	-1.22125200	-1.53622000
O	1.54630200	-1.89775800	0.40471700
C	3.79071100	-2.60129500	-0.19781800
H	3.63965600	-3.31233500	0.61998200
H	4.06095000	-3.16112800	-1.10037600
H	0.96325600	-0.46590500	-3.68933800
C	0.00505200	0.09474100	-3.71919600
O	-0.61532500	0.17156900	-2.56049100
O	-0.41564600	0.58925500	-4.75250200
C	4.92160100	-1.61081500	0.14800300
H	4.63942900	-1.04478900	1.04603500
H	5.01394800	-0.88315500	-0.66674100
C	6.26679200	-2.30751800	0.38366900

H	6.54338600	-2.87550900	-0.51593600
H	6.15961700	-3.04747400	1.18978600
C	7.39940400	-1.33495400	0.73672300
H	7.12093700	-0.76696700	1.63496200
H	7.50450400	-0.59626100	-0.06931400
C	8.74304800	-2.03317500	0.96955000
H	9.06492800	-2.58081400	0.07647300
H	9.52992800	-1.31406600	1.21963200
H	8.67788700	-2.75424500	1.79245900

Ilhex at T = 160°C

Zero-point = -2887.203337

Ru	0.26572800	-0.71158800	-0.88033700
P	0.52278100	1.33391500	-0.08755600
P	-1.84190300	-0.85647600	-0.06415500
C	-2.87124600	0.67185000	-0.29536900
H	-2.95589300	0.74712300	-1.38496200
H	-3.87039500	0.46626200	0.10018300
C	-0.97296700	2.41175900	-0.36341600
C	-2.34351200	2.02315000	0.26373500
C	-3.33060000	3.14317300	-0.19615600
H	-3.08091800	4.07831800	0.31906000
H	-3.23135400	3.33346900	-1.27460100
P	-5.12566400	2.83269100	0.07420400
H	-5.66472300	4.11142900	-0.23359400
H	-5.49647200	2.10050300	-1.08385200
O	-5.55943500	2.22983600	1.37944800
H	-0.70777400	3.42717900	-0.04768800
H	-1.08134200	2.42129600	-1.45188900
C	-2.28989300	2.04131700	1.80481600
H	-1.64336900	1.25950600	2.20422500
H	-1.89545100	3.00066600	2.15635800
H	-3.29041100	1.91084800	2.22281000
C	-2.11620400	-1.42443900	1.66441800
C	-3.29372500	-1.14483700	2.38327700
C	-1.13123200	-2.23682700	2.25657300
C	-3.47168700	-1.65663600	3.66990700
H	-4.07235100	-0.52364900	1.95645300
C	-1.32023100	-2.75143500	3.54165700
H	-0.22187000	-2.46184400	1.71068200
C	-2.48720200	-2.46032300	4.25065100
H	-4.37929600	-1.42634800	4.21573100
H	-0.55538100	-3.37899100	3.98562800
H	-2.63086300	-2.85709600	5.24912600
C	-2.81230200	-2.09655100	-1.03668600
C	-2.91105000	-1.94104300	-2.43544000
C	-3.42424300	-3.20717400	-0.42909200
C	-3.61712200	-2.87241700	-3.19807500

H	-2.41879800	-1.10514400	-2.91891300
C	-4.12451700	-4.13624100	-1.20204900
H	-3.35876500	-3.34357200	0.64256300
C	-4.22403700	-3.97126100	-2.58468800
H	-3.68497500	-2.74020900	-4.27200700
H	-4.59307300	-4.98718600	-0.72069400
H	-4.76798300	-4.69510100	-3.18063800
C	1.02138400	1.62005700	1.65927200
C	1.16289600	2.93095700	2.15616000
C	1.26268500	0.53394700	2.51411800
C	1.51724100	3.14488100	3.48714200
H	1.01193500	3.78122500	1.50000500
C	1.61808300	0.75574400	3.84879500
H	1.18454000	-0.47436100	2.12923700
C	1.73979900	2.05635600	4.33746400
H	1.62210000	4.15689900	3.86122300
H	1.79664000	-0.09057000	4.50230100
H	2.01141800	2.22563100	5.37301900
C	1.82424100	2.24190100	-1.02755700
C	1.57915100	2.68517100	-2.34126600
C	3.11015000	2.41106700	-0.48218500
C	2.59351400	3.29555500	-3.08028700
H	0.61306000	2.53303900	-2.80527300
C	4.12071300	3.01836200	-1.22917900
H	3.31932600	2.07301600	0.52539800
C	3.86479500	3.46396000	-2.52744900
H	2.38949400	3.62657900	-4.09197100
H	5.10653700	3.14275100	-0.79547800
H	4.65150300	3.93350600	-3.10652700
C	2.49157300	-1.88330000	-0.46430400
O	2.32033500	-1.22125200	-1.53622000
O	1.54630200	-1.89775800	0.40471700
C	3.79071100	-2.60129500	-0.19781800
H	3.63965600	-3.31233500	0.61998200
H	4.06095000	-3.16112800	-1.10037600
H	0.96325600	-0.46590500	-3.68933800
C	0.00505200	0.09474100	-3.71919600
O	-0.61532500	0.17156900	-2.56049100
O	-0.41564600	0.58925500	-4.75250200
C	4.92160100	-1.61081500	0.14800300
H	4.63942900	-1.04478900	1.04603500
H	5.01394800	-0.88315500	-0.66674100
C	6.26679200	-2.30751800	0.38366900
H	6.54338600	-2.87550900	-0.51593600
H	6.15961700	-3.04747400	1.18978600
C	7.39940400	-1.33495400	0.73672300
H	7.12093700	-0.76696700	1.63496200
H	7.50450400	-0.59626100	-0.06931400

C	8.74304800	-2.03317500	0.96955000
H	9.06492800	-2.58081400	0.07647300
H	9.52992800	-1.31406600	1.21963200
H	8.67788700	-2.75424500	1.79245900

Illhex

Zero-point = -2888.378165

Ru	0.20389800	-1.06509000	-0.65426900
P	0.64822400	1.18393900	-0.33431100
P	-1.94989200	-0.82501000	0.08403300
C	-2.79016300	0.74483800	-0.45611300
H	-2.86335200	0.62256900	-1.54195400
H	-3.80647800	0.70703700	-0.05274000
C	-0.76744000	2.28352200	-0.83922500
C	-2.15158400	2.12644200	-0.14872700
C	-3.05515500	3.21984300	-0.80462800
H	-2.72879000	4.20869300	-0.46141700
H	-2.95040800	3.20894500	-1.89916700
P	-4.86673700	3.10345000	-0.49415600
H	-5.30602300	4.35148000	-1.01374500
H	-5.30513700	2.22018000	-1.51528700
O	-5.33687700	2.76291300	0.89105900
H	-0.42739500	3.31998900	-0.73687200
H	-0.88725900	2.07747500	-1.90645000
C	-2.07798200	2.41811800	1.36347400
H	-1.49354100	1.66996300	1.89949200
H	-1.60128700	3.38864600	1.53723600
H	-3.08057900	2.44635600	1.79567000
C	-2.27199600	-0.99329800	1.88743000
C	-3.43360400	-0.48962800	2.50449500
C	-1.34277500	-1.71011000	2.66324300
C	-3.65046000	-0.69331000	3.86816900
H	-4.16703200	0.07172700	1.93719800
C	-1.57062500	-1.91556300	4.02668100
H	-0.44211100	-2.09643500	2.19980200
C	-2.72154800	-1.40695600	4.63070300
H	-4.54391600	-0.29252900	4.33270300
H	-0.84757600	-2.47169100	4.61304900
H	-2.89549400	-1.56342800	5.68913600
C	-3.12370600	-2.05536200	-0.64495800
C	-3.20478700	-2.15687700	-2.04919000
C	-3.91051000	-2.90821300	0.14649400
C	-4.06017400	-3.08749500	-2.63946900
H	-2.58440000	-1.52031300	-2.66986900
C	-4.76109300	-3.84119100	-0.45351400
H	-3.86363300	-2.84316600	1.22598200
C	-4.83935800	-3.93221500	-1.84369100
H	-4.11272900	-3.15454700	-3.72033600

H	-5.36256200	-4.49388900	0.16904600
H	-5.50054300	-4.65673500	-2.30498100
C	1.18853000	1.83644700	1.29784600
C	1.47104000	3.20732900	1.46179500
C	1.29773800	0.98006700	2.40464500
C	1.83724800	3.70806500	2.70997100
H	1.42002800	3.87764000	0.61077700
C	1.66555200	1.48900800	3.65463100
H	1.10987200	-0.07836400	2.28118400
C	1.93013200	2.84937200	3.81056100
H	2.05156400	4.76443200	2.82534800
H	1.74195700	0.81864200	4.50321400
H	2.21160900	3.24175500	4.78094700
C	1.98423100	1.76297700	-1.46581800
C	1.74297800	1.89550700	-2.84648600
C	3.28433900	1.98914400	-0.97878100
C	2.77754900	2.25953800	-3.71011300
H	0.76643500	1.68480700	-3.26262700
C	4.31361400	2.35043100	-1.84948900
H	3.49171300	1.88763500	0.07932800
C	4.06293800	2.48896600	-3.21585900
H	2.57513200	2.34993000	-4.77105000
H	5.31017200	2.52191400	-1.45839000
H	4.86401600	2.76748500	-3.89081200
C	2.47012200	-1.92422900	0.18749800
O	2.35560000	-1.52503700	-1.01119200
O	1.44707200	-1.84740100	0.95730600
C	3.77724400	-2.48149000	0.70033600
H	3.65926500	-2.72662700	1.76013000
H	3.96780900	-3.41973500	0.16239200
H	0.63571100	-1.65527100	-3.53234000
C	-0.07050700	-0.80067000	-3.63236800
O	-0.56406700	-0.36735700	-2.49791200
O	-0.34041500	-0.32753700	-4.72513400
H	0.05845700	-2.71992200	-1.43911700
H	-0.27620900	-2.83739300	-0.72352100
C	4.95828600	-1.52039400	0.47916400
H	4.99615900	-1.24738600	-0.58105700
H	4.77209300	-0.59043600	1.03346700
C	6.29963400	-2.11789400	0.91933400
H	6.48335100	-3.04693600	0.36067500
H	6.24423900	-2.40695800	1.97885100
C	7.48400100	-1.16417700	0.71709800
H	7.53573200	-0.87355000	-0.34079800
H	7.30102100	-0.23740600	1.27806300
C	8.82474000	-1.76655600	1.14904600
H	9.05231500	-2.67527400	0.58016500
H	9.64891600	-1.06264300	0.99367500

H 8.81428000 -2.03695100 2.21122900

TSIIIhex

Zero-point = -2888.376998

Ru	0.32194500	-0.98910000	-0.46519200
P	0.57420900	1.34449700	-0.54050500
P	-1.86744000	-0.85825000	0.11397000
C	-2.82020600	0.58700800	-0.59668300
H	-2.87772300	0.37338400	-1.66968400
H	-3.83885100	0.50938400	-0.20606600
C	-0.94292700	2.25725700	-1.14667900
C	-2.29852400	2.03783100	-0.41452200
C	-3.30140800	3.00147000	-1.12765400
H	-3.05261900	4.03600300	-0.86299500
H	-3.21175500	2.92251800	-2.22141000
P	-5.09524600	2.76843700	-0.78518400
H	-5.63285000	3.92726400	-1.41008000
H	-5.46510100	1.76867000	-1.72425900
O	-5.53835500	2.51512300	0.62627200
H	-0.71075500	3.32800800	-1.15786400
H	-1.06067200	1.94919700	-2.19144100
C	-2.22531900	2.44751800	1.06990200
H	-1.56337400	1.79667200	1.64143500
H	-1.83853300	3.46779900	1.16197800
H	-3.21734500	2.41108400	1.52539800
C	-2.29714800	-0.86761300	1.90806000
C	-3.55448100	-0.45703400	2.39221000
C	-1.34087400	-1.35273800	2.81814100
C	-3.83936900	-0.52179600	3.75649500
H	-4.31356000	-0.07261700	1.72112500
C	-1.63722000	-1.42188000	4.18291600
H	-0.36875100	-1.66464200	2.45601500
C	-2.88283500	-1.00542700	4.65399400
H	-4.80714500	-0.19201400	4.11637800
H	-0.89170300	-1.80042100	4.87356300
H	-3.10953500	-1.05500200	5.71297200
C	-2.93711700	-2.23373700	-0.52353700
C	-3.23171600	-2.32536400	-1.89752000
C	-3.40474600	-3.24589600	0.33179600
C	-3.97995200	-3.39239700	-2.39640600
H	-2.86130100	-1.57312800	-2.58432200
C	-4.14800700	-4.31526700	-0.17277600
H	-3.18943700	-3.19700900	1.39174100
C	-4.44033100	-4.39100600	-1.53533700
H	-4.19866100	-3.44639000	-3.45717700
H	-4.50000400	-5.08722800	0.50215300
H	-5.01890500	-5.22096400	-1.92395600
C	1.07764300	2.34120100	0.93035000



