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On the Importance of Decarbonylation as Side Reaction in the Ruthenium-Catalyzed Dehydrogenation of Alcohols: a Combined Experimental and Density Functional Study

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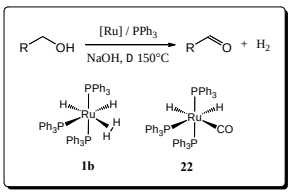
Abstract: We report a density functional study (B97-D2 level) of mechanism(s) operating in the alcohol decarbonylation occurring as an important side reaction during dehydrogenation catalysed by $[RuH_2(H_2)(PPh_3)_3]$. Using MeOH as substrate, three distinct pathways are fully characterized involving either neutral tris- or bis(phosphines), or anionic bis(phosphine) complexes after deprotonation. α-agostic formaldehyde and formyl complexes are key intermediates, and the computed rate-limiting barriers are similar between the various decarbonylation and dehydrogenation paths. Key steps are also studied for EtOH and iPrOH as substrates, rationalizing the known resistance of the latter toward decarbonylation. Kinetic isotope effects (KIEs) are predicted computationally for all pathways, and studied experimentally for one specific decarbonylation path designed to start from $[RuH\{OCH_3\}(PPh_3)_3]$. From the good accord between computed and experimental KIE (observed $k_H/k_D = 4$), the rate-limiting step for methanol decarbonylation is ascribed to the formation of the first agostic intermediate from a transient formaldehyde complex.

Keywords: Hydrogen generation • Mechanisms • Catalysis • Density Functional Theory • KIEs

Introduction

Hydrogen production from biomass derivatives has attracted increasing interest over the last decade and is now considered as a serious, more sustainable alternative to fossil energy sources. The key technological challenge we are facing today is to develop active catalysts that would allow for the conversion of biomass products into molecular hydrogen under mild conditions. Several homogenous catalysis systems have been developed, allowing conversion of simple organic substrates into molecular hydrogen without requiring any hydrogen acceptor.[1] Besides recent progress with formic acid as hydrogen carrier,[2] simple aliphatic alcohols have attracted particular interest,[3] because they can be readily obtained from biomass.[4] Hydrogen can be released *via* transition-metal catalyzed dehydrogenation of the substrates and the first very active system was developed by Morton and Cole-Hamilton, showing that high turnover frequencies (TOFs) for production of H_2 can be obtained at 150 °C, using the $[RuH_2(X)(PPh_3)_3]$ catalyst (where X = N_2, PPh_3 or H_2) in the presence of a base.[5] Several alcohol substrates have been screened, showing that methanol is only poorly converted whereas higher alcohols are more reactive. Subsequent studies report even higher activities at milder temperature, obtained by modifying the nature of the ligands and of the base.[3b-d] However, further progress is limited by the fundamental understanding of the developed systems, as the latter generally involve multistep reactions and a plethora of short-lived reaction intermediates that are hardly characterizable by routine physico-chemical methods. As a result, the reasons why one system is more active than another still remain difficult to rationalize, and the development of new, more active, systems is tied to the success of a rather empirical "trial-and-error" approach.



Scheme 1: Alcohol dehydrogenation catalysed by **1b**. The decarbonylation side-reaction affords the carbonyl complex **22** (compound labels consistent with those in reference [6]).

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Morton and Cole-Hamilton's system[5] represents a prototypical example of how complicated such catalytic systems can be. While it does produce the desired hydrogen, there are also a number of side reactions that limit its practical use. Not only can the produced aldehydes undergo aldol and Tischenko reactions under the reaction conditions, they can also react with the Ru catalyst in a decarbonylation reaction generating carbonyl complexes such as $[RuH_2(CO)(PPh_3)_3]$ (**22**, see Scheme 1). **22** is also active as a dehydrogenation catalyst,[5, 7] adding to the complexity of the system.[8] As **22** can be readily prepared under similar conditions (in methanol or ethanol, in presence of base and under a flux of hydrogen gas), [9] there should be a significant driving force for its formation under catalytic conditions, at the expense of dehydrogenation. Support for this scenario comes from the observation of higher TOFs for dehydrogenation under irradiation conditions,[5] which is expected to induce photodissociation of the coordinated CO ligands and regenerate the active catalyst **1**. A comprehensive picture of this catalytic system at the molecular level would therefore require the understanding of all these individual reactions, and detailed insights into the ways how they are (inter)connected.

We recently undertook a computational study of the mechanism for dehydrogenation catalysed by **1b**, comparing methanol, ethanol and 2-propanol as substrates.[6] Our results showed that the system can follow multiple reaction channels as several pathways with very close activation energies were characterized. Moreover, the nature of the rate-limiting step was found to depend on the nature of the substrate, and the height of the corresponding activation barriers was found to follow the experimental trends of TOFs (where ethanol reacts better than methanol).

We now present an extension of our first mechanistic study to the decarbonylation reaction. The same methodology, based on the density-functional theory (DFT) protocol validated previously[10] is employed, thus allowing for consistent comparisons with the dehydrogenation results.[6] The main questions to be addressed are: What is the precise mechanism of the decarbonylation reaction in the system? How does its activation energy compare with that of dehydrogenation? And why is the catalytic system more active with 2-propanol and ethanol than with methanol as substrate? To answer these questions, three alternative decarbonylation routes are investigated, which differ in the number of coordinated phosphine ligands and in the charge of the active species, and key barriers are evaluated for different alcoholic substrates. As it turns out, the barriers are rather similar for dehydrogenation and decarbonylation, both decreasing from methanol to ethanol, while, as expected because β□methyl rather than hydride abstraction would be required, higher decarbonylation barriers are obtained for 2-propanol. For methanol, the plausibility of the predicted reaction mechanism is validated through computation and the first experimental determination of a salient kinetic isotope effect (KIE).

Results and Discussion

This section is organized as follows: Using methanol as substrate, we first investigate a pathway where all three PPh_3 ligands remain coordinated to the metal (pathway **E**). Next, a reaction channel involving dissociation of one of them is explored (pathway **F**), followed by a path involving deprotonation in addition (pathway **G**). Subsequently, key parts of the pathways are recomputed for ethanol and 2-propanol as substrates and overall activation parameters of dehydrogenation and decarbonylation paths are compared. Finally, KIEs are evaluated for the turnover- and rate-limiting steps and compared to new experimental results for this property.

The labelling of the paths and intermediates is consistent with our previous study, where the pathways **A** to **D** have been described and involve complexes **1**-**18**.[6] Labeling of new intermediates and products starts with **19**.

The new (decarbonylation) paths are presented in Figures 1 and 3-5 along with the corresponding free energy profiles computed at an average computational level (noted ECP2 ; see Computational Details). The corresponding free energy differences of every elementary steps are gathered in Tables 1 and 2. In Table 3, we report the overall activation free energies for all the pathways using a higher computational level (noted ECP3) and a more elaborated approach to correct for the basis set superposition error (noted BSSE). BSSE is inherent in DFT calculations involving finite basis sets, and it can be significant at the ECP2 level *e.g.* as far as dissociation of bulky phosphines is concerned.[10] The use of the larger ECP3 basis sets and of a systematic BSSE correction is therefore required to be able to compare one pathway to another, as done in Table 3.

Reaction mechanisms involving methanol as substrate.

Pathway E. This channel involves ruthenium complexes retaining their three coordinated PPh_3 ligands, as suggested in the early study of Wilkinson et al.[11] It departs from the dehydrogenation pathway **B** (from Ref [6]) after formation of the product, formaldehyde, when it is still coordinated side-on to the metal (complex **9** in Figure 1). Rather than dissociating via the κ^1-coordinated intermediate **10** and closing the dehydrogenation cycle, formaldehyde can be further dehydrogenated affording H_2 and the carbonyl complex **22** (Scheme 1). A plausible stepwise process involves first transfer of one hydrogen atom affording a formyl complex **20**, followed by dissociation of H_2 to create a vacant coordination site. The latter can accept the second hydrogen atom, forming the decarbonylation product, **22** (Figure 1a). It turns out that the first H-transfer involves an additional intermediate, the α-agostic formaldehyde complex **19**, which is the highest point on the path (via $\mathbf{TS_{9perp\text{-}19}}$, see Figure 2).

The importance of agostic M...H-C bonds for organometallic chemistry is well recognised.[12] They are prevalent for aliphatic (or aromatic) C-H bonds and usually involve coordinatively unsaturated or electron-deficient metal centres (see also the following section). Because **9-*perp*** is an 18-electron complex with a fully saturated coordination sphere, little propensity for formation of an agostic bond is to be expected, consistent with our findings that this is an endothermic process with significant activation.

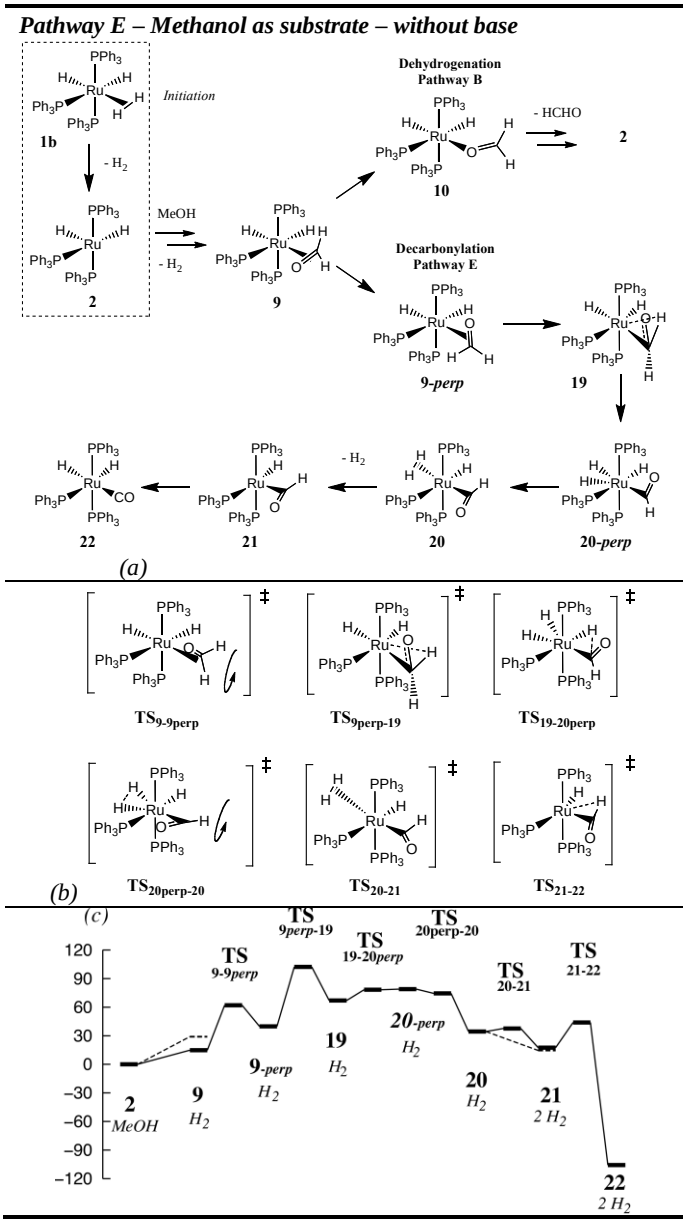

Figure 1: Reaction pathway **E** (decarbonylation) and its link with the previously investigated pathway **B** (dehydrogenation): schematic representation of *(a)* intermediates and *(b)* the transition states; *(c)* free energy profile (kJ/mol), with calculations carried at the B97-D2/ECP2 level of theory using methanol as model solvent. The dashed lines indicate BSSE corrected energies. Reaction energies are given in Table 1.

Decay of the agostic complex to the formyl derivative **20** is facile,[13] as is the further formation of the carbonyl complex **22**. Formyl complexes can be prepared by various routes (such as hydride addition to a metal-CO moiety),[14] and some are stable enough to be characterised through X-ray crystallography.[15] Usually they are quite reactive and are frequently invoked as intermediates in a variety of reactions, *e.g.* carbon monoxide hydrogenation.[16] Involvement of **20** in the path studied is thus entirely plausible.

In contrast to dehydrogenation, which is an endergonic process (cf. the computed driving force for **1b** + MeOH → **1b** + H_2CO + H_2, ΔG = + 50.5 kJ/mol),[6] formation of the carbonyl complex is strongly exergonic, cf. the reaction:

$$\mathbf{1b} + \mathrm{MeOH} \rightarrow \mathbf{22} + 3\ H_2, \quad \Delta G = -84.5\ \mathrm{kJ/mol} \quad (4)$$

Table 1: Reaction energies (ΔE), Correction Terms for BSSE (δE_{BSSE}), Solvation (δE_{solv}), Thermochemistry (δE_G), and Resulting Reaction Free Energies (ΔG) for pathways **E**-**G** (all data in kJ/mol).[a]

	ΔE	δE_{BSSE}	δE_{solv}[b]	δE_G	ΔG
Overall (methanol)					
MeOH → HCHO + H_2	100.4	0.0	2.1	-52.0	50.5
1b + MeOH → **22** + 3 H_2	-14.4	0.0	11.9	-81.9	-84.5
Pathway E (methanol)					
1b → **2** + H_2	69.9	-4.2	-0.2	-48.5	20.2
2 + MeOH → **9** + H_2	-17.6	14.2	16.4	16.1	29.1
9 → **9-*perp***	21.2	0.0	-0.5	4.4	25.0
9-*perp* → **19**	38.7	0.0	-5.4	-6.2	27.1
19 → **20-*perp***	18.8	0.0	-1.8	-5.0	12.0
20-*perp* → **20**	-40.5	0.0	-2.2	-1.8	-44.5
20 → **21**	23.5	-2.9	2.2	-42.6	-19.8
21 → **22**	-128.5	0.0	3.5	1.8	-123.2
9 → $\mathbf{TS}_{\mathbf{9\text{-}9perp}}$	41.8	0.0	-2.8	8.2	47.2
9-*perp* → $\mathbf{TS}_{\mathbf{9perp\text{-}19}}$	72.1	0.0	-4.8	-4.7	62.5
19 → $\mathbf{TS}_{\mathbf{19\text{-}20perp}}$	16.5	0.0	-1.3	-3.9	11.3
20-*perp* → $\mathbf{TS}_{\mathbf{20perp\text{-}20}}$	-0.8[c]	0.0	-1.8	-1.8	-4.5
20 → $\mathbf{TS}_{\mathbf{20\text{-}21}}$	17.0	0.0	2.7	-16.5	3.2
21 → $\mathbf{TS}_{\mathbf{21\text{-}22}}$	19.1	0.0	0.4	6.8	26.3
Pathway F (methanol)					
1b + MeOH → **13H** + H_2 + PPh_3	216.3	-28.0	-5.9	-87.7	94.6
13H → **23**-*perp* + H_2	52.0	-3.4	-5.6	-29.9	13.2
23-*perp* → **23**	1.0	0.0	2.3	-5.2	-1.9
23 → **24**	9.1	0.0	-1.7	-3.0	4.3
24 → **25**	-7.7	0.0	0.4	-4.0	-11.3
25 → **26b**-*trans*	-106.2	0.0	0.4	-19.7	-125.5
26b-*trans* → **26a**	13.3	0.0	4.1	-0.4	17.0
26a → **26b**-*cis*	-36.5	0.0	-0.8	14.4	-22.9
26b-*cis* → **27** + H_2	55.4	-3.3	-2.4	-41.9	7.8
27 + PPh_3 → **22**	-211.2	41.5	21.1	95.6	-52.9
13H → $\mathbf{TS}_{\mathbf{13H\text{-}23perp}}$	46.3	0.0	-3.2	-9.9	33.2
23-*perp* → $\mathbf{TS}_{\mathbf{23perp\text{-}23}}$	7.9	0.0	0.9	-3.2	5.6
23 → $\mathbf{TS}_{\mathbf{23\text{-}24}}$	13.4	0.0	0.1	2.1	15.5
24 → $\mathbf{TS}_{\mathbf{24\text{-}25}}$	10.4	0.0	1.7	-4.2	7.9
25 → $\mathbf{TS}_{\mathbf{25\text{-}26b\text{-}trans}}$	13.7	0.0	-5.9	-9.7	-2.0
26b-*trans* → $\mathbf{TS}_{\mathbf{26b\text{-}trans\text{-}26a}}$	18.8	0.0	2.4	1.3	22.4
26a → $\mathbf{TS}_{\mathbf{26a\text{-}26b\text{-}cis}}$	-0.2	0.0	-0.3	5.3	4.9
26b-*cis* → $\mathbf{TS}_{\mathbf{26b\text{-}cis\text{-}27}}$	49.7	0.0	-1.9	-14.8	32.9
27 + PPh_3 → $\mathbf{TS}_{\mathbf{27\text{-}22}}$	-75.0	0.0	16.8	59.0	0.8
Pathway G (methanol)					
1b + MeO^- → **13** + H_2 + PPh_3	35.4	-24.3	112.6	-63.7	60.0
13 → **28**	30.1	0.0	-7.5	-14.9	7.7
28 → **29a-*perp***	-5.0	0.0	-0.3	-12.2	-17.5
29a-*perp* → **29a**	1.4	0.0	-3.1	8.0	6.3
29a → **29b-*trans***	5.8	0.0	-4.8	-6.3	-5.3
29b-*trans* → **30** + H_2	19.0	-2.5	6.1	-31.4	-8.7
30 → **31**	-90.2	0.0	3.6	-2.6	-89.2
31 + MeOH → **26b-*cis*** + MeO^-	144.9	0.0	-113.4	-12.6	18.8
26b-*cis* → **27** + H_2	55.4	-3.3	-2.4	-41.9	7.8
27 + PPh_3 → **22**	-211.2	41.5	21.1	95.6	-52.9
13 → $\mathbf{TS}_{\mathbf{13\text{-}28}}$	91.9	0.0	-1.8	-18.7	71.4
28 → $\mathbf{TS}_{\mathbf{28\text{-}29a}}$	1.6	0.0	0.5	-7.2	-5.1
29a-*perp* → $\mathbf{TS}_{\mathbf{29aperp\text{-}29a}}$	3.1	0.0	-3.1	14.8	14.8
29a → $\mathbf{TS}_{\mathbf{29a\text{-}29btrans}}$	9.4	0.0	-7.5	1.2	3.2
29b-*trans* → $\mathbf{TS}_{\mathbf{29btrans\text{-}30}}$	18.6	0.0	13.9	-5.3	27.1
30 → $\mathbf{TS}_{\mathbf{30\text{-}31}}$	17.5	0.0	0.9	-4.0	14.5
26b-*cis* → $\mathbf{TS}_{\mathbf{26bcis\text{-}27}}$	49.7	0.0	-1.9	-14.8	32.9
27 + PPh_3 → $\mathbf{TS}_{\mathbf{27\text{-}22}}$	-75.0	0.0	16.8	59.0	0.8

a B97-D2/ECP2 energies. $\Delta G = \Delta E + \delta E_{BSSE} + \delta E_{solv} + \delta E_G$.
b MeOH has been used as solvent. *c* ΔE = +2.1 kJ/mol at the RI-BP86/ECP1 level

There is a substantial driving force for decarbonylation. Kinetic preferences of this route versus dehydrogenation will be discussed at the end of this section.

Pathway F. For the dehydrogenation step, Van der Sluys *et al.*[17] have proposed the transient dissociation of one PPh_3 ligands from **1**.[18] Our own computational results have corroborated this scenario, finding such paths competitive, if not preferred for the higher alcohols.[6] Because both tris-and bis(phosphine) intermediates are plausible intermediates,[6-7, 19] we now turn to a mechanistic alternative for decarbonylation involving phosphine dissociation. To make this path comparable to the one just discussed, we start from isomer **13H** on the dehydrogenation pathway **C**(neutral), see Figure 3a.

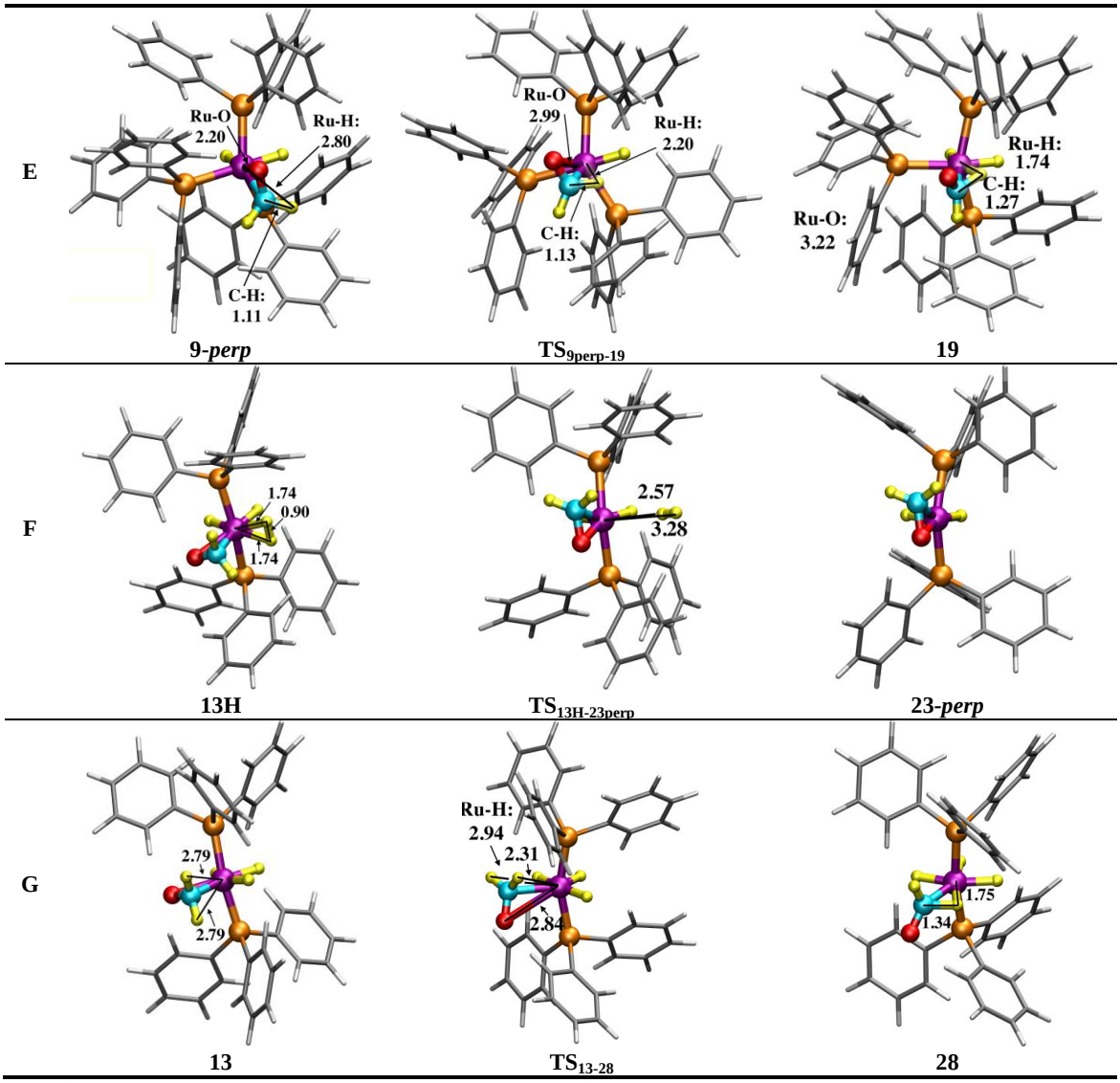

Figure 2: Structure of intermediates and transition states involved in the rate-limiting steps of the decarbonylation pathways **E**-**G**, with methanol as initial substrate. Paths **E** and **G**: Formation of the α-agostic complex **19** from **9-*perp***; Path **F**: Dissociation of H_2 and rotation of HCHO. RI-BP86/ECP1 optimized structures. Selected interatomic distances are given in Å. Additional snapshots are provided in Supporting Information (see Figures S1-S3).

Rather than expelling the aldehyde and closing the dehydrogenation cycle, this isomer can lose an H_2 ligand, forming the 16e-species **23-*perp*** (see Figure 2). The latter can form an α-agostic intermediate (**24**, akin to **19** on path **E**), which connects to **22**, i.e. the same final decarbonylation product as on path **E**, via a sequence of iomerization and ligand exchange reactions (Figure 3a).

Reaction energies are collected in Table 1 and the resulting free-energy profile is shown in Figure 3c. Interestingly, it is the dissociation of H_2 from **13H** that is indicated to be rate-limiting on the path (via **$TS_{13H\text{-}23perp}$**, see Figures 3b and 2). Again, the aldehyde rotation and the hydrogen transfer leading to the formyl complex **25** proceeds via a succession of almost barrierless processes, and a strong driving force is obtained for the formation of the carbonyl complex **26a**. The interconversion between non-classical and classical hydrides **26(b/a)** involves small activation barriers (below 22.4 kJ/mol), a feature which is consistent with the well-known fluxional behaviour of transition-metal hydrides, in which scrambling motions can be observed.[20] The relative stabilities of **26b-cis**, **26a** and **26b-trans** are known to result from a subtle balance between the interactions with the *cis*- hydrides[21] and the *trans*- carbonyl[22] ligands, and strongly depend on the nature of the metal and ancillary ligands.[23] Finally, loss of molecular hydrogen from **26b-cis** is facile, and a significant driving force for recoordination of a triphenylphosphine ligand is obtained, therefore generating **22**. Phosphine recoordination only involves a small activation barrier, in keeping with experimental data on the parent, tris-triphenylphosphine complex.[24]

Pathway G. Both pathways **E** and **F** depart from neutral complexes, following the observation that decarbonylation can be accomplished in the absence of base.[17] Dehydrogenation is facilitated by base, however,[5] so that under turnover conditions deprotonated, anionic intermediates are possible. We therefore studied another entry into decarbonylation, starting from the intermediate **13** (Figure 4a) on dehydrogenation path **C**. This anionic intermediate is related to neutral **13H** (Figure 3a) through simple deprotonation (i.e. **13H** + $MeO^- \rightarrow$ **13** + MeOH).

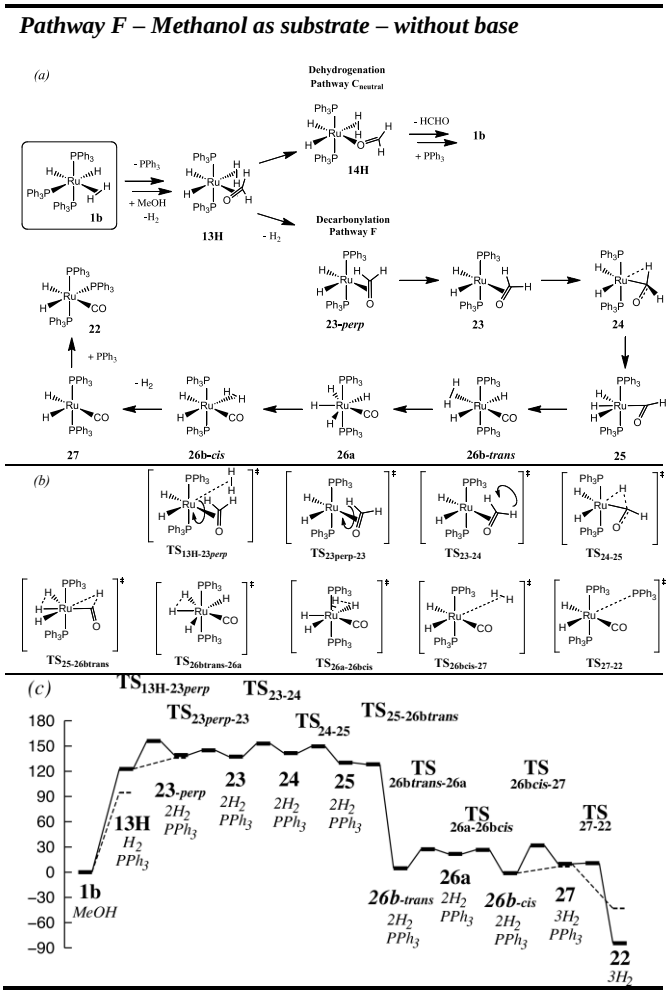

Figure 3: Reaction pathway **F** (decarbonylation) and its link with the previously investigated pathway **C** (dehydrogenation): schematic representation of *(a)* intermediates and *(b)* the transition states; *(c)* free energy profile (kJ/mol), with calculations carried at the B97-D2/ECP2 level of theory using MeOH as model solvent. The dashed lines indicate BSSE corrected energies. Reaction energies are given in Table 1.

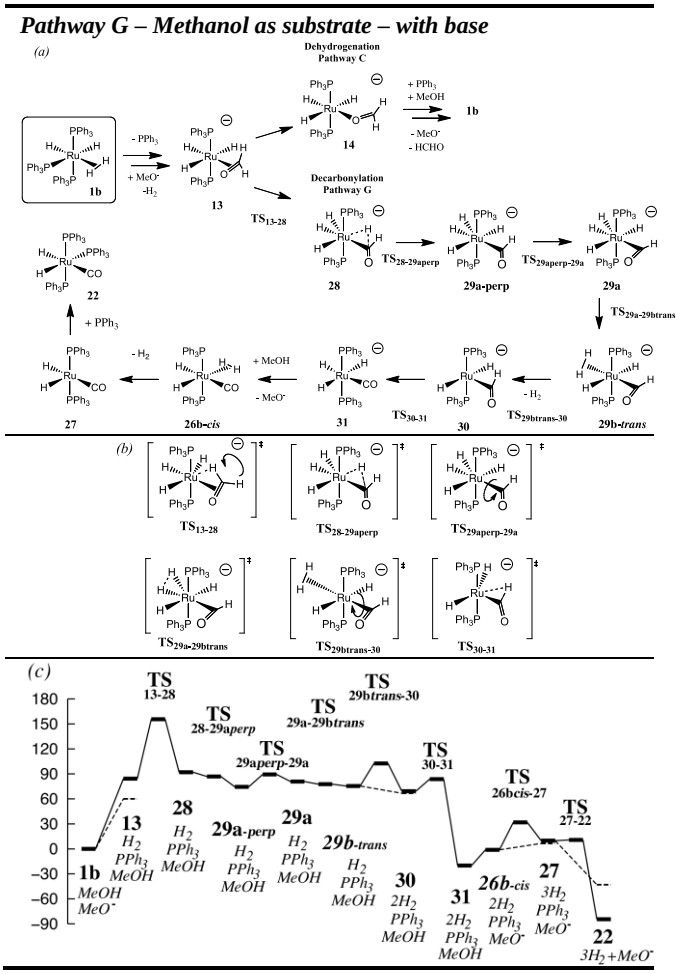

Figure 4: Reaction pathway **G** (decarbonylation) and its link with the previously investigated pathway **C** (dehydrogenation): schematic representation of (a) intermediates and *(b)* the transition states; *(c)* free energy profile (kJ/mol), with calculations carried at the B97-D2/ECP2 level of theory using MeOH as model solvent. The dashed lines indicate BSSE corrected energies. Reaction energies are given in Table 1.

Reaction energies are collected in Table 1 and the resulting free-energy profile is shown in Figure 4c. As with **9** (or **9**-*perp*) on pathway **E** (Figure 1a), **13** is coordinatively saturated, and formation of the first α-agostic intermediate **28** entails the largest kinetic impediment (via $\mathbf{TS_{13\text{-}28}}$, Figures 4b and 2). All further steps leading to the carbonyl complex **31** (ligand rotations, H-transfers and H_2 dissociation) are indicated to be facile, requiring little activation.