C	1.24798200	3.73714300	0.84249300
C	1.25390900	1.71222900	2.17344900
C	1.57344000	4.48380900	1.97420900
H	1.14194200	4.23700900	-0.11423500
C	1.58030500	2.46635100	3.30561100
H	1.14648300	0.63712100	2.24507000
C	1.73598000	3.84905800	3.21013600
H	1.70144300	5.55745900	1.89385700
H	1.70977900	1.96899500	4.26032900
H	1.98555500	4.43157200	4.08959200
C	1.81584000	1.87582900	-1.80635300
C	1.53638700	1.71327000	-3.17675200
C	3.08790800	2.34309800	-1.43146500
C	2.49310900	2.03440800	-4.14030500
H	0.58518900	1.30161000	-3.49082200
C	4.04469000	2.65536500	-2.39968000
H	3.33018100	2.46629800	-0.38329800
C	3.74938200	2.50845700	-3.75562600
H	2.25977300	1.90603800	-5.19156600
H	5.02060900	3.01327000	-2.09140200
H	4.49258800	2.75352300	-4.50553700
C	2.55425000	-1.48225100	0.66752700
O	2.52003200	-1.32349500	-0.58817100
O	1.47113900	-1.31402600	1.33437200
C	3.81929000	-1.89633000	1.38467500
H	3.77884100	-2.99013300	1.49152300
H	3.77965600	-1.49014800	2.40153500
H	-0.19198600	-1.99014000	-4.26638300
C	-0.04445600	-1.99391700	-3.17871800
O	-0.23660100	-0.91490600	-2.55529800
O	0.30003700	-3.09797200	-2.65259300
H	0.29564200	-2.87175800	-1.46456700
H	0.18587900	-2.69955200	-0.42578500
C	5.10941800	-1.48854000	0.66423500
H	5.08251400	-1.88031900	-0.35833100
H	5.13958400	-0.39526800	0.56852100
C	6.37207300	-1.97757300	1.38343500
H	6.33914100	-3.07316100	1.47381200
H	6.38393200	-1.59005300	2.41274100
C	7.67034400	-1.56892100	0.67592900
H	7.70337700	-0.47445700	0.58666100
H	7.65744600	-1.95569900	-0.35193100
C	8.93132000	-2.06162000	1.39299500
H	8.94397500	-3.15520900	1.46599900
H	9.83961900	-1.75386700	0.86437000
H	8.98914200	-1.66331000	2.41263500

IVhex

Zero-point = -2888.375896

Ru	-0.11394400	-0.79623200	0.87549300
P	-0.71936900	1.40909400	0.19106100
P	2.00724200	-0.66254000	0.10043900
C	2.72578700	1.02813900	-0.26042100
H	2.96597200	1.45077200	0.72138300
H	3.68237300	0.85215700	-0.75886700
C	0.69369600	2.57699300	-0.19497800
C	1.88660000	2.06563700	-1.05174600
C	2.77253800	3.32821100	-1.30216100
H	2.25808000	3.99037600	-2.00865400
H	2.91101100	3.90085400	-0.37290300
P	4.47647300	3.06012100	-1.94517100
H	4.84682900	4.39217200	-2.27716100
H	5.23165100	2.86599800	-0.75772200
O	4.69488000	2.03061800	-3.01609800
H	0.26907700	3.46639200	-0.67495000
H	1.08704500	2.88881800	0.78014400
C	1.42439700	1.52626800	-2.41879700
H	0.82766700	0.61912100	-2.31096600
H	0.80503700	2.26983200	-2.93126400
H	2.28306900	1.29459300	-3.05249400
C	2.38191300	-1.65874800	-1.41029100
C	3.41611900	-1.34851200	-2.31436500
C	1.61130600	-2.81581800	-1.63326800
C	3.66807700	-2.17710300	-3.40982800
H	4.02089000	-0.45731200	-2.20060400
C	1.87543200	-3.64430800	-2.72657000
H	0.79594900	-3.04655400	-0.95992800
C	2.90311800	-3.32739600	-3.61640300
H	4.46054200	-1.91629600	-4.10183800
H	1.27173900	-4.53124000	-2.88353400
H	3.10355900	-3.96734200	-4.46825900
C	3.32473200	-1.25031500	1.27142300
C	3.58916600	-0.52246600	2.44860700
C	4.03156800	-2.44334800	1.04752300
C	4.53798300	-0.97322300	3.36747400
H	3.04080300	0.38934300	2.65793400
C	4.97622100	-2.89396700	1.97310500
H	3.84414200	-3.01865200	0.14975200
C	5.23408000	-2.16155500	3.13261100
H	4.73196400	-0.39864200	4.26670800
H	5.51240900	-3.81694800	1.78323600
H	5.96941900	-2.51233400	3.84743100
C	-1.85965100	1.71393800	-1.24055100
C	-2.55238800	2.93087900	-1.38209100
C	-2.01955200	0.72367500	-2.22595800
C	-3.37087900	3.15606100	-2.48942700

H	-2.46801400	3.69388500	-0.61641700
C	-2.84238500	0.95454800	-3.33279600
H	-1.51558800	-0.22851400	-2.11393400
C	-3.51559400	2.16939500	-3.46887900
H	-3.90062000	4.09743100	-2.58435500
H	-2.95572700	0.18206100	-4.08540600
H	-4.15396800	2.34555500	-4.32718300
C	-1.59176900	2.35372200	1.52523600
C	-1.33623000	3.69862900	1.84606000
C	-2.58042100	1.66282100	2.25437400
C	-2.04995000	4.33634300	2.86551700
H	-0.58258500	4.26090300	1.30865200
C	-3.29267300	2.30600700	3.26732400
H	-2.77708900	0.62006600	2.03017300
C	-3.02953600	3.64301800	3.57708000
H	-1.83914600	5.37393100	3.10009600
H	-4.04981500	1.75924000	3.81850800
H	-3.58166500	4.13886600	4.36727000
C	-2.25246400	-1.94508400	0.08056800
O	-2.24555800	-1.39457800	1.22574700
O	-1.20333600	-1.85487300	-0.64486400
C	-3.46363600	-2.69785900	-0.41845200
H	-3.27334800	-3.01037000	-1.44978100
H	-3.55762700	-3.60854900	0.18880200
H	0.61101500	-0.28292400	4.77586200
C	0.45364800	-0.69153500	3.77315800
O	0.43016600	0.06757000	2.78957600
O	0.30309900	-1.97735700	3.72828300
H	0.29151600	-2.33959300	1.38774000
H	0.22638100	-2.21189300	2.70788600
C	-4.76129000	-1.87877500	-0.31835500
H	-4.89287100	-1.55338500	0.71989500
H	-4.65671800	-0.96717700	-0.92118300
C	-5.99578600	-2.66172400	-0.78021400
H	-6.09305600	-3.57706300	-0.17842800
H	-5.85150500	-2.99570600	-1.81795900
C	-7.29657600	-1.85410600	-0.68616400
H	-7.44024300	-1.52171200	0.35086400
H	-7.19739800	-0.93929300	-1.28597700
C	-8.52931700	-2.63796800	-1.14768600
H	-8.67457200	-3.54062500	-0.54304300
H	-9.44033400	-2.03550600	-1.06887600
H	-8.42964700	-2.95454700	-2.19239000

TSIVhex

Zero-point = -2888.345428

Ru	0.46242900	-0.83275400	-0.48340000
P	0.36854300	1.52430700	-0.45944600

P	-1.71746500	-1.01679500	0.10010100
C	-2.85486700	0.21772200	-0.72229400
H	-2.80925600	-0.05104600	-1.78301600
H	-3.86818000	-0.00657100	-0.37545000
C	-1.22180800	2.14844500	-1.21975800
C	-2.58735700	1.74183200	-0.59377800
C	-3.65905400	2.48592800	-1.45426400
H	-3.60140000	3.56107100	-1.24649200
H	-3.45553800	2.35784500	-2.52782200
P	-5.41856800	1.98945400	-1.24559400
H	-6.06354400	2.99122000	-2.02235000
H	-5.53399400	0.87058100	-2.11329900
O	-5.95565200	1.78291900	0.14043500
H	-1.16840100	3.24093900	-1.28681600
H	-1.17684000	1.77298700	-2.24916400
C	-2.72451700	2.23005200	0.86202600
H	-2.00902100	1.74318900	1.52537300
H	-2.54177900	3.30797200	0.91986700
H	-3.73121500	2.03268100	1.23741600
C	-2.16881900	-0.97047600	1.88561000
C	-3.49957100	-0.80783600	2.31780200
C	-1.15468000	-1.14428800	2.84332900
C	-3.80241700	-0.80519100	3.67912500
H	-4.30275100	-0.67482700	1.60227300
C	-1.46789400	-1.14718200	4.20653600
H	-0.12930800	-1.27391400	2.51868100
C	-2.78723000	-0.97469800	4.62586800
H	-4.82891800	-0.66860800	3.99926900
H	-0.67769500	-1.28359500	4.93659900
H	-3.02700800	-0.97200300	5.68310700
C	-2.55153800	-2.58355900	-0.44357000
C	-2.85867800	-2.79964500	-1.80235800
C	-2.81331200	-3.61519300	0.47581200
C	-3.42391700	-4.00660800	-2.22050200
H	-2.63244600	-2.03677500	-2.53802300
C	-3.37248900	-4.82211600	0.05082600
H	-2.58562900	-3.47114400	1.52471500
C	-3.68330100	-5.02045500	-1.29591100
H	-3.65734700	-4.15386600	-3.26922300
H	-3.57012000	-5.60438800	0.77500600
H	-4.12246500	-5.95611100	-1.62218400
C	0.59722200	2.57462700	1.04022300
C	0.32258700	3.95687800	1.04136700
C	1.06380400	1.97684300	2.22347200
C	0.50452900	4.71621000	2.19729100
H	-0.02899700	4.44412800	0.13895000
C	1.24371900	2.74286000	3.37953200
H	1.28311400	0.91575200	2.23046900

C	0.96360700	4.10925500	3.37027600
H	0.28714200	5.77833600	2.18442600
H	1.59994800	2.26725800	4.28649000
H	1.10028200	4.70028100	4.26859100
C	1.58663500	2.23121000	-1.66038300
C	1.71236600	1.58829000	-2.90884900
C	2.39732500	3.34393900	-1.38342700
C	2.60875700	2.07256300	-3.86167000
H	1.13855700	0.69017300	-3.11443600
C	3.29811500	3.81781800	-2.34143900
H	2.33512100	3.83602400	-0.42143900
C	3.40121500	3.18927800	-3.58286300
H	2.69983700	1.56417600	-4.81506600
H	3.92060300	4.67568600	-2.11229300
H	4.10247200	3.55801300	-4.32288800
C	2.75608400	-0.97991000	0.66453100
O	1.65407800	-1.01709600	1.32232200
O	2.70776800	-0.84635700	-0.59129200
C	4.07095100	-1.05137200	1.41079500
H	3.91351800	-1.64394800	2.31884800
H	4.30006200	-0.02947100	1.74747300
C	0.30248700	-2.25760200	-2.27093600
O	1.50034400	-2.54658700	-2.88040600
O	-0.17159900	-1.07923300	-2.52221100
H	-0.40404100	-3.09814600	-2.24890200
H	1.81991100	-3.40142500	-2.55858000
H	0.56973500	-2.49519200	-0.73004400
C	5.23505800	-1.59730000	0.57639900
H	5.31116000	-1.01430700	-0.34773700
H	5.00656500	-2.62642800	0.26894900
C	6.57065800	-1.57153000	1.32884300
H	6.48013700	-2.14679900	2.26191900
H	6.79793000	-0.53890000	1.63163500
C	7.74167600	-2.12486100	0.50691500
H	7.51568800	-3.15702600	0.20629400
H	7.83016000	-1.55097700	-0.42529900
C	9.07671500	-2.09197600	1.25762900
H	9.02905700	-2.68544300	2.17804400
H	9.89112700	-2.49351000	0.64557900
H	9.34735200	-1.06806400	1.54021300