The observed[5] complex **22** is readily obtained from **31** through re-protonation and release of H_2. The latter step (via $\mathbf{TS_{26bcis\text{-}27}}$) is indicated to be the most difficult on this section, but the overall barrier of ΔG = 51.7 kJ/mol relative to **31** (Table 3, 18.8 kJ/mol + 32.9 kJ/mol) is easily overcome under the reaction conditions.

Reaction mechanisms with other substrates (ethanol and 2-propanol).

We now turn to the reaction profiles when ethanol or 2-propanol are used as substrates instead of methanol. As a reaction mechanism coinciding with pathway **F** has been studied experimentally with ethanol,[17] we recomputed the full reaction profile with this substrate, in order to better understand the similarities and differences observed when moving from one alcohol to the other. We kept the same labelling as for methanol, adding either a "prime" or a "double prime" to denote the ethanol, and 2-propanol analogues, respectively.With ethanol, we found a very similar reaction profile (Figure 5, Table 4), in which the α-H transfer occurs via the formation of **23'** exhibiting an agostic interaction with the metal (although in this case a transient β-agostic interaction involving the $(CO)CH_3$ group is formed first, viz. **23**''). The transfer of the methyl group occurs in a concerted fashion via a three-membered ring (-[Ru]-$C(H_3)$-C(O)-), and involves only a small activation barrier. This step (i.e. **25'** → **26a**') is the reverse of migratory CO insertion into a metal-CH_3 bond, a process which is known to occur readily in certain types of complexes.[25] Formation of **25'** is also thermodynamically favourable, as are the methane decoordination and phosphine recoordination steps. Species related to **25'**, **26a'** and **27** have recently been characterized in a mechanistic study of alcohol decarbonylation at an Ir pincer complex.[26] Importantly, the rate-limiting step is the H_2 dissociation from **13H'**, as in the case of methanol, although the subsequent rearrangement of the β-agostic intermediate via $\mathbf{TS'_{23\text{-}24}}$ has a similar, only slightly lower barrier (see the two entries for pathway **F** with EtOH in Table 3).

Because only the very first steps are important to obtain the overall activation barrier, we did not repeat the calculations of the full remaining paths with ethanol or 2-propanol. Judging from the results for methanol, the barrier for pathway **E** is somewhat higher than those of pathways **F** and **G**, and this feature should be even more pronounced with the more bulky ethanol and 2-propanol

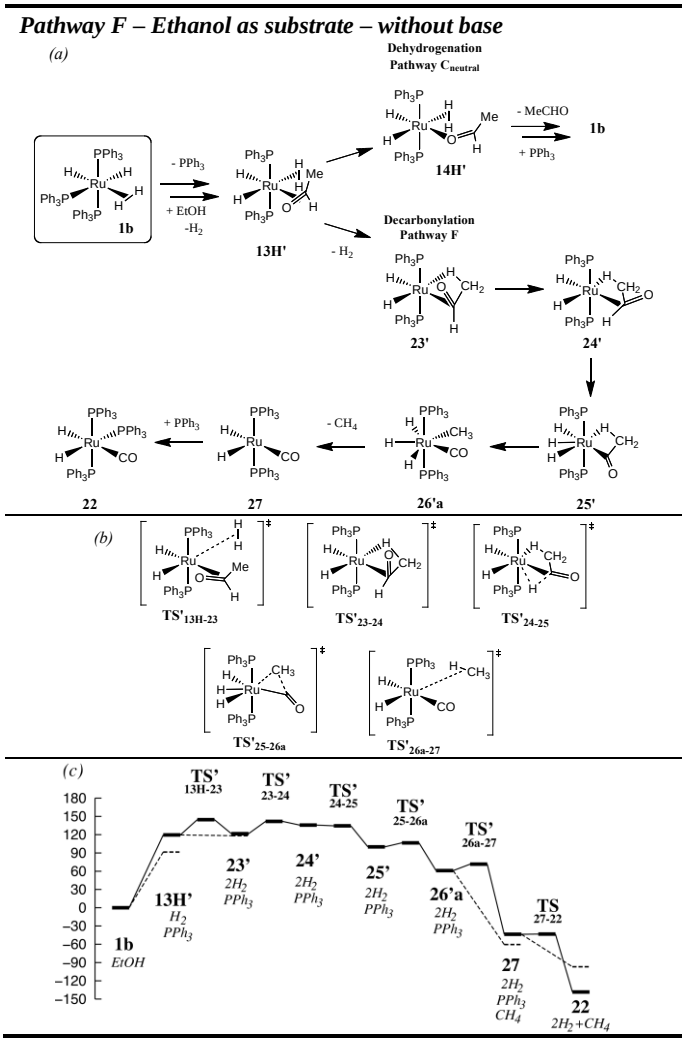

Figure 5: Reaction pathway **F** (decarbonylation) using EtOH as substrate and its link with the previously investigated pathway **C** (dehydrogenation); schematic representation of *(a)* intermediates and *(b)* the transition states; *(c)* free energy profile (kJ/mol), with calculations carried at the B97-D2/ECP2 level of theory using EtOH as model solvent. The dashed lines indicate BSSE corrected energies. Reaction energies are given in Table 2.

substrates.[27] We therefore only studied pathways **F** and **G** to gauge the possible spread of barriers between the mechanistic alternatives, focusing on the steps leading to the rate-limiting transition state. Overall activation barriers are reported in Table 3 and are discussed in more detailled in the next section.

On pathway **G**, these first steps are rather similar with MeOH and EtOH, with essentially identical barriers via $\mathbf{TS_{13\text{-}28}}$ and $\mathbf{TS'_{13\text{-}28}}$, respectively. Likewise, on pathway **F** (i.e. without base) similar barriers are obtained for EtOH and MeOH (slightly lower for the former, by ca. 10 kJ/mol, Table 3). It thus appears that both methanol and primary alcohols such as ethanol should decarbonylate similarly well. In contrast, the secondary alcohol iPrOH (or more specifically, its primary dehydrogenation product, acetone) is rather more resistant to decarbonylation,[28] making it a popular substrate for model studies of alcohol dehydrogenation.[3b, c] We were thus expecting rather high barriers on pathways **F** and **G** with 2-propanol. In fact, the very location of transition states proved tricky with that substrate, and those that could be found were indeed rather high in energy. Occasionally, somewhat unexpected departures from the paths established for MeOH and EtOH were found. For instance, the transition state resembling $\mathbf{TS"_{24\text{-}25}}$ on pathway **F** has a very high barrier of 182 kJ/mol (Table 3), but was found through IRC calculations to connect to a minimum with an unusual bis(β-agostic)

Table 2: Reaction energies (ΔE), Correction Terms for BSSE (δE_{BSSE}), Solvation (δE_{solv}), and Thermochemistry (δE_G), and Resulting Reaction Free Energies (ΔG) for pathway **F** with ethanol (all data in kJ/mol).[a]

	ΔE	δE_{BSSE}	δE_{solv} [b]	δE_G	ΔG
Overall (ethanol)					
EtOH → MeCHO + H_2	74.8	0.0	-1.8	-56.5	16.4
1b + EtOH → **22** + 2 H_2 + CH_4	-71.8	0.0	10.2	-76.8	-138.4
Pathway F (ethanol)					
1b + EtOH → **13H'** + H_2 + PPh_3	203.5	-28.0	-5.7	-78.3	91.5
13H' → **23'** + H_2	38.5	-3.1	-3.1	-33.4	-1.2
23' → **24'**	30.0	0.0	-6.1	-9.7	14.3
24' → **25'**	-32.2	0.0	-0.3	-3.2	-35.7
25' → **26'a**	-39.8	0.0	8.2	-7.6	-39.2
26'a → **27** + CH_4	-60.7	-16.8	-3.6	-40.2	-121.3
27 + PPh_3 → **22**	-211.2	41.5	20.7	95.6	-53.3
13H' → $\mathbf{TS'_{13H\text{-}23}}$	42.6	0.0	-0.2	-17.3	25.1
23' → $\mathbf{TS'_{23\text{-}24}}$	34.5	0.0	-5.8	-8.4	20.3
24' → $\mathbf{TS'_{24\text{-}25}}$	5.5	0.0	0.1	-6.8	-1.3
25' → $\mathbf{TS'_{25\text{-}26a}}$	3.1	0.0	4.6	-1.2	6.5
26'a → $\mathbf{TS'_{26a\text{-}27}}$	15.6	0.0	0.8	-5.9	10.6
27 + PPh_3 → $\mathbf{TS_{27\text{-}22}}$	-75.0	0.0	16.5	59.0	0.5

a B97-D/ECP2 energies. $\Delta G = \Delta E + \delta E_{BSSE} + \delta E_{solv} + \delta E_G$. *b* Solvent: EtOH.

Table 3: Refined Free Energies (in kJ/mol, at the B97-D2/ECP3 level) for Overall Activation Barriers of Pathways **A**-**D** (dehydrogenation, from Ref [6]) and **E**-**G** (decarbonylation).[a]

		ΔE	$\delta E'_{BSSE}$ [b]	δE_{solv}	δE_G	ΔG
	Methanol [c]					
A[d]	**1b** + MeO^- → $\mathbf{TS_{3\text{-}4}}$ + H_2	-64.4	20.9	153.1	13.4	123.0
B[e]	**9** + MeOH → $\mathbf{TS_{3Hb\text{-}7}}$ + HCHO	134.2	15.2	5.3	-5.8	148.9
C[b]	**1b** + MeO^- → $\mathbf{TS_{13\text{-}14}}$ + H_2 + PPh_3	118.0	-21.8	119.7	-84.9	131.0
$\mathbf{C_{neut.}}$	**1b** + MeOH → $\mathbf{TS_{13H\text{-}14H}}$ + H_2 + PPh_3	252.1	-19.4	-8.6	-91.5	132.6
D[d]	**13** + 2 MeOH→$\mathbf{TS_{16Hb\text{-}17}}$ + HCHO + MeO^-	286.2	1.3	-123.0	-51.9	113.0
E	**1b** + MeOH → $\mathbf{TS_{9perp\text{-}19}}$ + 2 H_2	152.9	8.7	12.6	-32.8	141.3
F	**1b** + MeOH → $\mathbf{TS_{13H\text{-}23perp}}$ + H_2 + PPh_3	251.2	-18.7	-7.8	-97.6	127.1
G	**1b** + MeO^- → $\mathbf{TS_{13\text{-}28}}$ + H_2 + PPh_3	91.1	-21.6	121.1	-82.4	108.1
	Ethanol [f]					
A[d]	**1b** + EtO^- → $\mathbf{TS'_{3\text{-}4}}$ + H_2	-56.9	18.0	138.1	18.0	117.2
B[d]	**2** + EtOH → $\mathbf{TS'_{3Hb\text{-}7}}$	15.1	25.9	20.9	60.7	122.6
C[d]	**1b** + EtO^- → $\mathbf{TS'_{13\text{-}14}}$ + H_2 + PPh_3	107.1	-20.5	111.3	-77.8	120.1
$\mathbf{C_{neut.}}$	**1b** + EtOH → $\mathbf{TS'_{13H\text{-}14H}}$ + H_2 + PPh_3	221.8	-18.5	-9.1	-89.9	104.4
D[g]	**13'** + 2 EtOH → $\mathbf{TS'_{16Hb\text{-}17}}$ + MeCHO + EtO^-	242.7	0.8	-117.2	-50.6	75.7
F[g]	**1b** + EtOH → $\mathbf{TS'_{13H\text{-}23}}$ + H_2 + PPh_3	236.8	-18.0	-5.3	-95.6	117.8
G	**1b** + EtO^- → $\mathbf{TS'_{13\text{-}28}}$ + H_2 + PPh_3	93.3	-20.2	110.5	-75.8	107.9
	2-propanol [h]					
A[b]	**1b** + $iPrO^-$ → $\mathbf{TS"_{3\text{-}4}}$ + H_2	-49.0	16.3	131.8	15.9	115.1
B[b]	**2** + *i*PrOH → $\mathbf{TS"_{3Hb\text{-}7}}$	4.6	25.1	20.5	62.8	113.0
C[b]	**1b** + $iPrO^-$ → $\mathbf{TS"_{13\text{-}14}}$ + H_2 + PPh_3	115.1	-19.7	104.2	-77.0	122.6
$\mathbf{C_{neut.}}$	**1b** + *i*PrOH → $\mathbf{TS"_{13H\text{-}14H}}$ + H_2 + PPh_3	208.5	-17.8	-10.7	-93.3	86.7
D[b]	**15H"** + *i*PrOH → $\mathbf{TS"_{13\text{-}14}}$ + H_2	-78.7	9.6	126.4	18.4	76.1
F	**1b** + *i*PrOH → $\mathbf{TS"_{24\text{-}25}}$ + 2 H_2 + PPh_3	323.7	-15.1	-14.1	-112.0	182.5
G	**1b** + $iPrO^-$ → $\mathbf{TS"_{28\text{-}29aperp}}$ + H_2 + PPh_3	125.4	-16.7	93.8	-60.0	142.5

a Additional data is provided in Supporting Information, namely the overall barrier considering different TDIs in pathways **B**, **D** and **E** (Table S2), and Free energy barriers involving lower (but close in energy) transition states on pathway **F** (Table S3). *b* BSSE computed at the B97-D2/ECP3 level, as the difference of intramolecular BSSE in the intermediate and the transition state (see Table S1 for details). *c* Model solvent: methanol. *d* from Ref [6]. *e.* Using complex **9** as TDI, as predicted by the Shaik's model (see Text for details). In pathway **B**, **2** is the TDI with ethanol and 2-propanol (see Table S4). *f* Model solvent: ethanol. *g* The *α*-H transfer is competitive in this case, as ΔG = 116.8 kJ/mol for: **1b** + EtOH → $\mathbf{TS'_{23\text{-}24}}$ + 2 H_2 + PPh_3 (see details in Table S3). *h* Model solvent: 2-propanol.

coordination mode of acetone without Ru···(C=O) contact (see Figure S5). A lower limit for the rate-limiting barrier on path **G** is 142.5 kJ/mol ($\mathbf{TS"_{28\text{-}29aperp}}$, see Table 3), where the IRC also leads to an analogue of intermediate **28"** with decoordinated acetone, forming a single agostic interaction with Ru (see Figure S5).

This feature should stem from the relative stabilities of η^2 *vs* η^1 binding modes that are different in formaldehyde, ethanal and acetone: the α-H/CH_3 transfer requires a η^2-coordination mode of the substrate, but the latter is less and less stable when moving from formaldehyde to acetone.[6] All in all, it appears from these results that the precise nature of the intermediates and, hence, the rate-limiting transition state, can change appreciably between EtOH and iPrOH, and that the latter substrate requires significantly higher barriers than the former.

Reaction kinetics: dehydrogenation *vs* decarbonylation

Contrasting the overall barriers for dehydrogenation of MeOH (pathways **A**-**D**, Table 3)[6] with those for its decarbonylation (**E**-**G**, Table 3) it appears that multiple pathways with comparable barriers are available for both processes.[29] For both reactions, there are pathways that are entropically favored at high temperatures (negative δE_G values, cf. **C**-**D** and **F**-**G**) as well as those that are disfavored (positive δE_G values, cf. **A, B** and **E**). Dehydrogenation and decarbonylation should thus be possible (and competing with one another) over a wide temperature range. Whenever the system departs from the dehydrogenation cycle into decarbonylation the original catalyst is depleted and subsequent turnover reduced This feature is thus consistent with the low TOF obtained when methanol is employed as substrate.[5a] When going to EtOH, all activation barriers are lowered by 6-28 kJ/mol for dehydrogenation and by up to 9 kJ/mol for decarbonylation. This result is therefore consistent with the increased TOF obtained with ethanol compared to methanol[5a] because dehydrogenation is more kinetically facile and because decarbonylation is also more demanding (namely, for EtOH, the lowest dehydrogenation path (**D**) is indeed more favorable than the lowest decarbonylation path (**G**), by ca. 30 kJ/mol). Given typical uncertainties of DFT, this result can still be regarded as compatible with both reactions occurring, but points to a somewhat more favourable dehydrogenation reaction over decarbonylation. For iPrOH this difference is much larger, at least 66 kJ/mol (compare paths **D** and **G**), in line with the pronounced resistance toward decarbonylation with this substrate.