Vhex

Zero-point = -2888.361105

Ru	0.53666100	-0.63957700	-0.38713200
P	0.17110700	1.57375200	-0.41719100
P	-1.62924300	-1.08664700	0.08084400
C	-2.87919600	-0.01934400	-0.79909400
H	-2.76851700	-0.30698700	-1.85040500

H	-3.87103700	-0.35200500	-0.47841200
C	-1.42960400	2.04871800	-1.25400200
C	-2.78080100	1.52497000	-0.69182500
C	-3.87629700	2.14118700	-1.61931100
H	-3.94043900	3.21984700	-1.43285200
H	-3.60794300	2.01556800	-2.67865900
P	-5.58168500	1.46273200	-1.47726300
H	-6.29636400	2.38028700	-2.29533100
H	-5.53901500	0.32712900	-2.32901900
O	-6.14929600	1.21707800	-0.10969000
H	-1.46386100	3.14212300	-1.31878200
H	-1.30089200	1.67979800	-2.27837700
C	-3.03853900	2.02205500	0.74479900
H	-2.31685800	1.61636900	1.45453300
H	-2.96031300	3.11330700	0.78838000
H	-4.04115200	1.73773100	1.07196900
C	-2.15485600	-1.11016200	1.84649100
C	-3.50555000	-1.04603900	2.23967700
C	-1.16193900	-1.24638500	2.83317900
C	-3.84927900	-1.10341800	3.59064100
H	-4.29428500	-0.94226200	1.50367300
C	-1.51490600	-1.31110900	4.18443000
H	-0.11980100	-1.29949700	2.53980400
C	-2.85541200	-1.23630000	4.56486600
H	-4.89186700	-1.04264900	3.88070300
H	-0.74041200	-1.41903400	4.93569900
H	-3.12731100	-1.28117800	5.61328800
C	-2.19992500	-2.74852800	-0.50833700
C	-2.26217200	-3.01062500	-1.89262100
C	-2.53367100	-3.77576100	0.39065300
C	-2.66350700	-4.26385800	-2.35705600
H	-1.95770100	-2.24573000	-2.59796500
C	-2.92695700	-5.03043200	-0.08214000
H	-2.49377400	-3.59458500	1.45725800
C	-2.99762600	-5.27647500	-1.45392600
H	-2.70737300	-4.45100800	-3.42424700
H	-3.18187100	-5.81220300	0.62439100
H	-3.30622700	-6.24979500	-1.81752300
C	0.23166100	2.62275900	1.09817900
C	-0.13833900	3.98249100	1.07495500
C	0.66244800	2.05736000	2.30960900
C	-0.08998000	4.74983200	2.23855500
H	-0.45585500	4.44623000	0.14777600
C	0.70779500	2.83161900	3.47344400
H	0.96713700	1.01822800	2.33234500
C	0.32947300	4.17375000	3.44178900
H	-0.37912700	5.79425800	2.20793400
H	1.03771100	2.38132500	4.40286300

H	0.36176500	4.77078000	4.34587300
C	1.38274100	2.38887000	-1.55047200
C	1.54096400	1.83815400	-2.83901500
C	2.16652100	3.49255900	-1.17743200
C	2.44836900	2.40291800	-3.73559800
H	0.99072600	0.94267600	-3.11356600
C	3.07702400	4.04766600	-2.08109100
H	2.07154100	3.91699900	-0.18618100
C	3.21580400	3.50948100	-3.36100400
H	2.56571400	1.96758000	-4.72177400
H	3.67827900	4.89844600	-1.78039700
H	3.92410000	3.94173100	-4.05866500
C	2.84703400	-0.70436200	0.76510200
O	1.76966600	-0.81179800	1.44275200
O	2.76472600	-0.49724100	-0.48988300
C	4.18947000	-0.78236900	1.45620200
H	4.05535600	-1.33492600	2.39187700
H	4.46050400	0.24588500	1.73734100
C	0.86558600	-2.17081900	-2.27977900
O	2.17401600	-2.16387300	-2.77608700
O	0.16064100	-1.01403600	-2.40117500
H	0.36087200	-3.04140300	-2.72289800
H	2.65107800	-1.46007900	-2.30531300
H	0.91434900	-2.47243000	-1.13972500
C	5.30251800	-1.39300700	0.59485100
H	5.37232100	-0.83207800	-0.34352400
H	5.02420300	-2.41879600	0.31944800
C	6.66267900	-1.40316300	1.30238400
H	6.58118700	-1.95657300	2.24923300
H	6.93865500	-0.37426900	1.57613800
C	7.78286000	-2.01754400	0.45337100
H	7.86266800	-1.46478600	-0.49232000
H	7.50665600	-3.04502500	0.18061300
C	9.14226300	-2.02361100	1.15965500
H	9.10227200	-2.59831800	2.09221900
H	9.91920700	-2.46807100	0.52900300
H	9.46199800	-1.00629900	1.41344500

Vlhex

Zero-point = -2889.533494

Ru	0.30711900	-1.04954900	-0.29461400
P	0.50456300	1.22707300	-0.58387600
P	-1.88873600	-0.86843200	0.23752800
C	-2.83936800	0.37657100	-0.77283300
H	-2.81123200	-0.05894100	-1.77731100
H	-3.87678300	0.33632800	-0.42689600
C	-0.94917800	1.96819400	-1.48037000
C	-2.36952500	1.85347900	-0.85708900

C	-3.31076200	2.59343500	-1.86118200
H	-3.11183900	3.67075700	-1.81376800
H	-3.10773900	2.27528200	-2.89423700
P	-5.12390400	2.36493200	-1.64012700
H	-5.62330400	3.32347300	-2.56421000
H	-5.37785700	1.15960800	-2.34645400
O	-5.69564900	2.42703500	-0.25326900
H	-0.72287900	3.02208000	-1.67644800
H	-0.94497900	1.44260800	-2.44018000
C	-2.46716100	2.57644900	0.50130900
H	-1.86540700	2.09061700	1.26956800
H	-2.10703500	3.60644900	0.40862900
H	-3.50411800	2.60613200	0.84328800
C	-2.33417700	-0.54918100	1.99632800
C	-3.58575600	-0.03600200	2.38817500
C	-1.39800700	-0.89438500	2.98797600
C	-3.88476900	0.13581400	3.74066800
H	-4.32846600	0.24185400	1.64923400
C	-1.70726900	-0.72611000	4.34053400
H	-0.42991600	-1.28606700	2.69648600
C	-2.94765600	-0.20967500	4.71852500
H	-4.84840900	0.54028200	4.02819400
H	-0.97757300	-0.99865200	5.09506500
H	-3.18502800	-0.07576100	5.76775600
C	-2.89980300	-2.36888800	-0.14829100
C	-2.87734800	-2.85716700	-1.46953900
C	-3.65856100	-3.04979500	0.81686400
C	-3.60560900	-3.99548300	-1.81428300
H	-2.26941400	-2.34838100	-2.20855400
C	-4.38156800	-4.19365100	0.46550200
H	-3.68872200	-2.68861400	1.83686800
C	-4.35906900	-4.66701700	-0.84697300
H	-3.57740200	-4.36270700	-2.83414900
H	-4.96249900	-4.71176700	1.22016600
H	-4.92066000	-5.55464700	-1.11470700
C	0.81436800	2.37094600	0.82485500
C	0.88334300	3.76414400	0.62303400
C	0.96483000	1.86348800	2.12510100
C	1.08047800	4.62591800	1.70087100
H	0.79632400	4.17313400	-0.37759100
C	1.16150200	2.73341000	3.20285400
H	0.94144200	0.79332300	2.28412000
C	1.21451400	4.11135100	2.99486700
H	1.13021200	5.69593400	1.53382900
H	1.27001400	2.32913700	4.20292300
H	1.36292800	4.78358300	3.83212200
C	1.88865500	1.62950500	-1.73928600
C	1.81357400	1.20176400	-3.07904500



C	3.05286800	2.28204300	-1.29927600
C	2.87179500	1.44163700	-3.95612200
H	0.94434400	0.64563500	-3.40800500
C	4.11120800	2.51223400	-2.18186300
H	3.13354300	2.61349600	-0.27170100
C	4.02252600	2.09767100	-3.51141800
H	2.80048800	1.10715500	-4.98522400
H	5.00338300	3.01629600	-1.82748200
H	4.84481200	2.27850600	-4.19417100
C	2.60172700	-1.34974900	0.85889500
O	1.52395100	-1.19821500	1.53288100
O	2.54418300	-1.30078700	-0.40771600
C	3.90724000	-1.60290600	1.58127200
H	3.89588600	-2.65462600	1.90166400
H	3.89648500	-1.01029800	2.50342900
C	0.18426300	-2.00173400	-3.15308900
O	1.29558100	-2.74014400	-2.64704700
O	-0.26950500	-0.98629600	-2.33198200
H	0.44807200	-1.56519200	-4.13702300
H	1.97269800	-2.10636800	-2.36115500
H	-0.57436900	-2.78711000	-3.32863400
H	0.07974600	-2.84456400	0.07667400
H	0.40459800	-2.86834000	-0.65130900
C	5.15907300	-1.31688600	0.74532100
H	5.12446100	-1.92206900	-0.16739500
H	5.14034100	-0.27131800	0.41258600
C	6.45861200	-1.59569000	1.50990800
H	6.47045200	-2.64449700	1.84082300
H	6.48340500	-0.98963400	2.42744600
C	7.72070000	-1.31340100	0.68494900
H	7.69563500	-1.91945500	-0.23064600
H	7.70858600	-0.26585300	0.35438400
C	9.01837400	-1.59378800	1.44941900
H	9.07533700	-2.64274600	1.76225600
H	9.89959900	-1.38264800	0.83465000
H	9.08785600	-0.97689200	2.35289300

TSVIhex

Zero-point = -2889.511463

Ru	0.31607700	-0.99663500	-0.39617900
P	0.56891100	1.34398300	-0.51452300
P	-1.86258200	-0.84595600	0.13932700
C	-2.79938600	0.51400300	-0.73127000
H	-2.76747600	0.21816700	-1.78639600
H	-3.84075100	0.45405800	-0.39943000
C	-0.91578800	2.19041300	-1.27378800
C	-2.31830700	1.98718100	-0.62903300
C	-3.27858300	2.86572000	-1.49503200

H	-3.06466200	3.92382900	-1.30263700
H	-3.10131300	2.69617700	-2.56769500
P	-5.09075300	2.63608000	-1.28245800
H	-5.58100900	3.70143500	-2.08757500
H	-5.36482600	1.52649800	-2.12837700
O	-5.65991800	2.54025700	0.10206900
H	-0.70832000	3.26384000	-1.34509300
H	-0.94275000	1.80679600	-2.30011600
C	-2.37538200	2.50771300	0.82074700
H	-1.73108300	1.93223100	1.48597100
H	-2.04157800	3.54953600	0.86447300
H	-3.39724100	2.45687600	1.20414500
C	-2.35043000	-0.71487200	1.91469800
C	-3.66996800	-0.43197700	2.31300600
C	-1.37613500	-0.96373800	2.89633300
C	-3.99996300	-0.37929900	3.66690800
H	-4.44269200	-0.24689800	1.57530900
C	-1.71643800	-0.91780400	4.25202000
H	-0.36100000	-1.19523900	2.59447800
C	-3.02382400	-0.62157700	4.63865000
H	-5.01720500	-0.14962700	3.96262700
H	-0.95803700	-1.11443300	5.00199500
H	-3.28501600	-0.58139900	5.69005600
C	-2.88992100	-2.31739200	-0.35047100
C	-3.90339200	-2.29487500	-1.32218500
C	-2.59596100	-3.54194500	0.28273100
C	-4.59858200	-3.46326400	-1.65597500
H	-4.16652700	-1.37450400	-1.82678100
C	-3.29273400	-4.70186900	-0.04800300
H	-1.80969900	-3.58128200	1.02858900
C	-4.29620100	-4.66708600	-1.02219100
H	-5.37803000	-3.42527800	-2.40891100
H	-3.05267200	-5.63353100	0.45186300
H	-4.83595000	-5.57065500	-1.28095100
C	0.93824800	2.38710000	0.96495400
C	0.94121800	3.79484500	0.89841800
C	1.21100200	1.76813000	2.19579400
C	1.19460100	4.55941500	2.03681300
H	0.75764800	4.29468200	-0.04622500
C	1.46459300	2.53938300	3.33501000
H	1.23197700	0.68712600	2.25176800
C	1.45247700	3.93191000	3.25992500
H	1.19130400	5.64171600	1.97159100
H	1.66862100	2.04755300	4.27956500
H	1.64459600	4.52771400	4.14489100
C	1.88601300	1.88018400	-1.70420600
C	1.80436400	1.42913000	-3.03750000
C	2.99441000	2.65380300	-1.32101400

C	2.79057200	1.77284900	-3.96232400
H	0.99126400	0.77376800	-3.32905700
C	3.98408600	2.98569300	-2.25079000
H	3.08585800	2.99999400	-0.29957200
C	3.88214800	2.55426300	-3.57348000
H	2.71235300	1.42112600	-4.98548400
H	4.83331900	3.58282100	-1.93743500
H	4.64939600	2.81617500	-4.29316400
C	2.59364200	-1.50090600	0.67911900
O	1.54811000	-1.28255600	1.38057600
O	2.51393800	-1.40915400	-0.58669100
C	3.88831700	-1.89182200	1.35787000
H	3.89731800	-2.98981800	1.42202800
H	3.85409700	-1.52430300	2.38890100
C	-0.37478200	-2.13638300	-3.01669100
O	0.83749700	-3.17447500	-2.46366800
O	-0.20168100	-0.96390500	-2.49206700
H	-0.21400800	-2.20861000	-4.10118300
H	1.67067900	-2.67396000	-2.55886300
H	-1.20866000	-2.75841100	-2.66403000
H	0.60328400	-2.98969900	-1.39476900
H	0.17146400	-2.69610200	-0.32534600
C	5.14627200	-1.40366900	0.62844900
H	5.11935700	-1.76514600	-0.40539200
H	5.12538300	-0.30777200	0.56629300
C	6.44297100	-1.85645200	1.30975700
H	6.45754300	-1.49772200	2.34927500
H	6.45981700	-2.95460900	1.36935100
C	7.70809200	-1.37074200	0.59093100
H	7.69267600	-1.72898000	-0.44729800
H	7.69094200	-0.27396700	0.53227400
C	9.00310300	-1.82652300	1.27078700
H	9.88658100	-1.46412700	0.73481300
H	9.06297300	-1.45419200	2.30003100
H	9.06534300	-2.92008300	1.31263500

TSVIhex at T=160°C

Zero-point = -2889.511463

Ru	0.31607700	-0.99663500	-0.39617900
P	0.56891100	1.34398300	-0.51452300
P	-1.86258200	-0.84595600	0.13932700
C	-2.79938600	0.51400300	-0.73127000
H	-2.76747600	0.21816700	-1.78639600
H	-3.84075100	0.45405800	-0.39943000
C	-0.91578800	2.19041300	-1.27378800
C	-2.31830700	1.98718100	-0.62903300
C	-3.27858300	2.86572000	-1.49503200
H	-3.06466200	3.92382900	-1.30263700

H	-3.10131300	2.69617700	-2.56769500
P	-5.09075300	2.63608000	-1.28245800
H	-5.58100900	3.70143500	-2.08757500
H	-5.36482600	1.52649800	-2.12837700
O	-5.65991800	2.54025700	0.10206900
H	-0.70832000	3.26384000	-1.34509300
H	-0.94275000	1.80679600	-2.30011600
C	-2.37538200	2.50771300	0.82074700
H	-1.73108300	1.93223100	1.48597100
H	-2.04157800	3.54953600	0.86447300
H	-3.39724100	2.45687600	1.20414500
C	-2.35043000	-0.71487200	1.91469800
C	-3.66996800	-0.43197700	2.31300600
C	-1.37613500	-0.96373800	2.89633300
C	-3.99996300	-0.37929900	3.66690800
H	-4.44269200	-0.24689800	1.57530900
C	-1.71643800	-0.91780400	4.25202000
H	-0.36100000	-1.19523900	2.59447800
C	-3.02382400	-0.62157700	4.63865000
H	-5.01720500	-0.14962700	3.96262700
H	-0.95803700	-1.11443300	5.00199500
H	-3.28501600	-0.58139900	5.69005600
C	-2.88992100	-2.31739200	-0.35047100
C	-3.90339200	-2.29487500	-1.32218500
C	-2.59596100	-3.54194500	0.28273100
C	-4.59858200	-3.46326400	-1.65597500
H	-4.16652700	-1.37450400	-1.82678100
C	-3.29273400	-4.70186900	-0.04800300
H	-1.80969900	-3.58128200	1.02858900
C	-4.29620100	-4.66708600	-1.02219100
H	-5.37803000	-3.42527800	-2.40891100
H	-3.05267200	-5.63353100	0.45186300
H	-4.83595000	-5.57065500	-1.28095100
C	0.93824800	2.38710000	0.96495400
C	0.94121800	3.79484500	0.89841800
C	1.21100200	1.76813000	2.19579400
C	1.19460100	4.55941500	2.03681300
H	0.75764800	4.29468200	-0.04622500
C	1.46459300	2.53938300	3.33501000
H	1.23197700	0.68712600	2.25176800
C	1.45247700	3.93191000	3.25992500
H	1.19130400	5.64171600	1.97159100
H	1.66862100	2.04755300	4.27956500
H	1.64459600	4.52771400	4.14489100
C	1.88601300	1.88018400	-1.70420600
C	1.80436400	1.42913000	-3.03750000
C	2.99441000	2.65380300	-1.32101400
C	2.79057200	1.77284900	-3.96232400

H	0.99126400	0.77376800	-3.32905700
C	3.98408600	2.98569300	-2.25079000
H	3.08585800	2.99999400	-0.29957200
C	3.88214800	2.55426300	-3.57348000
H	2.71235300	1.42112600	-4.98548400
H	4.83331900	3.58282100	-1.93743500
H	4.64939600	2.81617500	-4.29316400
C	2.59364200	-1.50090600	0.67911900
O	1.54811000	-1.28255600	1.38057600
O	2.51393800	-1.40915400	-0.58669100
C	3.88831700	-1.89182200	1.35787000
H	3.89731800	-2.98981800	1.42202800
H	3.85409700	-1.52430300	2.38890100
C	-0.37478200	-2.13638300	-3.01669100
O	0.83749700	-3.17447500	-2.46366800
O	-0.20168100	-0.96390500	-2.49206700
H	-0.21400800	-2.20861000	-4.10118300
H	1.67067900	-2.67396000	-2.55886300
H	-1.20866000	-2.75841100	-2.66403000
H	0.60328400	-2.98969900	-1.39476900
H	0.17146400	-2.69610200	-0.32534600
C	5.14627200	-1.40366900	0.62844900
H	5.11935700	-1.76514600	-0.40539200
H	5.12538300	-0.30777200	0.56629300
C	6.44297100	-1.85645200	1.30975700
H	6.45754300	-1.49772200	2.34927500
H	6.45981700	-2.95460900	1.36935100
C	7.70809200	-1.37074200	0.59093100
H	7.69267600	-1.72898000	-0.44729800
H	7.69094200	-0.27396700	0.53227400
C	9.00310300	-1.82652300	1.27078700
H	9.88658100	-1.46412700	0.73481300
H	9.06297300	-1.45419200	2.30003100
H	9.06534300	-2.92008300	1.31263500

Vllhex

Zero-point = -2889.536809

Ru	0.00617400	-1.16830300	-0.71536300
P	0.69050500	1.20140600	-0.48216300
P	-2.11899100	-0.77458000	-0.00794600
C	-2.80763400	0.90205000	-0.46780400
H	-2.92000700	0.84915100	-1.55492200
H	-3.81530500	0.93071500	-0.04373500
C	-0.71741500	2.35687200	-0.89537000
C	-2.05797400	2.21627200	-0.11350600
C	-2.93508300	3.40968500	-0.61488800
H	-2.52159300	4.34586700	-0.22161300
H	-2.90568400	3.48426100	-1.71194000

P	-4.72658900	3.38417900	-0.18783600
H	-5.10716500	4.70016800	-0.56810300
H	-5.29184700	2.62859500	-1.24916000
O	-5.13400700	2.95260700	1.19136900
H	-0.35235700	3.38522900	-0.79570700
H	-0.91103100	2.18822000	-1.95982000
C	-1.85698900	2.38290100	1.40551900
H	-1.27700400	1.56402700	1.83259600
H	-1.31516600	3.31058900	1.61715400
H	-2.82099500	2.42111200	1.91704500
C	-2.46985600	-0.97779000	1.78715000
C	-3.60164900	-0.41264200	2.40724700
C	-1.59319100	-1.76717900	2.55349300
C	-3.84077400	-0.62877300	3.76478300
H	-4.29331200	0.20935200	1.85110600
C	-1.84418200	-1.98354200	3.91167300
H	-0.71529500	-2.19816000	2.08801400
C	-2.96469500	-1.41507300	4.51870400
H	-4.70969700	-0.17955700	4.23156000
H	-1.16156900	-2.59538300	4.49091200
H	-3.15570500	-1.58038100	5.57291800
C	-3.43045900	-1.82599500	-0.78438400
C	-3.71642400	-1.68737200	-2.15755500
C	-4.11645400	-2.80498000	-0.04668800
C	-4.67121400	-2.50215800	-2.76746900
H	-3.17181600	-0.96168900	-2.75101700
C	-5.06811600	-3.61999000	-0.66451500
H	-3.91067300	-2.92840800	1.00902900
C	-5.35057700	-3.46949100	-2.02293000
H	-4.88006300	-2.38424800	-3.82502300
H	-5.58978000	-4.36976000	-0.08058100
H	-6.09143400	-4.10156200	-2.49872200
C	1.39337800	1.90875600	1.06673500
C	1.71430300	3.27669100	1.17174100
C	1.58964200	1.07678400	2.18187100
C	2.20989800	3.79786600	2.36641800
H	1.58964100	3.93058100	0.31536700
C	2.08759800	1.60524700	3.37758900
H	1.35602000	0.02147600	2.10871400
C	2.39453700	2.96246500	3.47309600
H	2.45284500	4.85216700	2.43536400
H	2.23092800	0.95330400	4.23184400
H	2.77732500	3.37034700	4.40148200
C	1.94082400	1.68700700	-1.75376300
C	1.61033500	1.57279300	-3.12001600
C	3.25217700	2.05493700	-1.40457500
C	2.56249900	1.84374900	-4.10291400
H	0.62894500	1.21454600	-3.40622200

C	4.20453400	2.31429900	-2.39542300
H	3.53424200	2.13382300	-0.36265500
C	3.86185500	2.21555900	-3.74601800
H	2.29494800	1.74349800	-5.14865000
H	5.21311000	2.58973900	-2.10859200
H	4.60285600	2.41276200	-4.51174700
C	2.21456800	-2.06674600	0.23918000
O	1.17174300	-1.85350200	0.95402100
O	2.14318600	-1.80227000	-1.00098000
C	3.48306000	-2.58844300	0.86567700
H	3.76796700	-3.50197600	0.32903200
H	3.26887400	-2.86007600	1.90392600
C	-0.47508800	-1.77118100	-2.67659800
O	-0.72877300	-0.48436700	-2.60918400
H	0.46657800	-2.09609300	-3.13833900
H	-1.31825500	-2.46061600	-2.76936000
H	-0.41166400	-2.71534700	-0.68904100
O	4.42140100	-1.12991100	-2.64343200
H	4.27013200	-0.17681700	-2.69204100
H	3.63012400	-1.45960900	-2.18446100
C	4.64017900	-1.57057400	0.78754500
H	4.81967300	-1.31799900	-0.26373300
H	4.33699800	-0.64582400	1.29806000
C	5.92933100	-2.10446100	1.42282200
H	5.74272800	-2.37353400	2.47298300
H	6.22272800	-3.03529600	0.91686200
C	7.09226900	-1.10653600	1.35406700
H	7.27586000	-0.84267300	0.30438100
H	6.79853700	-0.17438000	1.85638200
C	8.38330600	-1.64043400	1.98282700
H	9.19386600	-0.90686800	1.91863100
H	8.23851400	-1.88392200	3.04188400
H	8.72093600	-2.55298800	1.47842100