Table 4: Rate-limiting states (TDI and TDTS) and degree of TOF control (X_{TOF}, in %) for pathways **A**-**D** with methanol and 2-propanol, using Free Energy Profiles Computed at the B97-D2/ECP2 level from Reference [6].

	TDI	X_{TOF}(TDI)	TDTS	X_{TOF} (TDTS)
		Methanol		
A	**1b**	95	$\mathbf{TS_{3-4}}$	100
	4	5		
B	**7**	2	$\mathbf{TS_{3Hb-7}}$	100
	9	98		
C	**1b**	100	$\mathbf{TS_{13-14}}$	92
			$\mathbf{TS_{14-15}}$ [a]	8
$\mathbf{C_{neutral}}$	**1b**	100	$\mathbf{TS_{12H-13H}}$	1
			$\mathbf{TS_{13H-14H}}$	98
			$\mathbf{TS_{14H-15H}}$ [a]	1
D	**13**	92	$\mathbf{TS_{13-14}}$	32
	15H	4	$\mathbf{TS_{14-15}}$	3
	16Hb	4	$\mathbf{TS_{16Hb-17}}$	41
			$\mathbf{TS_{17-11}}$ [a]	11
			$\mathbf{TS_{11-12}}$	4
			$\mathbf{TS_{12-13}}$	9
		2-propanol		
D	**13"**	3	$\mathbf{TS"_{13-14}}$	100
	15H"	1		
	16Hb"	96		

a These transition states has not been located and a barrier-less process is assumed. See details in Supporting Information (Table S6).

Rate-limiting states and degree of TOF control. Shaik et *al.* introduced the idea that several steps dictate the overall kinetics of a catalytic reaction, and thus one should consider rate limiting *states* rather than rate-limiting *steps*.[30] The involvement of each intermediate (TDI) and transition state (TDTS) in the overall kinetics can be quantified as the "degree of TOF control", calculated according the model presented in reference [30-31]. When applying this model to the reaction pathways **A**-**D** (dehydrogenation) using the B97-D2/ECP2 free energies from reference [6], we found that the intermediates and transition states considered so far (in Table 2) indeed possess the largest degree of TOF control (almost 100% for pathways **A**-**C**, see Table 4). As a consequence, considering these complexes solely to estimate the overall activation of each path should indeed be a reasonable choice. One exception is found for pathway **B**, where the model indicates that the TDI is **9** rather than **2** with methanol, leading to a somewhat higher overall free energy barrier (148.9 kJ/mol) than previously reported (134.3 kJ/mol[6] ; see Tables 2 and S2). However, **2** should still be the TDI with ethanol and 2-propanol as the reaction **9'/9"** + MeOH → $\mathbf{TS_{3Hb-7}}$ + MeCHO/MeCO possesses a smaller free energy in these cases (see Tables 2 and S2) because **9'** and **9"** are higher on the reaction profile compared to **9**. Interestingly, Pathway **D** is somewhat special, since $\mathbf{TS_{16HB-17}}$ and $\mathbf{TS_{13-14}}$ have both large degree of TOF control (see Table 4), with $\mathbf{TS_{16HB-17}}$ showing the largest contribution (41 % *vs* 31 %).[32] With 2-propanol as substrate, the rate-limiting states are essentially **16Hb"** and $\mathbf{TS"_{13-14}}$. However, when the BSSE is taken into account, **15H"** is lower than **16Hb** on the reaction profile (see Figure S8 in Supporting Information of reference [6]), and thus the overall activation free energy is preferably computed from **15H"**, as reported in Table 2. As the Shaik's model only applies to (closed) catalytic cycles, the decarbonylation reaction (pathways **E**-**G**) has not been considered in this analysis,[33] and we considered the resting state of the system (**1b**) as the TDI and the highest transition state on the path as the TDTS for pathways **E**-**G**.

Isotope Effects. Regarding the highest transition states on each path, these mostly involve product decoordination, except for the dehydrogenation paths **A**, where it is β-hydride transfer to the metal, and the decarbonylation paths **E**-**G**, where it is formation of an H-agostic intermediate or H_2 dissociation (see Table 5). Because the extent of C-H bond breaking is quite variable in all these transition states, it appeared that they could be distinguishable through their kinetic isotope effects (KIEs), k_H/k_D. Large KIEs, on the order of 6 and above, are typically expected if C-H bond cleavage is involved in the rate-determining step.[34] Such KIEs can be readily calculated semi-classically[35] from the harmonic frequencies of the relevant isotopologues, and can be used to distinguish between alternative catalytic pathways.[36] Using methanol as substrate, we have now evaluated the H/D KIEs for the transition states listed in Table 2; the results are collected in Table 5. To gauge the effect of entropy and potential uncertainties from the low frequencies (which dominate the entropies), KIEs derived from computed enthalpies are reported (in parentheses) along with those obtained from free energies.

Small KIEs, between ca. 1 - 3, are predicted for dehydrogenation paths **A**-**C**, larger ones, between ca. 6 - 8, for paths $\mathbf{C_{neutral}}$ and **D**. These differences can be rationalized by inspecting the evolution of bond distances between their "optimal values" found in the intermediates and the ones found in the transition states (see last two columns in Table 5). For instance, the small value for path **A** (just around 1 actually) seems surprising, given that it involves a β-hydride transfer. However, while this transition state ($\mathbf{TS_{3-4}}$) indeed describes the rearrangement from a Ru-O-CH_3 to a Ru-H···CH_2=O moiety, it is the Ru-O contact that breaks predominantly at this point (Δd (Ru-O)= +1.05 Å), rather than the C-H bond (Δd(C-H) = +0.04 Å only. C-H breaks later on the reaction path, see Ref [6]). A small KIE is also predicted for pathway **C**, where the highest barrier is the partial decoordination of the HCHO product ($\mathbf{TS_{13-14}}$). Interestingly, a significantly larger KIE is predicted for pathway $\mathbf{C_{neutral}}$ because the partial decoordination of HCHO is accompanied by a rearrangement of the coordinated H_2 ligand that rotates from a perpendicular (in **13H**, see Figure 5) to a parallel (in $\mathbf{TS_{13H-14H}}$) orientation to relative to the equatorial plane.

Table 5: Computed $^{1}H/^{2}H$ and $^{12}C/^{13}C$ kinetic isotope effects (KIE). Values computed from enthalpies are in parenthesis (the corresponding enthalpies and free energies of activation are given in Tables S4 and S5).

	Rate-limiting step	KIE		Evolution of bond distances	
		$^{1}H/^{2}H$	$^{12}C/^{13}C$	Bond[a]	Δd, Å[b]
A	**β-H transfer**			C-H	+0.04
	1b + MeO^- → **TS_{3-4}** + H_2	0.79 (1.24)	1.013 (1.007)	Ru-H	-0.96
	1b + EtO^- → **TS'$_{3-4}$** + H_2	0.81 (1.37)		Ru-O	+1.05
	1b + $iPrO^-$ → **TS"$_{3-4}$** + H_2	0.91 (1.57)		Ru-C	-0.03
B	**H_2 dissociation**			Ru-Ha_{H2}	+0.64
	9 + MeOH → **TS_{3Hb-7} + HCHO**	4.13 (5.87)	0.989 (0.990)	Ru-Hb_{H2}	+1.00
				Ha_{H2}-Hb_{H2}	-0.21
C	**$\eta^2 \rightarrow \eta^1$ flipping of HCHO**			Ru-C	+0.79
	1b + MeO^- → **TS_{13-14}** + H_2 + PPh_3	1.87 (4.39)	1.006 (1.001)		
$C_{neutral}$	**$\eta^2 \rightarrow \eta^1$ HCHO and rotation of H_2**			Ru-C	+0.72
	1b + MeOH → **$TS_{13H-14H}$** + H_2 + PPh_3	7.49 (16.97)	1.007 (0.996)	Ha_{H2}-Hb_{H2}	+0.04
D	**H_2 dissociation**			Ru-Ha_{H2}	+2.00
	13 + 2 MeOH → $TS_{16Hb-17}$ +HCHO+ MeO^-	8.00 (12.48)	0.989 (0.985)	Ru-Hb_{H2}	+1.93
				Ha_{H2}-Hb_{H2}	-0.18
				Ru-C	-0.02
E	**H-agostic interaction**			Ru-H	-0.60
	1b + MeOH → **$TS_{9perp-19}$** + 2 H_2	1.63 (2.29)	1.003 (1.000)	C-H	+0.02
				Ru-C	+0.26
	7 → **$TS_{9perp-19}$**	3.05 (3.34)	1.007 (0.999)		
F	**H_2 dissociation**			Ru-Ha_{H2}	+1.54
	1b + MeOH → **$TS_{13H-23perp}$** + H_2 + PPh_3	7.08 (22.13)	1.007 (1.008)	Ru-Hb_{H2}	+0.83
				Ha_{H2}-Hb_{H2}	-0.14
G	**H-agostic interaction**			Ru-H	-0.48
	1b + MeO^- → **TS_{13-28}** + H_2 + PPh_3	1.88 (4.21)	1.012 (1.008)	C-H	+0.03
				Ru-C	+0.12

a Unless otherwise specified, C and H atoms are those of the coordinated CH_3O^- or HCHO ligands. Ha_{H2} and Hb_{H2} stand for the two hydrogens of coordinated H_2. *b* Difference in interatomic distances (*e.g.* atoms A and B), between the value in the transition state (**TS_{X-Y}**) and the preceding intermediate (**X**): Δd(A-B) = d(A-B in **TS_{X-Y}**) – d(A-B in **X**). For instance, in the next line, d(C-H) = 1.16 Å in **TS_{3-4}** and 1.12 Å in **3**, affording Δd = + 0.04 Å

Pathway **D** involves decoordination of H_2 from a Ru(H_2) complex, consistent with the large KIE. Experiments and further calculations are underway in our laboratories to test these predictions.

The decarbonylation path **F** shows a large KIE (ca. 7) expected from hydrogen involvement in the transition state. In the highest transition state (**$TS_{13H-23perp}$**, see Figure 2), the Ru-H(H_2) distance is significantly elongated (by 0.83 Å and 1.54 Å, see Table 5), giving rise to a large KIE. Paths **E** and **G** show smaller KIEs (1.63 and 1.88, respectively) corresponding to the formation of CH agostic intermediates via **$TS_{9perp-19}$** and **TS_{13-28}** (see Figure 2), where the Ru-H distance is indeed found to significantly shorten (by ca. 0.6 Å, see Figure 2 and Table 5) compared to the preceding intermediate on the path. We also note that the CH bond is not much elongated in these structures (+0.03 Å), a feature which is consistent with a smaller KIE compared to the one associated with the elimination of H_2 (path **F**).

In practice, KIEs are conveniently measured through competition experiments using a mixture of labeled and unlabeled substrate (e.g. CH_3OH and CD_3OD for k_H/k_D) and analyzing the isotope distribution in the product after partial conversion. For the decarbonylation reaction, this would seem rather difficult, however, because the reactant is stripped of its entire hydrogen content and the hydrogen gas that evolves is less straightforward to analyze. In this case, the $^{12}C/^{13}C$ KIE could be accessible through competition between regular and ^{13}C-enriched CH_3OH. Such effects are usually small and, thus, more difficult to calculate accurately. In fact, from the predicted $^{12}C/^{13}C$ KIEs (Table 5) little discrimination between the paths is predicted. However, a suitably $^{1}H/^{2}H$- *and* $^{12}C/^{13}C$-labeled substrate can be used to determine k_H/k_D of decarbonylation indirectly, as described in the following:

The deuterium isotope effect for the decarbonylation of methanol was measured by using the reaction of [RuHCl(PPh_3)$_3$] with NaOMe in methanol/ toluene, which has been shown to give [RuH_2(CO)(PPh_3)$_3$] *via* a series of intermediates, believed to be [RuH(OMe)(PPh_3)$_3$] (**7**), [RuH_2(CH_2=O)(PPh_3)$_3$] (**9**) and [RuH(CHO)(PPh_3)$_3$] (**21**).[11] To determine the deuterium isotope effect the reaction was carried out using equal amounts of $^{13}CH_3OH$ and CD_3OD each containing dissolved sodium to form the methoxide. This reaction should give [RuH_2(^{13}CO)(PPh_3)$_3$] from $^{13}CH_3OH$ and [RuHD(CO)(PPh_3)$_3$] from CD_3OD. Possible subsequent H/D exchange notwithstanding, the ratio of ^{13}CO:^{12}CO relates directly to the kinetic isotope effect k_H/k_D since the ^{13}C in the product comes only through H abstraction reactions, whilst the ^{12}CO comes only from D abstraction reactions.

We have used ^{13}CO NMR to determine the ^{13}CO:^{12}CO ratio. Figure 6 shows the ^{13}CO spectrum of [RuH_2(^{13}CO)(PPh_3)$_3$] obtained when using $^{13}CH_3OH$. We have also obtained similar spectra when using the mixture of $^{13}CH_3OH$ and CD_3OD and a mixture of CH_3OH and CD_3OD, run on the same spectrometer under identical conditions. The resonance at δ 207.0 ppm arises from the carbonyl (^{13}CO labelled). Whilst the resonances at δ 140.4 ppm (virtual triplet, CPP' spin system, 6C) and δ 138.6 ppm (d, 3P) are from the *ipso* carbon atoms of the phenyl groups on the mutually *trans* phosphines and the *cis* phosphine respectively. We used the resonance at δ 140.4 ppm as an "internal standard". Integration of the ^{13}CO signal and the signal at δ 140.4ppm gives a ratio of 100:6.34 for [RuH_2(^{13}CO)(PPh_3)$_3$]. In a sample obtained when using CH_3OH and CD_3OD (no ^{13}CO), the resonance at 207.0 is essentially absent with a maximum integral of 1.7 (should be 1 in the basis of 1 % natural abundance of CO) when the integral of the signal at 140.4 ppm is set at 6.34.

Integration of these two signals for the complex obtained from the mixture of $^{13}CH_3OH$ and CD_3OD gives a ratio of 80:6.34. 20 % of naturally abundant CO would contribute 0.2-0.3 to this signal, so this contribution can be ignored. This means that there is 80% of ^{13}CO in the mixture of complexes obtained when using $^{13}CH_3OH$ and CD_3OD and 20 % of ^{12}CO. This equates to a kinetic isotope effect (k_H/k_D) of 4.

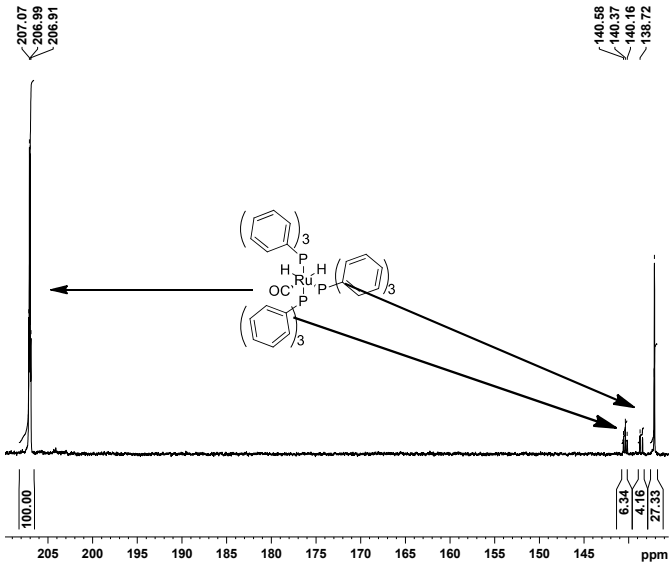

Figure 6: Part of the $^{13}C\{^1H\}$ NMR spectrum of $[RuH_2(^{13}CO)(PPh_3)_3]$ obtained from the reaction of $[RuHCl(PPh_3)_3]$ with $^{13}CH_3OH$ containing sodium in toluene.