VIIIhex

Zero-point = -2813.125839

Ru	0.31302000	-1.04957200	-0.66435100
P	0.64814600	1.39871800	-0.40146100
P	-1.88286100	-0.94608200	-0.08293800
C	-2.77104600	0.60919200	-0.62091900
H	-2.79968000	0.52772700	-1.71165600
H	-3.79910100	0.50008400	-0.26358200
C	-0.87771000	2.33906400	-0.93208700
C	-2.24089700	2.02083500	-0.24737700
C	-3.23560000	3.06963800	-0.84399400
H	-2.98848600	4.06155700	-0.44752500
H	-3.13255100	3.12886600	-1.93758300
P	-5.03368000	2.80084000	-0.55230000

H	-5.56156800	4.03839600	-1.01272300
H	-5.40118500	1.94340400	-1.62324800
O	-5.48912100	2.35612200	0.80746900
H	-0.66948900	3.41013600	-0.83095500
H	-0.96356500	2.13250900	-2.00437200
C	-2.18630300	2.23663900	1.27784800
H	-1.52599600	1.52077200	1.76865500
H	-1.80693800	3.23789300	1.50658000
H	-3.18293900	2.13716300	1.71323700
C	-2.30877000	-1.16714400	1.69389500
C	-3.55504300	-0.78448800	2.22785700
C	-1.36304500	-1.77963400	2.53564100
C	-3.83969000	-1.00418600	3.57582800
H	-4.30333900	-0.30226100	1.60961000
C	-1.65918500	-2.00158000	3.88397000
H	-0.39921300	-2.06987400	2.13501600
C	-2.89390900	-1.61389300	4.40555800
H	-4.79842200	-0.69581800	3.97647000
H	-0.92229600	-2.47624400	4.52242000
H	-3.12039200	-1.78284500	5.45218900
C	-2.99001800	-2.18319500	-0.90454000
C	-3.22385300	-2.10173200	-2.29200100
C	-3.56372900	-3.24428400	-0.18446400
C	-4.02003900	-3.05193000	-2.93310400
H	-2.76025000	-1.31128100	-2.87125600
C	-4.35633200	-4.19433000	-0.83300000
H	-3.39502300	-3.32601700	0.88186000
C	-4.58980700	-4.09964600	-2.20577600
H	-4.19056100	-2.97576600	-4.00134400
H	-4.79309400	-5.00589000	-0.26205500
H	-5.20778100	-4.83663400	-2.70557500
C	1.10255400	2.18490000	1.20252900
C	1.16029600	3.58526100	1.35010300
C	1.36709000	1.37390700	2.31892800
C	1.46742700	4.15601300	2.58490500
H	0.97585100	4.22934500	0.49731300
C	1.67331000	1.95198600	3.55526700
H	1.33404100	0.29609600	2.21351700
C	1.72138100	3.33917800	3.69154600
H	1.50793700	5.23477500	2.68536100
H	1.86973700	1.31430700	4.40982900
H	1.95536500	3.78492800	4.65148800
C	1.90129200	2.08677200	-1.57316800
C	1.74258900	1.82708700	-2.95013100
C	3.03866900	2.79152500	-1.14396100
C	2.68412400	2.29181900	-3.86822700
H	0.90690100	1.22328800	-3.28638000
C	3.98127300	3.24631300	-2.07020900



H	3.19047300	2.98653300	-0.09025500
C	3.80389600	3.00560900	-3.43285100
H	2.54934600	2.08374300	-4.92395000
H	4.85392900	3.78784600	-1.72237100
H	4.53617100	3.36090700	-4.14879000
C	2.56727000	-1.63557700	0.38713600
O	1.47968800	-1.54872700	1.06997300
O	2.52062800	-1.38540100	-0.84931400
C	3.84454500	-2.05310300	1.07981800
H	3.76024500	-3.13153300	1.27654100
H	3.86294300	-1.57199800	2.06506500
C	0.02695300	-1.73660600	-2.63329400
O	-0.40059000	-0.49402100	-2.60871900
H	1.02855200	-1.93706100	-3.03609600
H	-0.70956000	-2.53438400	-2.76089200
H	0.11535100	-2.63935700	-0.63256200
C	5.12031400	-1.75443600	0.28631100
H	5.04324800	-2.22270800	-0.70121100
H	5.18711800	-0.67473700	0.10249900
C	6.38876300	-2.23846900	0.99900200
H	6.45580200	-1.76942600	1.99164100
H	6.31554400	-3.32070000	1.18113100
C	7.67427300	-1.94533500	0.21504000
H	7.60613400	-2.41334300	-0.77623600
H	7.74790800	-0.86436400	0.03429100
C	8.94082500	-2.43299500	0.92564500
H	9.83969900	-2.20906100	0.34172100
H	9.05421900	-1.95617400	1.90617500
H	8.91190400	-3.51660300	1.08833700

TSIIIhex

Zero-point = -2813.120824

Ru	0.32344700	-1.05114400	-0.59496500
P	0.60343800	1.31401800	-0.44510700
P	-1.86758800	-0.92405600	-0.00264000
C	-2.79338800	0.54480800	-0.69640400
H	-2.81863400	0.34739400	-1.77350900
H	-3.82175600	0.46101900	-0.33209400
C	-0.88428900	2.22195500	-1.11973800
C	-2.27980100	1.99217300	-0.47120000
C	-3.24086600	2.95990800	-1.23449100
H	-3.00625600	3.99348200	-0.95325500
H	-3.09053700	2.88327100	-2.32157700
P	-5.05051300	2.72974500	-0.98954700
H	-5.55132500	3.88290900	-1.65436100
H	-5.37012800	1.72064500	-1.93650000
O	-5.56921000	2.49256300	0.39887300
H	-0.66068500	3.29474400	-1.12095200

H	-0.92447700	1.91038800	-2.17005000
C	-2.29444700	2.38694500	1.01886600
H	-1.65620800	1.73838500	1.61975000
H	-1.92790600	3.41104700	1.14371900
H	-3.30997800	2.33476900	1.41759600
C	-2.27641000	-0.95115800	1.79315200
C	-3.53577000	-0.55876100	2.28765500
C	-1.30455000	-1.42089000	2.69431300
C	-3.80752500	-0.62493600	3.65429400
H	-4.30575400	-0.19164400	1.61898800
C	-1.58722300	-1.48999400	4.06208600
H	-0.33237600	-1.72328300	2.32348600
C	-2.83440100	-1.09085200	4.54367800
H	-4.77711300	-0.31052100	4.02292300
H	-0.83003400	-1.85549000	4.74696000
H	-3.05010500	-1.14071300	5.60492000
C	-2.96735600	-2.26255000	-0.66316400
C	-3.19551500	-2.35460800	-2.05159000
C	-3.54416100	-3.22677100	0.18062700
C	-3.99182100	-3.37587500	-2.57226400
H	-2.71982100	-1.64731400	-2.72204100
C	-4.33606100	-4.24927800	-0.34795400
H	-3.38077500	-3.17535000	1.24960400
C	-4.56616100	-4.32439700	-1.72245200
H	-4.15790300	-3.43329200	-3.64239100
H	-4.77565200	-4.98345800	0.31775600
H	-5.18431900	-5.11652900	-2.12901100
C	1.02670000	2.22440000	1.10039800
C	1.02164100	3.63222900	1.16417800
C	1.35541300	1.49442300	2.25522200
C	1.33068900	4.28924400	2.35505400
H	0.78290500	4.21712300	0.28292100
C	1.66310300	2.15886900	3.44675700
H	1.37247100	0.41194600	2.21200300
C	1.64928000	3.55259700	3.50022400
H	1.32151900	5.37278700	2.39122500
H	1.91003000	1.58329000	4.33176100
H	1.88460800	4.06513900	4.42588400
C	1.89135200	1.88019400	-1.64493400
C	1.83176400	1.35872900	-2.95384400
C	2.93225900	2.76048500	-1.30925400
C	2.77758300	1.74026400	-3.90536200
H	1.07127600	0.62526000	-3.20611800
C	3.88067500	3.13047400	-2.26733000
H	3.00844400	3.15347400	-0.30361800
C	3.80206600	2.62873500	-3.56671000
H	2.72291400	1.33018700	-4.90781400
H	4.68103000	3.80891300	-1.99348600

H	4.53937900	2.91750800	-4.30712800
C	2.59074800	-1.60689000	0.46854500
O	1.52466300	-1.49366900	1.17168900
O	2.52027400	-1.39226200	-0.77786000
C	3.88626900	-2.01789400	1.13287900
H	3.87562300	-1.63112600	2.15816200
H	3.86343900	-3.11374700	1.22323800
C	0.02184100	-2.27254600	-2.36352800
O	-0.33921100	-1.02600500	-2.62732700
H	1.01648200	-2.59602600	-2.69790200
H	-0.75495400	-3.04225800	-2.44709400
H	0.14940900	-2.68635400	-0.80138400
C	5.14677000	-1.57927100	0.37920500
H	5.09487000	-1.95533400	-0.64836800
H	5.15746400	-0.48466400	0.29931200
C	6.43809900	-2.06080500	1.05117300
H	6.47790300	-1.68625000	2.08456900
H	6.42261800	-3.15790500	1.12848200
C	7.70761100	-1.62575000	0.30811900
H	7.66714000	-2.00008000	-0.72365200
H	7.72300800	-0.53008600	0.23149500
C	8.99713400	-2.11008800	0.97859000
H	9.88396100	-1.78380100	0.42523400
H	9.08232000	-1.72321600	2.00070800
H	9.02651400	-3.20424200	1.03771000

IXhex

Zero-point = -2813.136806

Ru	0.45261600	-0.74146700	-0.58113500
P	0.33823400	1.43906100	-0.30068400
P	-1.71105900	-1.00386100	-0.02808800
C	-2.86798200	0.23458700	-0.79141800
H	-2.76520400	0.02574300	-1.86225000
H	-3.88979100	-0.02594100	-0.49854300
C	-1.20266200	2.18155000	-1.04721500
C	-2.61026000	1.74725500	-0.54587100
C	-3.61868200	2.55100300	-1.42717700
H	-3.57165200	3.61223000	-1.15472400
H	-3.34893600	2.48076600	-2.49108900
P	-5.38749200	2.04881600	-1.35117400
H	-5.98773500	3.09348500	-2.10675300
H	-5.45135100	0.97890600	-2.28246100
O	-6.00220100	1.76952600	-0.01035000
H	-1.11697500	3.27211400	-0.98075000
H	-1.10836300	1.90759000	-2.10279500
C	-2.84231500	2.14782400	0.92492100
H	-2.18385400	1.60882500	1.60648600
H	-2.64705600	3.21696800	1.06025400

H	-3.87720300	1.95336900	1.21531800
C	-2.19853600	-1.15763700	1.74094700
C	-3.50972100	-0.92791100	2.19895600
C	-1.22268700	-1.59424600	2.65567100
C	-3.83036700	-1.11909600	3.54415500
H	-4.28405500	-0.59211000	1.51909600
C	-1.55274600	-1.78969100	3.99927900
H	-0.21096500	-1.77726900	2.31108000
C	-2.85358000	-1.55024000	4.44581000
H	-4.84170500	-0.93019800	3.88539100
H	-0.79227200	-2.12841600	4.69418900
H	-3.10699000	-1.69829700	5.48938000
C	-2.37055700	-2.57935100	-0.74375800
C	-2.18607600	-2.81219900	-2.12225400
C	-3.01797800	-3.55477700	0.03365300
C	-2.65481700	-3.99038800	-2.70503400
H	-1.65898900	-2.06630300	-2.70913800
C	-3.47847900	-4.73374200	-0.55788500
H	-3.16568500	-3.39339400	1.09371100
C	-3.30056400	-4.95355500	-1.92511500
H	-2.50865300	-4.15886100	-3.76637900
H	-3.97724000	-5.47873600	0.05182900
H	-3.65906400	-5.87049900	-2.37892900
C	0.50022800	2.19790400	1.36901100
C	0.28382000	3.57609100	1.56748000
C	0.86328200	1.39956000	2.46510900
C	0.40713000	4.13440700	2.83900100
H	0.03137000	4.21463000	0.72826300
C	0.98475500	1.96575400	3.73845100
H	1.06108900	0.34585800	2.31231700
C	0.75228800	3.32780100	3.92850400
H	0.23578400	5.19542400	2.98111300
H	1.26044500	1.33838300	4.57853600
H	0.84302300	3.76327100	4.91698000
C	1.64479500	2.31330900	-1.26965800
C	1.64949500	2.17173500	-2.67097500
C	2.66267600	3.06284800	-0.65621500
C	2.63714800	2.78928800	-3.43769600
H	0.89742400	1.54763900	-3.13976200
C	3.65386500	3.67088700	-1.43074100
H	2.68024900	3.17554700	0.42039400
C	3.64079700	3.54078200	-2.82034800
H	2.63031700	2.67348200	-4.51585800
H	4.43466600	4.24599700	-0.94577000
H	4.41118300	4.01461000	-3.41794200
C	2.72337600	-1.47239900	0.37721200
O	1.67989800	-1.41260700	1.11913700
O	2.64029000	-1.09846600	-0.83456400

C	4.01774200	-2.01620100	0.94205900
H	4.00419100	-3.10383500	0.77940000
H	4.00091100	-1.86880400	2.02716800
C	0.68582100	-1.07769700	-3.43662400
O	-0.19133600	-0.44911500	-2.53250100
H	1.72517400	-0.72290800	-3.34605600
H	0.35200200	-0.87275100	-4.46792000
H	0.70938900	-2.17856000	-3.32551100
C	5.27730000	-1.41268800	0.30869300
H	5.22395000	-1.54349000	-0.77747100
H	5.28535400	-0.32880900	0.48373100
C	6.57087700	-2.03106500	0.85178800
H	6.60979800	-1.90583800	1.94380500
H	6.55945400	-3.11622700	0.67276000
C	7.83815200	-1.43079000	0.22986600
H	7.84981900	-0.34717200	0.40979900
H	7.79798000	-1.55551400	-0.86060900
C	9.13002000	-2.05281200	0.76942400
H	9.16349700	-3.13057100	0.57243800
H	10.01513400	-1.60340800	0.30711200
H	9.21463200	-1.91391700	1.85348600

Xhex

Zero-point = -2814.310531

Ru	0.32889300	-1.04492900	-0.46965500
P	0.53836300	1.24855100	-0.43876900
P	-1.87708400	-0.92779500	0.05719700
C	-2.81354000	0.44831800	-0.77736100
H	-2.76515400	0.15965700	-1.83301800
H	-3.85692800	0.36054800	-0.45910500
C	-0.91131100	2.11435100	-1.22533600
C	-2.33782600	1.91901900	-0.63742300
C	-3.26530700	2.80444600	-1.53032600
H	-3.06207900	3.86198700	-1.32349300
H	-3.05355000	2.63998200	-2.59698300
P	-5.08139200	2.55661800	-1.36300100
H	-5.56656200	3.64154200	-2.14403000
H	-5.33259600	1.46758800	-2.23876200
O	-5.66908400	2.42133600	0.01199800
H	-0.67959400	3.18424000	-1.26865000
H	-0.90342900	1.72824000	-2.24889400
C	-2.44490900	2.43517400	0.81141800
H	-1.84719500	1.84255900	1.50428300
H	-2.08499800	3.46761300	0.87291700
H	-3.48401700	2.41501400	1.14743700
C	-2.35255600	-0.87347500	1.83519800
C	-3.60771100	-0.41921900	2.28392700
C	-1.42836900	-1.36328400	2.77597000

C	-3.92299500	-0.44974300	3.64354300
H	-4.33933600	-0.02893000	1.58570800
C	-1.75340000	-1.39684100	4.13459300
H	-0.45620800	-1.70706700	2.43986300
C	-2.99825900	-0.93948800	4.57011000
H	-4.88915200	-0.08868400	3.97684000
H	-1.03245100	-1.77843000	4.84915900
H	-3.24803800	-0.96179000	5.62476300
C	-2.86360300	-2.36035700	-0.57451700
C	-2.71687500	-2.70306900	-1.93431900
C	-3.72472100	-3.11901100	0.23364700
C	-3.42755300	-3.77814500	-2.46812000
H	-2.03169700	-2.12274500	-2.54593600
C	-4.42889900	-4.19837700	-0.30875700
H	-3.84735000	-2.86975000	1.28008300
C	-4.28424900	-4.52859300	-1.65684300
H	-3.30794800	-4.03410300	-3.51523600
H	-5.08988100	-4.77875700	0.32514800
H	-4.83200100	-5.36658400	-2.07276600
C	0.84254200	2.17285800	1.12376200
C	0.90770800	3.58075900	1.12816300
C	0.99463700	1.48038200	2.33550300
C	1.10094200	4.27594100	2.32084000
H	0.82080800	4.13159900	0.19801700
C	1.18784100	2.18389600	3.52918000
H	0.97893500	0.39808700	2.33511700
C	1.23561900	3.57764300	3.52559600
H	1.14750200	5.35904400	2.31243200
H	1.29890200	1.63781600	4.45915600
H	1.38131200	4.12035900	4.45253100
C	1.92308300	1.82191700	-1.51605100
C	1.83842500	1.62943600	-2.90779200
C	3.09608900	2.37770000	-0.97717800
C	2.89438000	2.00688600	-3.73754600
H	0.96245200	1.14839600	-3.32432500
C	4.15262300	2.74588600	-1.81352200
H	3.18340700	2.52802100	0.09157800
C	4.05310200	2.56693400	-3.19414100
H	2.81568900	1.85319500	-4.80810200
H	5.05142000	3.17380900	-1.38376900
H	4.87377000	2.85534200	-3.84095700
C	2.62824500	-1.53944600	0.60562600
O	1.57149200	-1.46018300	1.32439500
O	2.53805900	-1.34569800	-0.64427100
C	3.95215300	-1.88338400	1.25595400
H	3.94151200	-2.96507800	1.45325300
H	3.97330700	-1.40159100	2.24042000
C	0.44169900	-1.48258100	-3.35058400

O	-0.29901100	-0.71473700	-2.44321600
H	1.53174300	-1.37253800	-3.22711400
H	0.19428200	-1.17835900	-4.38247500
H	0.21724700	-2.56785300	-3.27617400
H	0.29540700	-2.80213900	-1.03435900
H	0.10688000	-2.85025300	-0.25879900
C	5.18150800	-1.50877500	0.42178500
H	5.11063700	-1.99771800	-0.55612300
H	5.16447800	-0.43057300	0.21830200
C	6.50084800	-1.88829000	1.10460100
H	6.56157500	-1.39850200	2.08762000
H	6.51112600	-2.96964200	1.30576000
C	7.73988800	-1.51779900	0.27958000
H	7.72987000	-0.43773900	0.07931000
H	7.67871200	-2.00725500	-0.70175600
C	9.05764600	-1.89969000	0.96122400
H	9.11194600	-2.97941400	1.14226900
H	9.92164800	-1.62226100	0.34826200
H	9.16297600	-1.39822100	1.93031300

TSXhex

Zero-point = -2814.280822

Ru	0.52154700	-0.79291100	-0.65714900
P	0.42369500	1.50982800	-0.30731000
P	-1.66281600	-1.04824800	-0.07046300
C	-2.83018500	0.27730000	-0.67774900
H	-2.86080900	0.13650800	-1.76436100
H	-3.82518900	0.04140000	-0.28844100
C	-1.17085900	2.24444800	-0.95133200
C	-2.53682700	1.77258100	-0.37456200
C	-3.60178000	2.63033800	-1.13250500
H	-3.53455600	3.66913300	-0.78802800
H	-3.39666900	2.64070300	-2.21342500
P	-5.36746000	2.13284200	-0.99850400
H	-5.99341700	3.22497900	-1.66021000
H	-5.48273700	1.12569200	-1.99565200
O	-5.92248400	1.76831300	0.34628000
H	-1.10655000	3.33510500	-0.86739000
H	-1.13878100	2.02149100	-2.02470300
C	-2.66904400	2.07353900	1.13210000
H	-1.95191300	1.50800000	1.72774700
H	-2.48954200	3.13587200	1.32566200
H	-3.67485900	1.82721500	1.48082700
C	-2.08040900	-1.22327700	1.72356200
C	-3.41830400	-1.25210300	2.16151200
C	-1.05092100	-1.39144100	2.66338700
C	-3.71479700	-1.41697700	3.51351500
H	-4.23378000	-1.15215100	1.45442300

C	-1.35623600	-1.56445300	4.01756200
H	-0.02011800	-1.39739400	2.33456700
C	-2.68345000	-1.57082600	4.44542100
H	-4.74880700	-1.42769600	3.83849200
H	-0.55259800	-1.69564800	4.73385800
H	-2.91737400	-1.70061400	5.49592700
C	-2.51115600	-2.57598500	-0.69940400
C	-3.73776600	-2.58379200	-1.38388600
C	-1.87739700	-3.80719600	-0.44152100
C	-4.30932300	-3.78863200	-1.80655900
H	-4.25959400	-1.65981500	-1.59704500
C	-2.45257600	-5.00597900	-0.85901500
H	-0.92515900	-3.81972300	0.07776600
C	-3.67021400	-5.00017900	-1.54614000
H	-5.25514200	-3.77520800	-2.33650500
H	-1.94965000	-5.94365800	-0.65129300
H	-4.11485500	-5.93242900	-1.87442000
C	0.66850400	2.32957900	1.32925600
C	0.35976200	3.68817900	1.54366000
C	1.19946300	1.58326800	2.39496100
C	0.57036800	4.27752200	2.79032200
H	-0.04188300	4.29147900	0.73766400
C	1.40855800	2.17874400	3.64271700
H	1.44323500	0.53940900	2.24144500
C	1.09383900	3.52245900	3.84402900
H	0.32526900	5.32293300	2.94031600
H	1.81471700	1.58794000	4.45613100
H	1.25321800	3.98118900	4.81305000
C	1.63477700	2.39093900	-1.39530000
C	1.80093600	1.90063800	-2.70685400
C	2.39429700	3.49695700	-0.97951200
C	2.68703000	2.52862100	-3.58325300
H	1.27235000	1.00447000	-3.01967900
C	3.28235200	4.11599200	-1.86322500
H	2.30426600	3.86944500	0.03257400
C	3.42556700	3.63915400	-3.16692700
H	2.81228600	2.13684200	-4.58665600
H	3.86479600	4.96700600	-1.52794300
H	4.11721400	4.12043800	-3.84912200
C	2.80678700	-1.15225600	0.43273000
O	1.71237500	-1.27095400	1.09590200
O	2.74089800	-0.79253200	-0.77792700
C	4.12823100	-1.40726100	1.12208300
H	3.97251800	-2.19979500	1.86274700
H	4.36767900	-0.49902200	1.69477400
C	-0.93838600	-1.00033800	-3.55657300
O	0.25748100	-0.88142500	-2.82037000
H	-0.69639200	-1.25616600	-4.59811600



H	-1.49527000	-0.04894600	-3.57305000
H	-1.60837800	-1.77869800	-3.16660300
H	0.50573300	-1.95612300	-2.07125000
H	0.65833600	-2.47279300	-1.25668800
C	5.27937300	-1.74523900	0.16855500
H	5.03199500	-2.66065100	-0.38408800
H	5.36288500	-0.95196800	-0.58222400
C	6.61763300	-1.92662800	0.89451600
H	6.86189900	-1.00633200	1.44524200
H	6.52157800	-2.71647000	1.65390600
C	7.77700500	-2.27223200	-0.04860700
H	7.87120500	-1.48376800	-0.80736300
H	7.53358200	-3.19214400	-0.59727600
C	9.11497400	-2.44807900	0.67653900
H	9.92072200	-2.69433200	-0.02289400
H	9.40272100	-1.53213200	1.20554200
H	9.06136600	-3.25333300	1.41837700

Xlhex

Zero-point = -2814.289143

Ru	-0.12517100	-0.61780800	1.13695500
P	-0.70879200	1.45485500	0.04317600
P	1.99365800	-0.68337200	0.33151200
C	2.73276900	0.90672000	-0.33696600
H	3.03557500	1.45119600	0.56674400
H	3.65988300	0.62033500	-0.84089300
C	0.74395100	2.52358100	-0.45165400
C	1.91076200	1.86555000	-1.24201100
C	2.83845800	3.05259400	-1.65684200
H	2.33210100	3.65003700	-2.42436200
H	3.02694600	3.72171000	-0.80412400
P	4.50750400	2.62868600	-2.30837600
H	4.92729000	3.89015700	-2.81167700
H	5.29426400	2.53891400	-1.12973700
O	4.63645900	1.46823900	-3.25337800
H	0.35973500	3.37401100	-1.02738300
H	1.15218400	2.92219700	0.48542200
C	1.40247500	1.18692700	-2.52915500
H	0.81466300	0.29463800	-2.30873300
H	0.76195300	1.87471900	-3.09077500
H	2.23649200	0.89629300	-3.17006400
C	2.25017800	-1.92706300	-1.01170600
C	3.07460600	-1.72553600	-2.13493700
C	1.62730700	-3.17932000	-0.84572100
C	3.26538700	-2.75205100	-3.06477800
H	3.57047500	-0.77904600	-2.31385600
C	1.82704400	-4.20012700	-1.77534900
H	0.97688400	-3.33768500	0.00538700