When comparing this result to the predictions in Table 5 one should bear in mind that the latter are designed for intermediates occurring during catalytic turnover for dehydrogenation (e.g. **13** in Figure 4), whereas the former result is derived from another precursor, presumably **7**. The latter is an intermediate on dehydrogenation pathway **B**,[6] from which our pathway **E** departs at a later point (after **9**, see Figure 1). A likely scenario for interpretation of our experimental result is thus a "partial" path **E** starting from **7** as detailed in Figure 7.

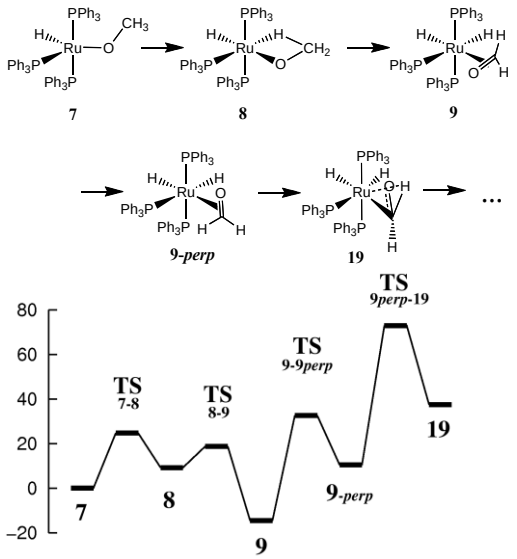

Figure 7: Section of decarbonylation pathway **E** starting from methoxide complex **7** on pathway **B;** top: schematic representation of the key intermediates, bottom: free energy profile (kJ/mol, B97-D2/ECP2 level in methanol). For continuation of the path after **19** see Figure 1.

The deuterium KIE computed for this section is ca. 3 (see **7** → $\mathbf{TS_{9perp\text{-}19}}$ entry in Table 5), in very good qualitative agreement with experiment. It thus appears that we have designed a specific entry into one of the possible decarbonylation pathways, pathway **E**, and that it is indeed formation of the first agostic intermediate that is rate-limiting on this path.[37] The computed features of the key transition state, $\mathbf{TS_{9perp\text{-}19}}$, should thus be reliable (i.e. the extent of C-H, Ru-H, and Ru-C bond cleavage/formation, see Δd values in Table 5 for path **E**).

Under catalytic turnover conditions, the other pathways **F** and **G** should become accessible as well (the latter in particular in the presence of base, because it has the lowest computed overall activation barrier for decarbonylation, cf. Table 3). Since similar k_H/k_D values around ca. 2 - 4 are predicted for the full pathways **E** and **G**, they would not be clearly distinguishable through the deuterium KIE under catalytic turnover conditions. On the other hand involvement of pathway **F** would be indicated through a noticeably higher KIE, because here H_2 dissociation is rate-limiting, with a predicted k_H/k_D of ca. 7 - 22 (depending on whether free energies or enthalpies are used in the evaluation, cf. values in parentheses in Table 5)

For decarbonylation of benzaldehyde at a Rh^I center, k_H/k_D = 1.77 has been determined previously and, on the basis of DFT calculations, ascribed to migratory CO extrusion.[38] While these results imply little C-H or metal-H involvement in the transition state, the KIE in our system is much larger, and is found consistent with the formation of a CH agostic interaction on the rate-limiting step. Overall, the combination of measured and modelled KIEs appears to be a fruitful and promising technique to gain mechanistic insights into alcohol decarbonylation and, possibly, dehydrogenation.[39]

Conclusion

We have presented a computational mechanistic study for alcohol decarbonylation at a classic homogeneous Ru catalyst, an important side reaction in hydrogen production from alcohols. For methanol as substrate, at least three pathways have been identified, which involve α-agostic aldehyde and formyl complexes as key intermediates, and which are characterised by similar rate-limiting barriers. These barriers are of the same order of magnitude as those found for dehydrogenation, consistent with the observation that both are competing reactions. The nature of the rate-limiting step depends on the active catalyst (i.e. 18e or 16e complex), on the involvement of base, but also on the nature of the substrate. For methanol the highest barrier is generally found for a rearrangement of the coordinated dehydrogenation product, formaldehyde, to form an α-CH-agostic intermediate. For ethanol, similar rearrangements of coordinated acetaldehyde are found to be rate-limiting, now involving β-CH-agostic intermediates. Once these CH agostic intermediates are formed, all subsequent steps, H or Me transfer, as well as elimination of H_2 or CH_4, are indicated to be fast and exergonic.

On going from methanol to ethanol, the barriers for formation of the first agostic intermediate are slightly decreased without base, and rather similar with base, and are found to be competitive with those for dehydrogenation. Decarbonylation can therefore deplete the original dehydrogenation catalyst and limit the subsequent turnover for H_2 generation. Moreover, our DFT results suggest that this feature is more marked with methanol than with ethanol, which is consistent with the lower TOF observed with MeOH compared to EtOH. 2-propanol as substrate (or rather, the resulting acetone) is much more resistant toward decarbonylation, and only very high-lying transition states could be located. As a result, only dehydrogenation should be involved in this case.

For all dehydrogenation and decarbonylation paths studied in this system so far, we have computed H/D (as well as $^{12}C/^{13}C$) KIEs, to gauge their potential usefulness as mechanistic probe into the nature of the rate-limiting transition state. While the $^{12}C/^{13}C$ KIEs appear to be of lesser diagnostic value in that respect, predicted H/D KIEs cover a wide range, and may prove a useful link between theory and experiment. We have measured this KIE in a reaction involving decarbonylation of methanol, and found a value compatible with that predicted for the pathway accessible under these conditions, indicating noticeable, but not very pronounced C-H bond activation in the key transition state. Because of the complicated nature of the underlying potential energy surfaces with their multiple, sometimes cross-linked reaction channels it appears that quite detailed computational studies are required to interpret the observations.

Computational Details

We followed our recently developed protocol[10] based on geometry optimizations and computation of thermochemistry corrections at a fairly low computational level, whereas refined energies are obtained using a larger basis set in conjunction with the B97-D2 functional.[40] The latter allows for a more accurate description of non-covalent interactions which have been demonstrated to be critically important when bulky ligands are considered.[41] Solvent effects are also taken into account via the use of a continuum model. In details, the following steps are involved:

Geometries and thermodynamic corrections. Geometries of complexes **22 – 31** were fully optimized at the RI-BP86/ECP1 level, i.e. employing the exchange and correlation functionals of Becke[42] and Perdew,[43] respectively, in conjunction with the SDD basis on Ru, denoting the small-core Stuttgart–Dresden relativistic effective core potential (ECP) together with its valence basis set,[44] and the standard 6-31G(d,p) basis for all other elements, except the C and H atoms of phenyl rings on which the smaller 3-21G basis were used[45] (hereafter denoted as the "ECP1" basis sets) and suitable auxiliary basis sets for the fitting of the Coulomb potential.[46] Harmonic frequencies were computed analytically and were used without scaling to obtain enthalpic and entropic corrections at the experimentally used temperature of 150 °C.[5a] The corresponding correction terms δE_G were estimated at the RI-BP86/ECP1 level and have been obtained as the difference of the reaction energy of a given step ($\Delta E_{RI\text{-}BP86/ECP1}$) and the corresponding free energy ($\Delta G_{RI\text{-}BP86/ECP1}$):

$$\delta E_G = \Delta G_{RI\text{-}BP86/ECP1} - \Delta E_{RI\text{-}BP86/ECP1} \qquad (1)$$

The entropic contributions have been evaluated at a pressure of 1354 atm in order to model the changes in entropy for a condensed phase.[47] The corresponding correction terms (δE_G) for each step of the catalytic cycles are gathered in Tables 1-3 along with other correction terms *(vide infra)*.

The transition states (denoted $\mathbf{TS_{x\text{-}y}}$) were characterized by a single imaginary frequency and visual inspection of the corresponding vibrational mode ensured that the desired minima **x** and **y** were connected. The reaction pathways have been investigated more closely by following the Intrinsic Reaction Coordinate (IRC)[48] starting from $\mathbf{TS_{x\text{-}y}}$ and leading to the intermediates **x** and **y**.

The initial structures of the complexes were constructed by hand, and were derived from those of our previous study.[6]

Energies. Refined energies were obtained from single-point calculations (on the RI-BP86/ECP1 geometries) using the same SDD ECP on Ru[44] and a larger basis set (hereafter noted ECP2), namely 6-311+G(d,p), on all elements except for all the C and H phenyl atoms, where the 6-31G(d,p) basis was used, in conjunction with the B97-D2 functional,[40] as in our previous study.[6] The latter follows the DFT-D2 general approach of Grimme,[40, 49] in which the functional energies are corrected by an atomic pair-wise additive term accounting for the long-range non-covalent interactions. B97-D2 has been successfully employed to study other Ru catalyzed reactions,[50] and has recently been shown to perform well at describing several "bulky" transition metal-complexes.[51] Its performance has also been tested against other density functionals in our previous study on dehydrogenation, and it has been show to provide an overall good agreement *e.g.* with the M06-L functional[52] (see Footnote 32 in Ref [6], see also Ref. [53]).

Energies have been corrected for the basis set superposition error (BSSE) using the counterpoise method.[54] The BSSE energy corrections (noted δE_{BSSE}) are gathered in Tables 1 and 2. Estimates of the solvation effects were computed using the Conductor-like screening model (COSMO),[55] with a dielectric constant $\varepsilon = 32.63$ to model the experimentally used methanol solvent, $\varepsilon = 24.55$ to model ethanol and $\varepsilon = 20.18$ for 2-propanol. We defined the δE_{solv} energy correction as the difference between the reaction energy in the continuum (including the outlaying charge correction[56] ; noted ΔE_{COSMO}) and in the gas phase (ΔE), at the B97-D2/ECP2 level:

$$\delta E_{solv} = \Delta E_{COSMO} - \Delta E \qquad (2)$$

Both counterpoise and COSMO corrections were calculated by performing single-point calculations at the B97-D2/ECP2 level on the RI-BP86/ECP1 geometries. The final ΔG values are calculated as a sum of all energy correction terms, added to the raw B97-D2/ECP2 gas phase reaction energies (ΔE):

$$\Delta G = \Delta E + \delta E_{solv} + \delta E_{BSSE} + \delta E_G. \qquad (3)$$

Where ΔE, δE_{solv} and δE_{BSSE} are computed at the B97-D2/ECP2 level and δE_G at the RI-BP86/ECP1 level (*vide supra*).

KIEs have been computed at the RI-BP86/ECP1 level, at T = 423 K and P = 1354 atm. In case of the $^1H/^2H$ KIEs, all hydrogen atoms, except phenyl hydrogens, have been substituted with deuterium.

Consistently to our previous study on dehydrogenation,[6] activation barriers have been recomputed using a larger basis set (hereafter noted ECP3), where all P, O, C and H atoms are described by the 6-311+G(d,p) basis set (and the same SDD ECP on Ru), using the same B97-D2 functional (in the gas phase and in the continuum). The basis set error is then computed considering the difference in intra-molecular BSSE between the intermediates and transition states. The resulting corrections (noted $\delta E'_{BSSE}$) are gathered in Table 3. More details are given in Ref.[6] Intramolecular BSSE energies are provided in Supporting Information (see Table S1).

All RI-BP86 calculations have been performed with the Gaussian03 software,[57] whereas B97-D2 (gas phase and COSMO) calculations were performed with the Turbomole package.[58]

Experimental Section

Materials. All manipulations were carried out under dinitrogen using glovebox and standard Schlenk-line techniques (dinitrogen was dried through a Cr(II)/silica packed glass column). $RuCl_3 \bullet 3H_2O$ was purchased from Alfa Aesar and used as received. Sodium methoxide was prepared by reacting sodium metal (supplied by Lancaster Synthesis in mineral oil; the small pieces were washed with hexane) with degassed CH_3OH, CD_3OD or $^{13}CH_3OH$. Triethylamine was purchased from Fischer Scientific and degassed before use. Toluene and diethyl ether were dried using a Braun Solvent Purification System. Methanol was dried and degassed by distillation from magnesium methoxide under dinitrogen. All gases were purchased from BOC gases. All solvents and deuterated solvents, which were not previously dried, were only degassed prior to use.

Instruments. $^{13}C\{^1H\}$ NMR spectra were recorded on a Bruker Avance II 400 MHz Spectrometer (^1H NMR at 400 MHz and ^{13}C NMR at 100 MHz) at room temperature.

^{31}P and ^{1}H NMR were recorded on Bruker Avance II 400 MHz and on a Bruker Avance 500 MHz Spectrometers. ^{1}H and $^{13}C\{^{1}H\}$ spectra are referenced to TMS and the residual proton signal of the solvent was used as internal standard.

Syntheses. $[RuCl_2(PPh_3)_3]$[59] and $[RuHCl(PPh_3)_3]$[60] were prepared by published procedures and all observations and NMR data were in accordance with those reported in the literature. $[RuH_2(CO)(PPh_3)_3]$ was prepared by an adaptation of a literature method.[11]

Sodium methoxide was prepared by reacting sodium metal with CH_3OH, CD_3OD or $^{13}CH_3OH$, under an inert atmosphere of dinitrogen and the formed solution was subsequently added to a suspension of $[RuHCl(PPh_3)_3]$ (0.015 g, 0.016 mmol) in toluene (3 ml). After refluxing the reaction mixture for 1 hour at 100 °C, the resulting orange solution was cooled to room temperature and evaporated to dryness. The recovered solid was washed once with dry and degassed methanol, in order to remove the methoxide, and dried *in vacuo*. The collected yellow solid was finally analysed *via* NMR spectrometry (toluene-d_8, 298 K). The ^{1}H and ^{31}P spectral data are identical to those described in the literature.[61] $^{13}C\{^{1}H\}$: 207.3, q, J_{CP} = 8.3 Hz, CO; 140.4, vt, $J_{CP+CP'}$ = 40.8 Hz, $C_{ipso,}$ mutually trans phosphines; 138.6, d, J_{CP} = 28.4 Hz, C_{ipso} unique phosphine; 134.4-133.9, m, Ar; 128.2, s, Ar; 127.3-127.1, m, Ar.

$[RuH_2(^{13}CO)(PPh_3)_3]$ was prepared as above for $[RuH_2(CO)(PPh_3)_3]$ except that the methoxide was obtained by reacting sodium (0.01 g, 0.43 mmol) with $^{13}CH_3OH$ (0.2 ml, 4.94 mmol). $J_{HC\ (trans)}$ = 18.3 Hz; $J_{HC\ (cis)}$ = 6.4 Hz; J_{PC} = 7.2 Hz to mutually *trans* P, 9.5 Hz to unique P.

Mixture of $[RuH_2(^{13}CO)(PPh_3)_3]$ and $[RuHD(CO)(PPh_3)_3]$, as above for $[RuH_2(CO)(PPh_3)_3]$ except that the methoxide was obtained by reacting equal amounts of $^{13}CH_3OH$ (0.2 ml, 4.94 mmol) and CD_3OD (0.2 ml, 4.94 mmol), each containing sodium metal (0.01 g, 0.43 mmol).

Mixture of $[RuH_2(CO)(PPh_3)_3]$ and $[RuHD(CO)(PPh_3)_3]$, as above for $[RuH_2(CO)(PPh_3)_3]$ except that the methoxide was obtained by reacting equal amounts of CH_3OH (0.2 ml, 4.94 mmol) and CD_3OD (0.2 ml, 4.94 mmol), each containing sodium metal (0.01 g, 0.43 mmol) to form the methoxide.

Note that in all cases where H and D are used together in the sources of methanol, H and D are incorporated into both hydride sites.

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[33] Closing a cycle from **22** would require the decoordination of the CO ligand *e.g.* via an exchange with H_2 to afford **1b**. This process is very demanding thermodynamically (ΔG = +135 kJ/mol at the B97-D2/ECP2 level) and would certainly require further activation either by irradiation or by an homogeneous catalyst.

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[45] Structures have been determined without corrections for the basis set superposition error (BSSE), since the latter is found to have only a little influence on geometries. This feature has been investigated in our previous study on a similar tris-triphenylphosphine complex and only small structural differences have been obtained when going from ECP1 to the larger ECP2 basis set, where BSSE is expected to be smaller (see Reference 10). On the other hand, we note that the influence of BSSE on reaction energies has been carefully considered herein, and counterpoise energy corrections have been made for each investigated step.

[46] Generated automatically according to the procedure implemented in Gaussian 09.

[47] Following the argument in Martin, R. L.; Hay, P. J.; Pratt, L. R. *J. Phys. Chem. A* **1998**, *102*, 3565-3573, where this simple procedure has been proposed as adjustment for the concentration of water molecules in the liquid, and where the necessary value for the pressure has been derived from the experimental density of liquid water. Such an elevated pressure is designed to model the change in entropy existing in condensed phase when the number of particle vary during a given reaction. For instance, in the case of the dissociation of PPh_3 from **1b**, δE_G = -95.8 kJ/mol at P = 1354 atm, whereas it is -120.9 kJ/mol at P = 1 atm (both at T = 423 K).

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Entry for the Table of Contents

Hydrogen generation

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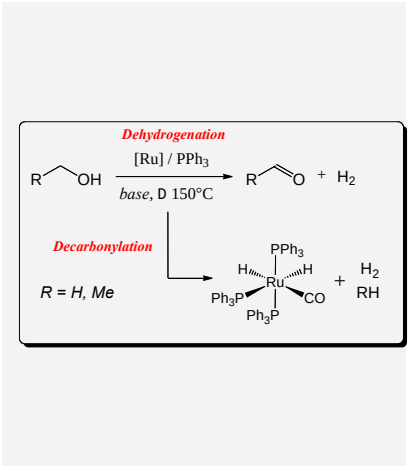
On the Importance of Decarbonylation as Side Reaction in the Ruthenium-Catalyzed Dehydrogenation of Alcohols: a Combined Experimental and Density Functional Study



Decarbonylation *vs* dehydrogenation: Combination of density functional theory calculations and isotopic labelling experiments shed light on the mechanism of the decarbonylation reaction, which is an important side-reaction in the Ru-catalyzed production of hydrogen from alcohols by dehydrogenation. It is shown that multiple reaction pathways are operating and that decarbonylation is competitive with dehydrogenation as far as simple primary alcohols are considered as substrates.

On the Importance of Decarbonylation as Side Reaction in the Ruthenium-Catalyzed Dehydrogenation of Alcohols: a Combined Experimental and Density Functional Study.

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– Supporting information –

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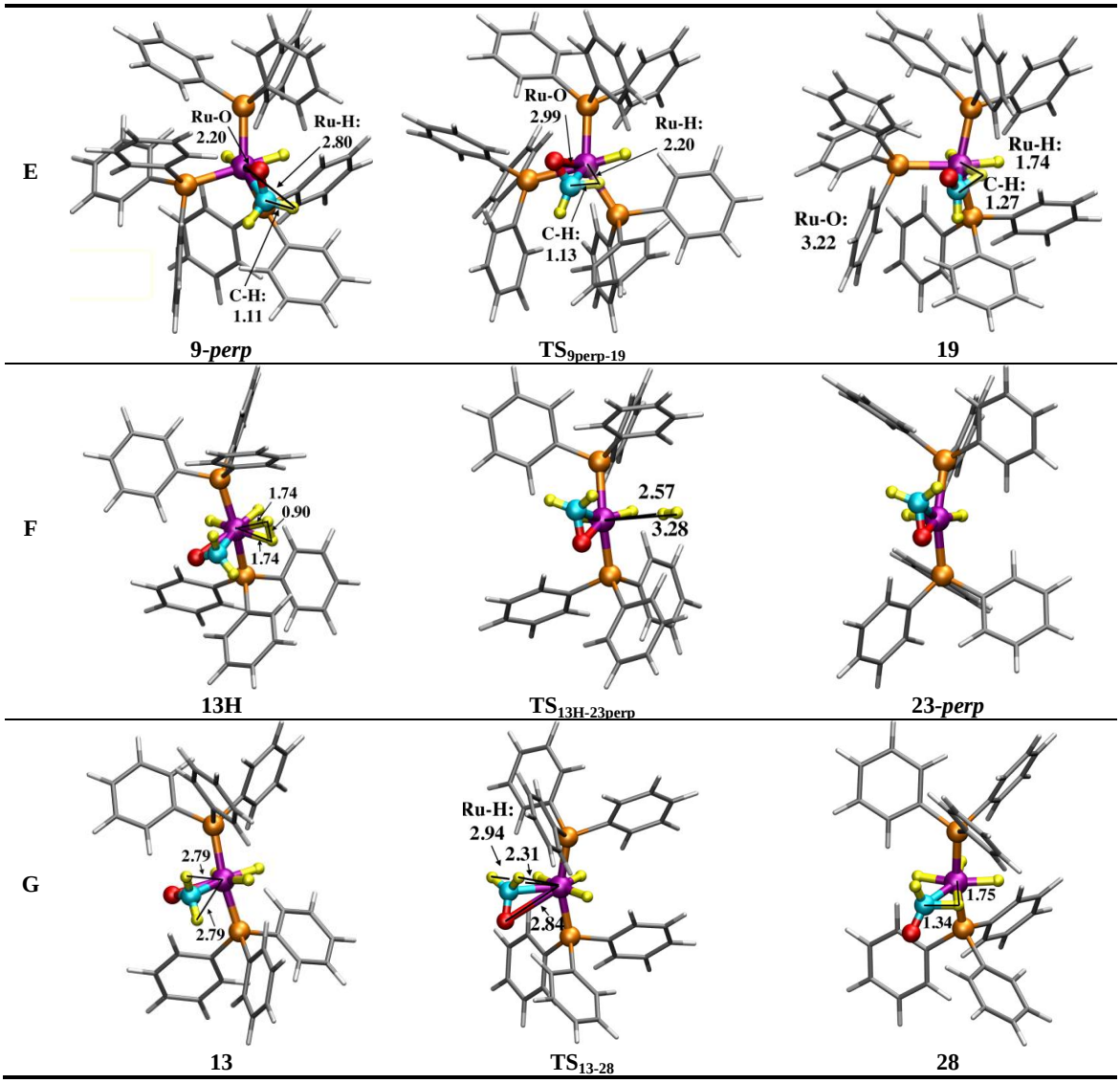


Figure 2 (colour version): Structure of intermediates and transition states involved in the rate-limiting steps of the decarbonylation pathways **E**-**G**, with methanol as initial substrate. Paths **E** and **G**: Formation of the α-agostic complex **19** from **9-*perp***; Path **F**: Dissociation of H_2 and rotation of HCHO. RI-BP86/ECP1 optimized structures. Selected interatomic distances are given in Å. Additional snapshots are provided in Supporting Information (see Figures S1-S3).

Table S1: BSSE corrections at the ECP3 level, in kJ/mol.[(a)]

Global									
1b [(b)]			**2** [(b)]			**$TS_{9perp-19}$**			**$TS_{13H-23perp}$**	
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H_2	1.7		*Vac*	0.0		**HCHO**	6.6		**H_2**	0.6
$P_{ax}1$	12.6		**$P_{ax}1$**	12.6		**$P_{ax}1$**	14.5		**HCHO**	6.1
$P_{ax}2$	12.6		**$P_{ax}2$**	12.1		**$P_{ax}2$**	12.7		**$P_{ax}1$**	8.8
P_{eq}	15.5		**P_{eq}**	15.5		**P_{eq}**	17.2		**$P_{ax}2$**	8.1
Total	42.3		**Total**	40.2		**Total**	51.0		**Total**	23.6
Methanol										
TS_{23-24}			**TS_{24-25}**			**TS_{13-28}**			**$TS_{13H-14H}$**	
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
Vac	0.0		***Vac***	0.0		***Vac***	0.0		**H_2**	1.4
HCHO	5.5		**HCHO**	6.2		**HCHO**	5.5		**$P_{ax}1$**	7.5
$P_{ax}1$	7.4		**$P_{ax}1$**	7.2		**$P_{ax}1$**	7.0		**$P_{ax}2$**	8.0
$P_{ax}2$	7.9		**$P_{ax}2$**	7.8		**$P_{ax}2$**	8.2		**HCHO**	6.0
Total	20.8		**Total**	21.2		**Total**	20.7		**Total**	22.9
Methanol										
9			**TS_{3Hb-7}** [(b)]			**$TS_{16Hb-17}$** [(b)]				
H	0.0		**H**	0.0		**H**	0.0			
H	0.0		**H_2**	0.8		**H**	0.0			
P_{eq}	17.5		**MeO^-**	18.0		**H_2**	0.4			
HCHO	7.7		**$P_{ax}1$**	14.6		**$P_{ax}1$**	7.9			
$P_{ax}1$	14.1		**$P_{ax}2$**	15.1		**$P_{ax}2$**	7.5			
$P_{ax}2$	14.1		**P_{eq}**	20.1		**MeOH**	8.4			
Total	53.4		**Total**	68.6		**Total**	23.8			

[(a)] **$BSSE_n$** values for each ligand. The sum of all contribution ("Total") corresponds to the intramolecular BSSE (**$E_{intra-BSSE}$**) of a given complex.

[(b)] From: Sieffert, N.; Bühl, M. *J. Am. Chem. Soc.* **2010**, *132*, 8056.

Table S1 (continued): BSSE corrections at the ECP3 level, in kJ/mol.[(a)]

Ethanol									
TS'$_{13H-14H}$			**TS'$_{23-24}$**			**TS'$_{13H-23}$**			**TS'$_{13-28}$**	
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H_2	1.2		*Vac*	0.0		**H_2**	0.5		**H**	0.0
$P_{ax}1$	7.9		**$P_{ax}1$**	8.1		**$P_{ax}1$**	8.7		**$P_{ax}1$**	7.7
$P_{ax}2$	8.0		**$P_{ax}2$**	8.8		**$P_{ax}2$**	8.3		**$P_{ax}2$**	8.3
MeCHO	6.7		**MeCHO**	7.9		**MeCHO**	6.8		**MeCHO**	6.1
Total	23.8		**Total**	24.8		**Total**	24.3		**Total**	22.1

Ethanol									
9'			**TS'$_{3Hb-7}$** *(b)*			**TS'$_{16Hb-17}$** *(b)*				
H	0.0		**H**	0.0		**H**	0.0			
H	0.0		**H_2**	0.9		**H**	0.0			
P_{eq}	17.5		**EtO^-**	15.2		**H_2**	0.4			
MeCHO	8.8		**$P_{ax}1$**	14.7		**$P_{ax}1$**	8.0			
$P_{ax}1$	14.3		**$P_{ax}2$**	15.3		**$P_{ax}2$**	7.5			
$P_{ax}2$	14.7		**P_{eq}**	19.7		**EtOH**	7.8			
Total	55.3		**Total**	65.8		**Total**	23.7			

Table S1 (continued): BSSE corrections at the ECP3 level, in kJ/mol.[(a)]

2-propanol									
TS"$_{13H-14H}$			**9"**			**TS"$_{13H-23}$**			**TS"$_{3Hb-7}$** [(b)]	
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H	0.0		**H**	0.0		**H**	0.0		**H**	0.0
H_2	1.2		**P_{eq}**	17.4		**H_2**	0.4		**H_2**	0.8
$P_{ax}1$	6.6		**Me_2CO**	9.6		**$P_{ax}1$**	9.2		**$P_{ax}1$**	14.9
$P_{ax}2$	8.4		**$P_{ax}1$**	14.2		**$P_{ax}2$**	8.7		**$P_{ax}2$**	15.5
Me_2CO	8.3		**$P_{ax}2$**	14.9		**Me_2CO**	7.5		**Me_2CO**	13.5
Total	24.5		**Total**	56.1		**Total**	25.8		**Total**	44.7

2-propanol									
TS"$_{16Hb-17}$ [(b)]			**TS"$_{24-25}$**			**TS"$_{28-29aperp}$**			
H	0.0		**H**	0.0		**H**	0.0		
H	0.0		**H**	0.0		**H**	0.0		
H_2	0.4		-	-		**H**	0.0		
$P_{ax}1$	8.1		**$P_{ax}1$**	8.4		**$P_{ax}1$**	7.9		
$P_{ax}2$	7.9		**$P_{ax}2$**	9.8		**$P_{ax}2$**	8.7		
***i*PrOH**	8.3		**Me_2CO**	9.0		**Me_2CO**	9.0		
Total	24.7		**Total**	27.2		**Total**	25.6		

Table S2: Additional Refined Free Energies (in kJ/mol, at the B97-D2/ECP3 level) for Selected Activation Barriers of Pathways **B, D** and **E**.

		ΔE	**$\delta E'_{BSSE}$** [a]	**δE_{solv}**	**δE_G**	**ΔG**
	Methanol [b]					
B	**1b** + MeOH → **TS_{3Hb-7}** + H_2	91.3	26.8	20.5	13.8	152.4
B	**2** + MeOH → **TS_{3Hb-7}**	21.8	28.9	21.3	62.3	134.3
D	**1b** + MeOH → **$TS_{16Hb-17}$** + PPh_3	185.4	-18.5	-2.0	-63.4	101.5
E	**1b** + MeOH → **$TS_{9perp-19}$** + 2 H_2	152.9	8.7	12.6	-32.8	141.3
E	**2** + MeOH → **$TS_{9perp-19}$** + H_2	83.4	10.8	13.3	15.7	123.1
	Ethanol [c]					
B	**1b** + EtOH → **TS'_{3Hb-7}** + H_2	84.8	23.5	20.0	12.1	140.4
B	**9** + EtOH → **TS'_{3Hb-7}** + MeCHO	105.9	10.5	1.4	-22.5	95.3
D	**1b** + EtOH → **$TS'_{16Hb-17}$** + PPh_3	178.6	-18.6	-2.7	-56.2	101.1
	2-propanol [d]					
B	**1b** + *i*PrOH → **TS''_{3Hb-7}** + H_2	74.3	2.4	19.9	14.1	110.7
B	**9** + *i*PrOH → **TS''_{3Hb-7}** + Me_2CO	51.3	13.8	-0.1	-38.6	26.4
D	**1b** + *i*PrOH → **$TS''_{16Hb-17}$** + PPh_3	170.7	-17.6	-2.4	-58.4	92.4

a BSSE computed at the B97-D2/ECP3 level, as the difference of intramolecular BSSE in **1b** and the transition state (see Table S1 for details). *b* Model solvent: methanol. *c* Model solvent: ethanol. *d* Model solvent: 2-propanol.

Table S3: Additional Refined Free Energies (in kJ/mol, at the B97-D2/ECP3 level) for Selected Activation Barriers of Pathway **F**.

	ΔE	**$\delta E'_{BSSE}$** [a]	**δE_{solv}**	**δE_G**	**ΔG**
Methanol [b]					
1b + MeOH → **$TS_{13H-23perp}$** + H_2 + PPh_3	251.2	-18.7	-7.8	-97.6	127.1
1b + MeOH → **TS_{23-24}** + 2 H_2 + PPh_3	270.2	-21.5	-7.9	-120.7	120.1
1b + MeOH → **TS_{24-25}** + 2 H_2 + PPh_3	276.8	-21.1	-7.7	-130.0	118.0
Ethanol [c]					
1b + EtOH → **TS'_{13H-23}** + H_2 + PPh_3	236.8	-18.0	-5.3	-95.6	117.8
1b + EtOH → **TS'_{23-24}** + 2 H_2 + PPh_3	268.0	-17.5	-13.5	-120.2	116.8
2-propanol [d]					
1b + *i*PrOH → **$TS''_{13H-23perp}$** + H_2 + PPh_3	245.9	-16.5	-3.8	93.3	132.3
1b + *i*PrOH → **TS''_{23-24}** + 2 H_2 + PPh_3	323.7	-15.1	-14.1	-112.0	182.5

a BSSE computed at the B97-D2/ECP3 level, as the difference of intramolecular BSSE in **1b** and the transition state (see Table S1 for details). *b* Model solvent: methanol. *c* Model solvent: ethanol. *d* Model solvent: 2-propanol.