C	2.64524200	-3.98940300	-2.88759100
H	3.90018700	-2.57662200	-3.92587000
H	1.33923800	-5.15777400	-1.63170700
H	2.79667500	-4.78249000	-3.61104500
C	3.41383100	-1.11039700	1.45313500
C	3.26843400	-1.05468500	2.84826900
C	4.67364200	-1.44083100	0.91654800
C	4.36039000	-1.30647500	3.68539100
H	2.30476100	-0.84502900	3.29468400
C	5.75935200	-1.69136600	1.75565500
H	4.80027300	-1.53025500	-0.15620900
C	5.60666300	-1.62001400	3.14325000
H	4.22710500	-1.26517100	4.76071200
H	6.72069900	-1.95103200	1.32663100
H	6.45054000	-1.81903200	3.79403100
C	-1.79290200	1.54388400	-1.45796400
C	-2.40316700	2.74948500	-1.85092400
C	-2.00031200	0.39088900	-2.23491500
C	-3.18994400	2.80208300	-3.00188700
H	-2.27747600	3.64170800	-1.24708900
C	-2.79225100	0.44906800	-3.38600000
H	-1.54768400	-0.54603100	-1.93275200
C	-3.38467600	1.65206000	-3.77271600
H	-3.65560900	3.73674800	-3.29388400
H	-2.94255600	-0.44671800	-3.97830200
H	-3.99834000	1.69471800	-4.66530800
C	-1.63129000	2.60871300	1.16405800
C	-1.25470100	3.93276800	1.44652800
C	-2.78734400	2.08978500	1.78555200
C	-2.00992200	4.71604600	2.32640300
H	-0.37678800	4.36781000	0.98577200
C	-3.53917400	2.87701400	2.65669800
H	-3.08016300	1.06248000	1.59394800
C	-3.15184100	4.19219600	2.93170100
H	-1.70344300	5.73527800	2.53406600
H	-4.42364900	2.46135400	3.12638100
H	-3.73442800	4.80051500	3.61378300
C	-2.21205200	-1.90266400	0.45102100
O	-1.12291400	-1.91712600	-0.22193000
O	-2.27292700	-1.16749200	1.48480200
C	-3.38251300	-2.75233100	0.01649200
H	-3.46774400	-3.58130000	0.73264300
H	-3.14543000	-3.18944500	-0.95836700
C	-0.05038200	0.39929600	3.44136200
O	0.35090600	-0.59261500	4.34752600
H	0.25658900	1.37120800	3.84161800
H	-1.12433200	0.42969900	3.25736100
H	0.60772700	0.39232400	2.47729700

H	0.26840700	-1.99033300	1.93682600
H	0.13078300	-1.43748900	3.92279500
C	-4.70821000	-1.97519500	-0.02923400
H	-4.88501400	-1.52230800	0.95303800
H	-4.61387300	-1.14692200	-0.74385000
C	-5.90078000	-2.85640100	-0.41885000
H	-5.71120900	-3.31854600	-1.39844900
H	-5.98841300	-3.68737600	0.29603600
C	-7.22929700	-2.09114100	-0.47016100
H	-7.14021500	-1.26089500	-1.18383100
H	-7.41758500	-1.62989300	0.50882400
C	-8.42026500	-2.97359500	-0.85739100
H	-9.35225900	-2.39945800	-0.88518100
H	-8.27640000	-3.42176900	-1.84730000
H	-8.55582800	-3.79282900	-0.14195900

## S12. Cartesian coordinates of the optimized stationary points along the side reaction

### Ru<sub>2</sub><sup>ace</sup>-H-acetic

Zero-point = -2959.099255

Ru	-0.01040000	-0.86923900	-0.85165800
P	-1.99043200	-0.30016600	0.35957000
P	1.21508600	0.84054500	-0.02846300
C	0.62963200	1.70047500	1.52804200
H	0.87748000	1.01359000	2.34479400
H	1.27552900	2.57275400	1.65630500
C	-1.76485100	0.85194900	1.82020100
C	-0.86117200	2.10816000	1.66281800
C	-1.03623900	2.90017200	2.99841500
H	-2.03733600	3.34695400	3.01961500
H	-0.97050600	2.22616900	3.86562900
P	0.17012900	4.24341800	3.35771800
H	-0.45250000	4.86652600	4.47393600
H	1.22848600	3.54851900	4.00206700
O	0.59184000	5.15857700	2.24464100
H	-2.76018100	1.17248500	2.14933200
H	-1.34242400	0.22919700	2.61817400
C	-1.32817300	3.01198500	0.50581000
H	-1.19982800	2.52377400	-0.46158000
H	-2.39102000	3.25165800	0.61569500
H	-0.76202500	3.94578600	0.49318800
C	1.58879700	2.21516200	-1.20556800
C	1.88126700	3.53241700	-0.80248400
C	1.62283600	1.90266100	-2.57803000
C	2.19952100	4.50645200	-1.75114500
H	1.84378100	3.82854900	0.23863600
C	1.95098900	2.88070700	-3.52000700
H	1.37100300	0.89998900	-2.89886800

C	2.23981600	4.18315800	-3.10944900
H	2.41040900	5.51803100	-1.42380800
H	1.97266200	2.62296700	-4.57301300
H	2.48835100	4.94318600	-3.84154800
C	2.91776500	0.38398100	0.56254000
C	3.06740800	-0.42517500	1.70668200
C	4.07032300	0.76957400	-0.14133900
C	4.33349600	-0.82677000	2.13576000
H	2.19248500	-0.75711800	2.25461600
C	5.33599300	0.36138500	0.28816300
H	3.97865500	1.38774100	-1.02530400
C	5.47302500	-0.43355900	1.42736900
H	4.43156400	-1.44775600	3.01929800
H	6.21393800	0.66975200	-0.26809000
H	6.45612800	-0.74270200	1.76357900
C	-3.47299400	0.44160900	-0.47447300
C	-4.74995600	0.39396800	0.11533300
C	-3.32037600	1.09601900	-1.70968100
C	-5.84158300	1.00010400	-0.50745000
H	-4.89456500	-0.13460600	1.05090700
C	-4.41803500	1.70115600	-2.32919800
H	-2.34894900	1.11339900	-2.18885800
C	-5.67743000	1.65810100	-1.72973100
H	-6.82034200	0.95319200	-0.04304400
H	-4.28504800	2.20400200	-3.28080200
H	-6.52735200	2.12680000	-2.21264600
C	-2.76797000	-1.76152500	1.19297600
C	-3.27842000	-1.75429600	2.50311100
C	-2.85096700	-2.95265300	0.44412700
C	-3.85844100	-2.90381000	3.04880200
H	-3.23020000	-0.85819900	3.10942300
C	-3.43579900	-4.09502400	0.99202200
H	-2.44443600	-2.97956500	-0.56110100
C	-3.94010000	-4.07516900	2.29517500
H	-4.24677500	-2.88011100	4.06110600
H	-3.49232000	-5.00250800	0.40097200
H	-4.39083100	-4.96506300	2.71954500
C	-1.17916600	-1.35817800	-3.07010000
O	-1.10176600	-2.28369400	-2.20469900
O	-0.69352100	-0.21055300	-2.78591800
C	-1.86527400	-1.57867900	-4.39311300
H	-2.88963200	-1.19437900	-4.32989000
H	-1.34885500	-1.03189100	-5.18542300
H	-1.90408100	-2.64342700	-4.62848200
H	1.36820500	-1.29390100	-1.69384600
C	4.92954200	-3.35826500	-0.43342700
O	4.97829200	-2.83230500	-1.47471100
O	4.91234200	-3.90047200	0.60474900

C	1.29043200	-3.10310800	0.62171000
O	0.49755500	-2.15845900	0.80905000
O	1.94306400	-3.26717800	-0.49909800
C	1.54998200	-4.13161200	1.68267400
H	2.62356300	-4.18723300	1.88153200
H	1.23321700	-5.11352100	1.31746000
H	1.68428600	-2.45518700	-1.09999300
H	0.99961000	-3.88386300	2.58969200

### Ru<sub>2</sub><sub>ace</sub>-H-CO<sub>2</sub>

Zero-point = -2959.070886

Ru	0.45274300	-0.86424900	0.56306300
P	0.98687700	1.40093200	-0.41560000
P	-1.77722300	-0.83334000	0.01365200
C	-2.24205200	0.30791800	-1.38897700
H	-1.84329800	-0.18166100	-2.28462000
H	-3.33092100	0.24006700	-1.45876300
C	-0.27844300	1.94977600	-1.68364500
C	-1.79914900	1.79965800	-1.39155600
C	-2.50223700	2.50523400	-2.59746600
H	-2.34119700	3.58654800	-2.51663900
H	-2.05607600	2.18779600	-3.55123600
P	-4.31373100	2.23674300	-2.80340400
H	-4.63246400	3.25329800	-3.74341900
H	-4.36875200	1.08293100	-3.62937300
O	-5.17425500	2.18130400	-1.57345200
H	-0.07509800	3.00201200	-1.91267200
H	-0.03609600	1.37015100	-2.58207400
C	-2.19818900	2.54503200	-0.10396600
H	-1.75823900	2.08539700	0.78246400
H	-1.84474900	3.58070500	-0.14486000
H	-3.28229600	2.55405000	0.02205700
C	-2.92887000	-0.42844700	1.38904600
C	-4.21140500	0.11199300	1.16794900
C	-2.53253600	-0.72946600	2.70542100
C	-5.06850000	0.34838800	2.24385600
H	-4.55261600	0.37625500	0.17421800
C	-3.40030500	-0.49462700	3.77514200
H	-1.54379500	-1.12872000	2.88899400
C	-4.66718900	0.04432100	3.54729200
H	-6.04761900	0.77425100	2.05843700
H	-3.08112600	-0.73124500	4.78383000
H	-5.33760400	0.22984400	4.37862900
C	-2.47691400	-2.41006800	-0.64843300
C	-2.00040800	-2.93543500	-1.86636100
C	-3.46381900	-3.11977300	0.05644700
C	-2.50710300	-4.13690200	-2.36281900
H	-1.21358700	-2.42701700	-2.40972700

C	-3.96383900	-4.32311200	-0.44637200
H	-3.84239200	-2.73362000	0.99388300
C	-3.48984900	-4.83323200	-1.65552000
H	-2.12598500	-4.53206900	-3.29753500
H	-4.72477700	-4.85891900	0.10937400
H	-3.87886100	-5.76792100	-2.04223100
C	1.21702000	2.88799700	0.65445600
C	1.92039800	4.01952100	0.20254600
C	0.67009000	2.89877100	1.95088100
C	2.05280300	5.14199600	1.02089700
H	2.38532300	4.01193500	-0.77650100
C	0.80583800	4.02646100	2.76509000
H	0.15710200	2.02149600	2.32687700
C	1.49227200	5.14977500	2.30112700
H	2.60073500	6.00614600	0.66278100
H	0.37767700	4.02280100	3.76125900
H	1.59916600	6.02241100	2.93510500
C	2.51656900	1.38124000	-1.44182900
C	2.66346000	2.12965000	-2.62655600
C	3.58475800	0.57020800	-1.01761700
C	3.85208400	2.06847200	-3.35664400
H	1.85824000	2.75648400	-2.99060700
C	4.76881900	0.50395700	-1.75626700
H	3.48651800	-0.02262000	-0.11711700
C	4.90310600	1.25534400	-2.92475300
H	3.95234200	2.64974800	-4.26661700
H	5.55920400	-0.15944100	-1.42310500
H	5.81817900	1.19968400	-3.50296700
C	1.81754700	-0.43367600	2.67202700
O	2.42145000	-0.87757000	1.65259800
O	0.54981200	-0.24827400	2.58209900
C	2.54014800	-0.08340700	3.94185900
H	2.67113300	1.00351400	3.98401700
H	1.94991200	-0.38553500	4.81024100
H	3.52169900	-0.55837300	3.96338000
H	0.01006700	-2.23373100	1.25971200
C	1.14825600	-2.43960000	-0.54010300
O	1.71686500	-3.49224000	-0.36965800
O	0.82108500	-1.64929800	-1.45507900
C	5.22031700	-2.75550800	0.04939900
O	6.23797800	-2.10181600	-0.04002900
O	4.38545900	-2.85279900	-1.00573700
C	4.78700300	-3.48169000	1.30774000
H	4.49134700	-4.51264100	1.09003700
H	5.60611000	-3.47389800	2.02663100
H	3.91894000	-2.96738700	1.73325100
H	3.54907800	-3.29989800	-0.76928700