Table S4: Correcting Terms for Enthalpies and Free energies of activation (in kJ/mol) for the rate-limiting steps of pathways **A**-**G**. Comparisons of different isotopomers (RI-BP86/ECP1 level).[a]

		^{1}H, ^{12}C		^{2}H		^{13}C	
		δE_H	δE_G	δE_H	δE_G	δE_H	δE_G
A	**1b** + MeO^- → **$TS_{3\text{-}4}$** + H_2	-6.2	13.5	-5.4	12.7	-6.2	13.5
B	**9** + MeOH → **$TS_{3Hb\text{-}7}$** + HCHO	-14.4	-11.0	-10.1	-7.1	-14.4	-11.0
C	**1b** + MeO^- → **$TS_{13\text{-}14}$** + H_2 + PPh_3	-22.1	-85.1	-16.9	-82.9	-22.1	-85.1
C_{neut}	**1b** + MeOH → **$TS_{13H\text{-}14H}$** + H_2 + PPh_3	-34.1	-91.5	-24.2	-84.4	-34.2	-91.5
D	**13** + 2 MeOH → **$TS_{16Hb\text{-}17}$** +HCHO+MeO^-	-22.4	-51.7	-13.6	-44.4	-22.5	-51.8
E	**2** + MeOH → **$TS_{9perp\text{-}19}$** + H_2	-22.8	15.7	-13.4	22.4	-22.8	15.7
F	**1b** + MeOH → **$TS_{13H\text{-}23perp}$** + H_2 + PPh_3	-33.5	-97.6	-22.7	-90.7	-33.5	-97.5
G	**1b** + MeO^- → **$TS_{13\text{-}28}$** + H_2 + PPh_3	-21.3	-82.4	-16.3	-80.2	-21.3	-82.4

a $\delta E_H = \Delta H - \Delta E$ and $\delta E_G = \Delta G - \Delta E$ (see Table S5 for the values of ΔE, ΔH and ΔG).

Table S5: Enthalpies and Free energies of activation (in kJ/mol) for the rate-limiting steps of pathways **A**-**G**. Comparisons of different isotopomers (RI-BP86/ECP1 level).

		^{1}H, ^{12}C		^{2}H		^{13}C	
	ΔE	**ΔH**	**ΔG**	**ΔH**	**ΔG**	**ΔH**	**ΔG**
A	-72.0	-78.2	-58.5	-77.4	-59.3	-78.2	-58.4
B	164.7	146.9	158.9	153.2	163.9	146.9	158.8
C	-11.1	-33.3	-96.3	-28.1	-94.1	-33.3	-96.2
C_{neut}	178.0	143.8	86.5	153.8	93.6	143.8	86.5
D	374.5	352.0	322.7	360.9	330.0	352.0	322.7
E	95.6	72.8	111.3	82.2	118.1	72.8	111.4
F	179.4	145.9	81.9	156.8	88.7	145.9	81.9
G	-41.8	-63.1	-124.2	-58.0	-122.0	-63.1	-124.1

Table S6: Full data on the calculations of the degree of TOF control by the Shaik's model. B97-D2/ECP2 level. BSSE corrections have been applied only in steps **3 → 7** (10.2 kcal/mol) and **3Ha → 11H** (9.8 kcal/mol). "Ei" and "Ets" are free energies in kcal/mol, "Xi" and "Xts" are the degree of TOF control. The temperature is in K.

Pathway A:

TOF=-0.92E+05 1/s
Temperature= 423.00

Ei	Ets	Xi	Xts		
0.00	9.40	0.95	0.00	(1b)	(TS1b-2)
5.10	5.10	0.00	0.00	(2)	(no TS)
10.80	27.50	0.00	1.00	(3)	(TS3-4)
14.60	14.60	0.05	0.00	(4)	(no TS)
17.90	17.90	0.00	0.00	(5)	(no TS)
12.10				(1b)	

Pathway B:

TOF=-0.93E+03 1/s
Temperature= 423.00

Ei	Ets	Xi	Xts		
0.00	0.00	0.00	0.00	(2)	(no TS)
5.80	5.80	0.00	0.00	(3)	(no TS)
13.30	22.80	0.00	1.00	(3Hb)	(TS3Hb-7)
7.00	12.90	0.02	0.00	(7)	(TS7-8)
9.20	11.50	0.00	0.00	(8)	(TS8-9)
3.50	24.20	0.98	0.00	(9)	(TS9-10)
15.50	15.50	0.00	0.00	(10)	(no TS)
12.10				(2)	

Pathway C-anionic

TOF=-0.18E+03 1/s
Temperature= 423.00

Ei	Ets	Xi	Xts		
0.00	9.40	1.00	0.00	(1b)	(TS1b-2)
5.10	5.10	0.00	0.00	(2)	(no TS)
10.80	10.80	0.00	0.00	(3)	(no TS)
14.30	18.90	0.00	0.00	(11)	(TS3-11)
18.80	19.70	0.00	0.00	(12)	(TS12-13)
10.90	32.70	0.00	0.92	(13)	(TS13-14)
30.60	30.60	0.00	0.08	(14)	(no TS)
25.60	25.60	0.00	0.00	(15)	(no TS)
17.90	17.90	0.00	0.00	(5)	(no TS)
12.10				(1b)	

Pathway C-neutral

TOF=-0.88E+04 1/s
Temperature= 423.00

Ei	Ets	Xi	Xts		
0.00	9.40	1.00	0.00	(1b)	(TS1b-2)
5.10	5.10	0.00	0.00	(2)	(no TS)

```
 10.80 10.80  0.00  0.00  (3)    (no TS)
 14.30 14.30  0.00  0.00  (3Ha)  (no TS)
 15.20 16.50  0.00  0.00  (11H)  (TS11H-12H)
 20.20 25.20  0.00  0.01  (12H)  (TS12H-13H)
 20.10 29.50  0.00  0.98  (13H)  (TS13H-14H)
 26.00 26.00  0.00  0.02  (14H)  (no TS)
 24.60 24.60  0.00  0.00  (15H)  (no TS)
 12.10                    (1b)
```

Pathway D

```
TOF=-0.75E+07 1/s
 Temperature= 423.00
  Ei Ets Xi Xts
  0.00 22.70  0.92  0.32  (13)    (TS13-14)
 20.60 20.60  0.00  0.03  (14)    (TS14-15)
 15.70 15.70  0.00  0.00  (15)    (no TS)
 13.70 13.70  0.04  0.00  (15H)   (no TS)
 14.00 23.10  0.03  0.41  (16Hb)  (TS16Hb-17)
 22.00 22.00  0.00  0.11  (17)    (no TS)
 16.40 21.10  0.00  0.04  (11)    (TS11-12)
 20.90 21.80  0.00  0.09  (12)    (TS12-13)
 12.10                    (13)
```

Pathway D – 2-propanol

```
TOF= 0.29E+02 1/s
 Temperature= 423.00
  Ei Ets Xi Xts
  0.00 19.20  0.03  1.00  (13”)    (TS”13-14)
  8.70  8.70  0.00  0.00  (14”)    (no TS)
  1.40  1.40  0.00  0.00  (15”)    (no TS)
 -1.00 -1.00  0.01  0.00  (15H”)   (no TS)
 -4.90  5.00  0.96  0.00  (16Hb”)  (TS”16Hb-17)
  4.00  4.00  0.00  0.00  (17”)    (no TS)
  1.10  7.00  0.00  0.00  (11”)    (TS”11-12)
  4.20  7.50  0.00  0.00  (12”)    (TS”12-13)
 -2.00                    (13”)
```

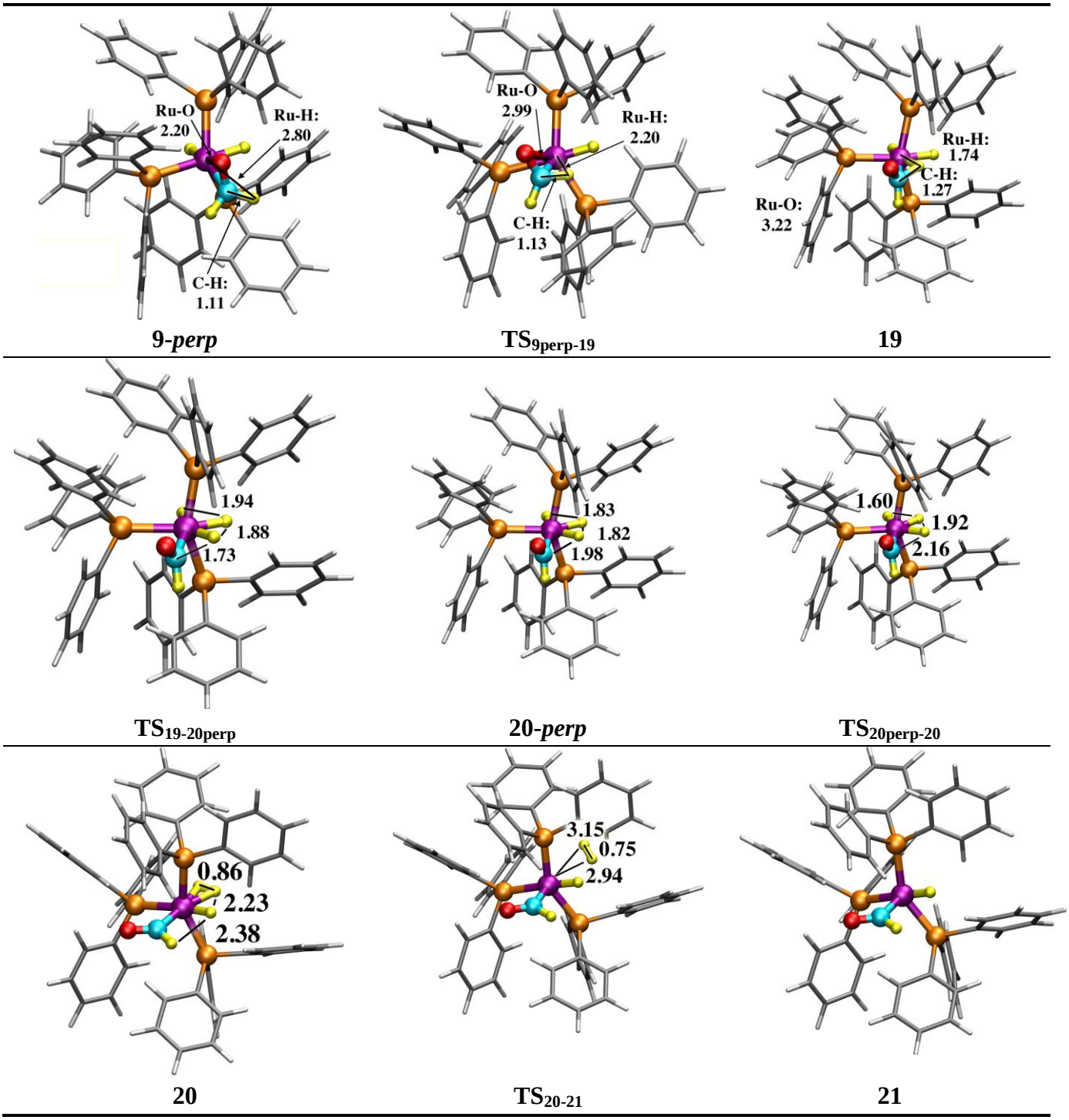
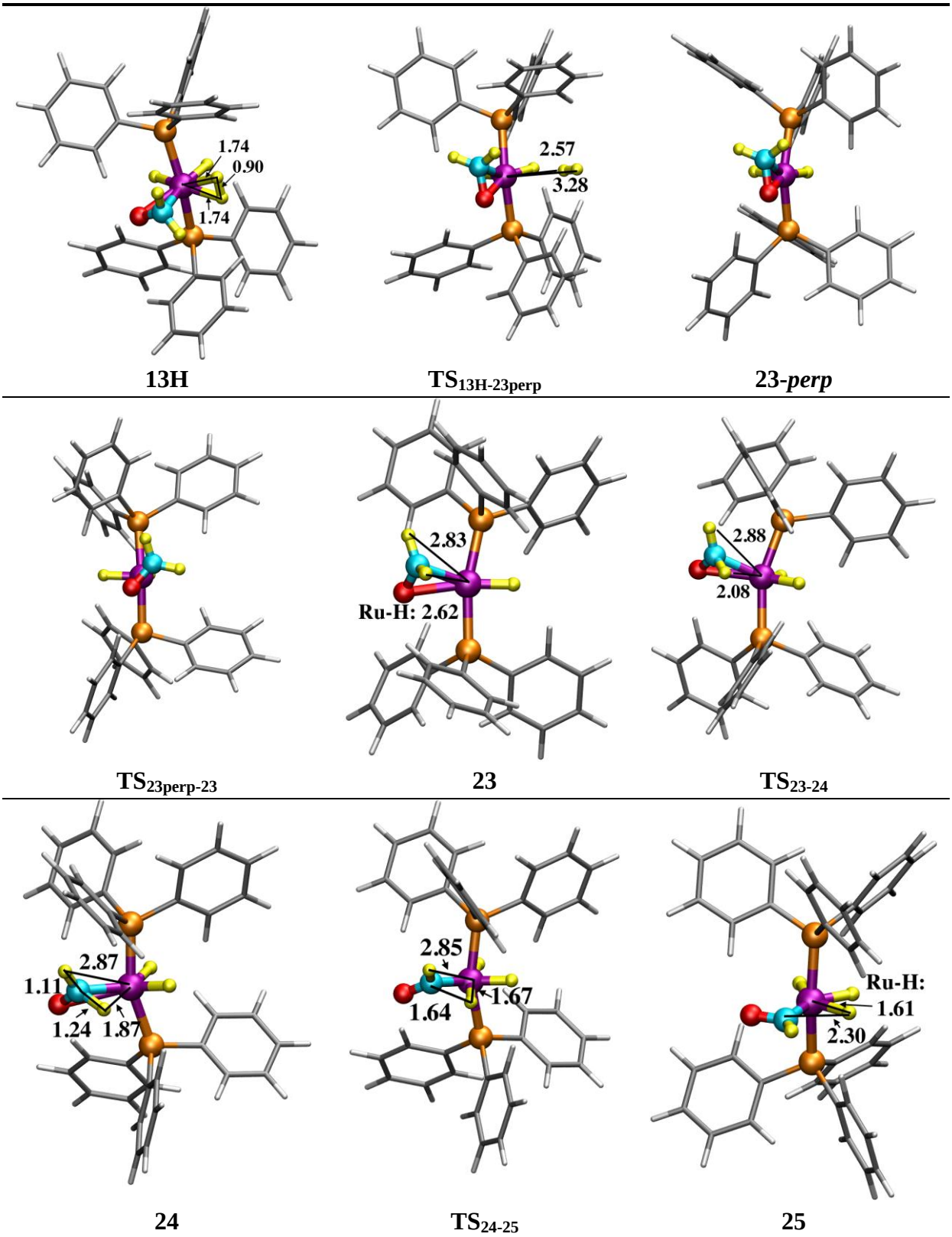


Figure S1: Structures of the intermediates and transition states involved in the first α-H transfer in Pathway **E** with methanol. Selected interatomic distances are given in Å.