**Ru<sub>2</sub>dec-H-CO<sub>2</sub>**

Zero-point = -3273.377282

Ru	-1.08858000	-0.65622900	0.69375400
P	-3.28861000	-1.27277500	-0.37741100
P	-1.29316000	1.59586200	0.34301500
C	-3.00063600	2.24019100	-0.07361200
H	-3.52127000	2.26332200	0.89058400
H	-2.84640300	3.28436200	-0.35922500
C	-4.45528400	0.17764400	-0.55686100
C	-3.90735900	1.52439400	-1.11448000
C	-5.17916000	2.40561100	-1.33612800
H	-5.74824900	1.99989700	-2.18093500
H	-5.84102000	2.36673000	-0.45837800
P	-4.92495900	4.19994800	-1.66439800
H	-6.22793300	4.58177800	-2.08391100
H	-4.89093500	4.75871300	-0.35955400
O	-3.79575700	4.60963100	-2.56585800
H	-5.29265100	-0.14737900	-1.18512400
H	-4.85238900	0.35534600	0.44954500
C	-3.21273600	1.33026000	-2.47596900
H	-2.27945200	0.77267100	-2.37578100
H	-3.86204700	0.76963800	-3.15629400
H	-2.98194500	2.29263200	-2.93586400
C	-0.17064800	2.25775300	-0.95628800
C	-0.51924400	3.32617700	-1.80543000
C	1.12042600	1.70054500	-1.05389300
C	0.40006500	3.81347400	-2.73702200
H	-1.49940100	3.78596300	-1.77152300
C	2.03441300	2.20250900	-1.98286900
H	1.41490200	0.88625300	-0.40363600
C	1.67641400	3.25425400	-2.82812200
H	0.11181100	4.63024500	-3.38860900
H	3.02496500	1.76621500	-2.03978400
H	2.38668400	3.63743500	-3.55206000
C	-0.94831300	2.70093400	1.78432400
C	-1.71544000	2.56782600	2.95940000
C	0.06780400	3.66961100	1.74237700
C	-1.47130300	3.39159200	4.05837600
H	-2.47656400	1.79942900	3.02912500
C	0.30693600	4.48954100	2.84801700
H	0.67211200	3.78034400	0.85147800
C	-0.46106900	4.35508800	4.00506900
H	-2.06218700	3.27125300	4.95926500
H	1.09591000	5.23143700	2.80174100
H	-0.27030900	4.99055900	4.86210900
C	-3.41896800	-2.12563200	-2.01176600
C	-4.57715400	-2.83747700	-2.37491000
C	-2.35129200	-2.05008000	-2.92462800

C	-4.67026100	-3.44325400	-3.62835500
H	-5.39500000	-2.93687300	-1.67026900
C	-2.45150600	-2.65912400	-4.17875600
H	-1.44260000	-1.52881500	-2.64791700
C	-3.60958300	-3.35230500	-4.53399300
H	-5.56658500	-3.99174100	-3.89504200
H	-1.62270300	-2.59085300	-4.87450000
H	-3.68408400	-3.82542300	-5.50635200
C	-4.25258000	-2.39429800	0.72152600
C	-5.63763100	-2.27812900	0.93730300
C	-3.54906400	-3.43000600	1.36635700
C	-6.30271700	-3.17911400	1.77293500
H	-6.20676300	-1.48845200	0.46190200
C	-4.22055100	-4.32788700	2.19715100
H	-2.47734900	-3.51962300	1.22731000
C	-5.59650900	-4.20512800	2.40286200
H	-7.37029500	-3.07631900	1.93175100
H	-3.66397300	-5.11533700	2.69219600
H	-6.11368900	-4.89976600	3.05453400
C	0.16410200	-2.51654300	-0.50030400
O	-0.39884800	-2.79045400	0.60052000
O	0.05824900	-1.31933600	-0.95424500
C	0.90507400	-3.55522700	-1.29531900
H	0.24575400	-3.93782200	-2.08249600
H	1.78142500	-3.11094100	-1.77237000
H	1.20008000	-4.38354300	-0.64964000
H	0.36196300	-0.19768700	1.12728800
C	-0.87387900	-0.64759500	2.72112400
O	-0.04369000	-0.77454800	3.59449000
O	-2.11979200	-0.52845800	2.60818200
C	3.30651000	-0.76611700	2.27293800
O	2.80035600	-0.13833200	1.35706900
O	2.63891500	-1.24132600	3.32466100
C	4.78636500	-1.10049600	2.35428000
H	4.87469500	-2.18818400	2.47289100
H	5.16800100	-0.67600100	3.29214900
H	1.67804500	-1.00543300	3.27532600
C	5.59388600	-0.60447500	1.15473600
H	5.17809500	-1.03933700	0.23753400
H	5.45957900	0.47938800	1.05649500
C	7.08668400	-0.93856600	1.25924500
H	7.49591500	-0.50187900	2.18176800
H	7.21329300	-2.02634400	1.35943800
C	7.90410700	-0.44269500	0.05963700
H	7.49510700	-0.87977900	-0.86259000
H	7.77687400	0.64477100	-0.03984700
C	9.39933400	-0.77105900	0.15596800
H	9.52659600	-1.85870200	0.25480200



H	9.80796200	-0.33456900	1.07865900
C	10.21519100	-0.27296900	-1.04385200
H	10.08753800	0.81467300	-1.14245100
H	9.80634700	-0.70935200	-1.96659500
C	11.71073300	-0.60005300	-0.94924200
H	11.83970600	-1.68772900	-0.85156300
H	12.12067200	-0.16401200	-0.02674900
C	12.52633100	-0.10101400	-2.14886900
H	12.39801800	0.98578900	-2.24597700
H	12.11705200	-0.53697000	-3.07055100
C	14.01874900	-0.43181000	-2.04653400
H	14.18135500	-1.51397900	-1.98359600
H	14.57251000	-0.06291600	-2.91627400
H	14.46437900	0.01998400	-1.15279400

**Ru<sub>2</sub><sub>hex</sub>-H-decanoic**

Zero-point = -3273.366735

Ru	-0.44452700	-0.04485300	0.88138800
P	-1.28199400	1.96271800	-0.15896500
P	-1.97690800	-1.40346600	-0.03846800
C	-2.97416100	-0.79048300	-1.50450200
H	-2.29889900	-0.86365500	-2.36339300
H	-3.76250800	-1.52893700	-1.67131800
C	-2.45681600	1.71916200	-1.60062100
C	-3.57508900	0.64212900	-1.47750400
C	-4.45070400	0.83166600	-2.75767500
H	-5.01611700	1.76708600	-2.66854500
H	-3.81860500	0.92701500	-3.65364500
P	-5.65547900	-0.49272200	-3.18134800
H	-6.37632300	0.13857200	-4.23284500
H	-4.86437100	-1.41033500	-3.92362200
O	-6.48758500	-1.10161600	-2.09047100
H	-2.92041300	2.68568800	-1.83197500
H	-1.82082700	1.44335600	-2.44896300
C	-4.46922100	0.88274000	-0.24595700
H	-3.91896700	0.72799400	0.68374400
H	-4.84280500	1.91225000	-0.24307400
H	-5.32529100	0.20472100	-0.25019700
C	-3.25336200	-2.06942300	1.12754600
C	-4.54659200	-2.46322300	0.73417700
C	-2.87759300	-2.23467400	2.47462500
C	-5.43587200	-3.00422400	1.66537200
H	-4.89272200	-2.33854800	-0.28427300
C	-3.76874400	-2.78655400	3.39804500
H	-1.89400900	-1.91202400	2.79076000
C	-5.04907800	-3.17157000	2.99677800
H	-6.43133200	-3.29002400	1.34514600
H	-3.46098300	-2.90775700	4.43076600

H	-5.74245000	-3.59371600	3.71555300
C	-1.34205100	-2.98622900	-0.79110900
C	-0.63296600	-2.96502700	-2.00700200
C	-1.48580700	-4.21534900	-0.12395000
C	-0.09331500	-4.13628800	-2.54111300
H	-0.48536000	-2.02932900	-2.53329500
C	-0.93694100	-5.38470600	-0.65724900
H	-2.02415800	-4.25703000	0.81417000
C	-0.24204100	-5.35080200	-1.86744000
H	0.44607700	-4.10082500	-3.48187000
H	-1.05906600	-6.32206800	-0.12611300
H	0.17889400	-6.25986900	-2.28152900
C	-2.14452100	3.31155900	0.78491500
C	-2.24962500	4.62216800	0.28328400
C	-2.73937700	3.01029100	2.02309900
C	-2.94388700	5.60119300	0.99523000
H	-1.77358700	4.88234300	-0.65564000
C	-3.43453100	3.99492800	2.73185700
H	-2.64242300	2.01146900	2.43198000
C	-3.54089700	5.28881100	2.21995300
H	-3.01441200	6.60780000	0.59791300
H	-3.89086900	3.74722400	3.68399600
H	-4.07893800	6.05109800	2.77201400
C	0.06409100	2.95555200	-0.97201100
C	-0.00423900	3.51573000	-2.26028900
C	1.25711300	3.11004600	-0.23511300
C	1.08741700	4.20483000	-2.80010000
H	-0.90786600	3.42253400	-2.85080300
C	2.34218200	3.80390400	-0.77507800
H	1.33058800	2.66808900	0.75400700
C	2.26327700	4.34954100	-2.06060900
H	1.01360600	4.63647700	-3.79267700
H	3.24909000	3.91722300	-0.19103400
H	3.10632400	4.88886100	-2.47758000
C	-0.15746400	0.96399100	3.20878000
O	0.79159300	1.09843400	2.38081400
O	-1.22587800	0.36581200	2.83351700
C	-0.07148900	1.53016600	4.60344100
H	-0.57508100	2.50337000	4.62473700
H	-0.57774400	0.87250900	5.31383700
H	0.97158500	1.67007800	4.89207100
H	0.14818500	-1.39866000	1.55761300
C	1.76488300	-3.61324300	1.25636600
O	2.36825000	-3.23630800	0.32696300
O	1.20214900	-4.03238500	2.19121600
C	1.47972700	-0.00205100	-1.69403700
O	1.13447400	-0.23194600	-0.55060500
O	0.54443600	0.16329200	-2.66203100

C	2.92586300	0.11863500	-2.11585200
H	3.10129400	-0.58816200	-2.94019400
H	3.05684500	1.12697700	-2.53652000
H	0.97269500	0.43692600	-3.48604300
C	3.91840300	-0.11968700	-0.97482700
H	3.71308000	0.60157600	-0.17633500
H	3.73555400	-1.11021300	-0.54594700
C	5.37668400	0.00178600	-1.43253900
H	5.57099200	-0.71909600	-2.24015900
H	5.54593500	0.99796200	-1.86716600
C	6.37994200	-0.23172800	-0.29578000
H	6.20840300	-1.22692200	0.13717000
H	6.18386300	0.48694100	0.51222400
C	7.84411000	-0.11389000	-0.73732400
H	8.01426800	0.88222300	-1.17100000
H	8.03868900	-0.83281700	-1.54624500
C	8.84654700	-0.34851500	0.39992600
H	8.67607400	-1.34438100	0.83313400
H	8.65129600	0.36970600	1.20901600
C	10.31153600	-0.23110400	-0.03891100
H	10.48299200	0.76510200	-0.47197300
H	10.50759700	-0.94945100	-0.84812600
C	11.31408400	-0.46616700	1.09819900
H	11.14316800	-1.46155900	1.53038400
H	11.11843900	0.25167800	1.90645100
C	12.77476900	-0.34708800	0.65175400
H	12.98568300	0.64958700	0.24717100
H	13.46425400	-0.51987300	1.48466800
H	13.01061600	-1.07666200	-0.13157300

### S13. References

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