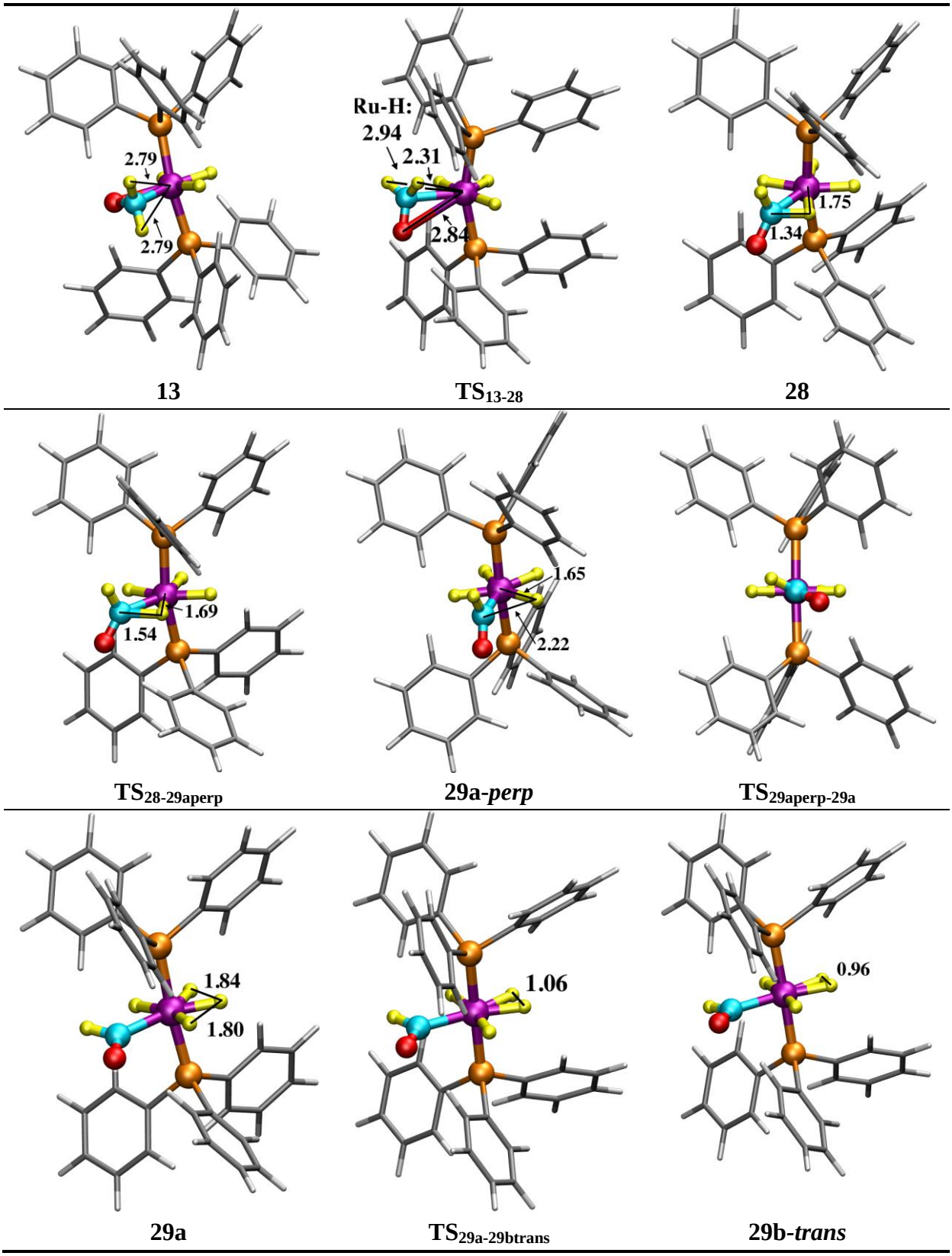


13H **$TS_{13H-23perp}$** **23-*perp***

$TS_{23perp-23}$ **23** **TS_{23-24}**

24 **TS_{24-25}** **25**

Figure S2: Structures of the intermediates and transition states involved in the first α-H transfer in Pathway **F** with methanol. Selected interatomic distances are given in Å.



13 **$TS_{13\text{-}28}$** **28**

$TS_{28\text{-}29aperp}$ **29a-*perp*** **$TS_{29aperp\text{-}29a}$**

29a **$TS_{29a\text{-}29btrans}$** **29b-*trans***

Figure S3: Structures of the intermediates and transition states involved in the first α-H transfer in Pathway **G** with methanol. Selected interatomic distances are given in Å.

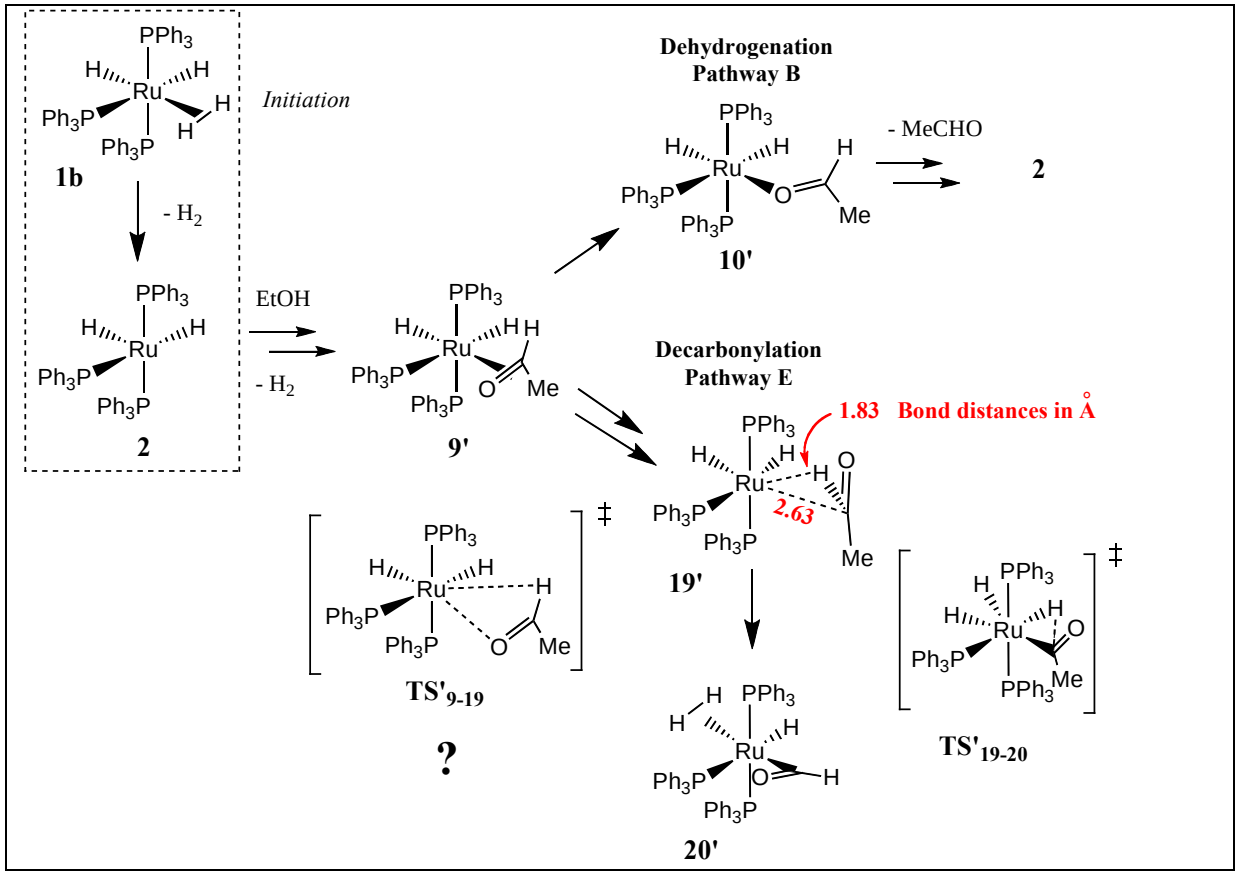


Figure S4: Decarbonylation of formadehyde via pathway **E**, showing the partial decoordination of MeCHO in **19'** that occurs when following the IRC starting from **TS'$_{19\text{-}20}$**. The transition state **TS'$_{9\text{-}19}$** connecting **9** and **19** has not been located as the transition state search leads to **10'**.

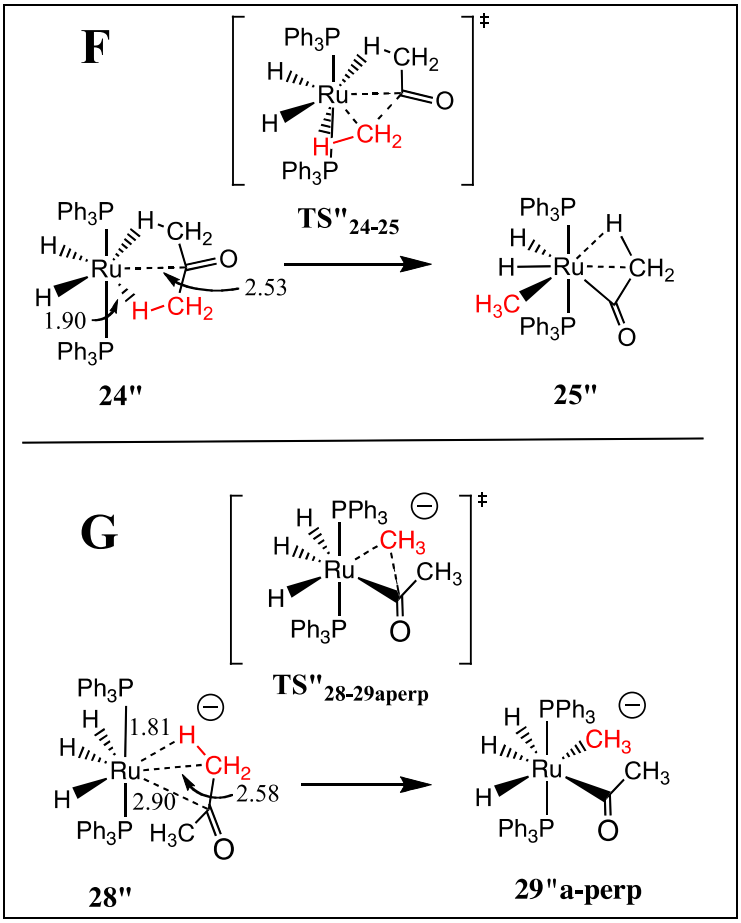


Figure S5: The key α-CH_3 transfer involved in the decarbonylation of acetone in pathways **F** and **G**. The IRC calculation affords complexes **24"** and **28"** with decoordinated acetone. Selected bond distances are given in Å**.**

METHANOL

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Complex 9-perp

Ru	0.003264	0.301300	-0.579867
P	-2.117925	1.097622	-0.083214
P	2.189928	1.068581	-0.131777
P	-0.008499	-2.050850	-0.048337
C	-2.224457	2.910844	0.401166
C	-4.455496	-0.680829	3.588004
C	-3.053221	-0.600539	3.600375
C	-2.365368	-0.083281	2.489695
C	-3.421820	1.065584	-1.416523
C	-3.909641	-0.187619	-1.863605
C	-4.838607	-0.255715	-2.912751
C	-5.288734	0.919529	-3.539682
C	-4.809511	2.165376	-3.105899
C	-3.884640	2.241025	-2.049448
C	2.241643	2.698216	0.780741
C	-1.417727	3.880016	-0.237756
C	1.213224	3.053819	1.679724
C	1.290066	4.243736	2.423940
C	2.391124	5.101054	2.274458
C	3.416576	4.765325	1.373207
C	3.345345	3.573467	0.635225
C	3.223799	1.484765	-1.620392
C	2.589284	2.036592	-2.757877
C	3.346054	2.439782	-3.869460
C	4.743194	2.293835	-3.867198
C	5.383305	1.737693	-2.747750
C	-1.559484	5.245955	0.057000
C	4.631322	1.335182	-1.631042
C	3.412607	0.116485	0.909669
C	3.831119	0.568491	2.183228
C	4.708116	-0.205237	2.963880
C	5.187686	-1.433793	2.483263
C	4.781974	-1.891181	1.217625
C	3.898683	-1.128092	0.438925
C	-1.477706	-3.022615	-0.678440
C	-1.405330	-3.751863	-1.888578
C	-2.539928	-4.403779	-2.402332
C	-2.501030	5.670738	1.008196
C	-3.761229	-4.352473	-1.711467
C	-3.845062	-3.634910	-0.505928
C	-2.719432	-2.965378	0.002584
C	0.059968	-2.604878	1.731517
C	-0.579524	-3.775233	2.207025
C	-0.454853	-4.163004	3.552078
C	0.317215	-3.397183	4.441540
C	0.967048	-2.241345	3.977588
C	0.838274	-1.845912	2.635960
C	1.352738	-3.125116	-0.762985
C	-3.301398	4.719193	1.660700
C	1.753775	-4.339339	-0.160492
C	2.758249	-5.129588	-0.743781
C	3.372796	-4.722012	-1.940672
C	2.981657	-3.518056	-2.549801
C	1.982491	-2.718785	-1.964629
C	-3.170478	3.353835	1.357181
C	-3.067290	0.358876	1.346374
C	-4.481505	0.278433	1.347282
C	-5.166920	-0.239041	2.459276
H	-3.567182	-1.109296	-1.383078
H	-5.205018	-1.233527	-3.240643
H	-6.008760	0.862674	-4.362082
H	-5.157088	3.086178	-3.585468
H	-3.522382	3.215587	-1.712196
H	-2.803143	-2.405777	0.938138
H	-4.790876	-3.586878	0.043177
H	-4.640289	-4.871824	-2.105890
H	-2.461574	-4.962131	-3.340862
H	-0.452463	-3.823531	-2.420116
H	1.289954	-4.658083	0.777330
H	3.060944	-6.064543	-0.260601
H	4.153820	-5.340713	-2.394898
H	3.456669	-3.189679	-3.480405
H	1.672119	-1.773771	-2.428727
H	-1.272550	-0.046705	2.496874
H	-2.483983	-0.956558	4.464342
H	-4.991124	-1.089888	4.450469
H	-6.260203	-0.296815	2.441390
H	-5.040300	0.613928	0.469474
H	-3.806899	2.626303	1.867351
H	-0.655414	3.551054	-0.951582
H	-0.917731	5.974563	-0.448228
H	-2.605661	6.734673	1.243475
H	-4.035927	5.036824	2.408005
H	4.145636	3.318940	-0.065823
H	4.275244	5.431914	1.242848
H	2.446855	6.030923	2.849507
H	0.474642	4.504890	3.105471
H	0.337766	2.405088	1.773019
H	1.499607	2.111744	-2.772713
H	5.135078	0.893952	-0.766667
H	6.471280	1.615469	-2.739626
H	2.838070	2.858284	-4.744191
H	5.330030	2.605574	-4.737198
H	3.574133	-1.507569	-0.533930
H	3.479036	1.533061	2.558034
H	5.023080	0.162707	3.946006
H	5.871989	-2.033873	3.091294
H	5.139529	-2.851350	0.833741
H	-1.189577	-4.374388	1.524780
H	1.351227	-0.948047	2.280868
H	1.585800	-1.644869	4.655545
H	0.416446	-3.703068	5.487958
H	-0.961838	-5.067944	3.902947
H	-0.029700	0.528325	1.013862
O	0.519222	-0.139692	-2.671197
C	-0.785179	-0.107285	-2.605529
H	-1.363269	-1.054254	-2.632349
H	0.062285	1.838566	-1.091333
H	-1.320822	0.781313	-2.994112

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Complex 19

Ru	-0.070417	0.511419	-0.363900
P	-2.342698	0.973743	-0.060301
P	2.173140	1.172606	-0.104429
P	0.144134	-1.889957	0.005269
C	-2.689247	2.750468	0.440748
C	-4.811249	-1.153028	3.316556
C	-3.420593	-0.995005	3.436018
C	-2.690000	-0.376240	2.407281
C	-3.494079	0.842158	-1.527166
C	-3.758984	-0.445117	-2.060734
C	-4.542192	-0.592487	-3.216113
C	-5.065573	0.538284	-3.865850
C	-4.807664	1.817480	-3.348413
C	-4.028102	1.971463	-2.188215
C	2.326155	2.947889	0.487801
C	-2.045840	3.810614	-0.243113
C	1.356587	3.484747	1.367498
C	1.497859	4.782982	1.886477
C	2.600762	5.573541	1.523933
C	3.564876	5.056446	0.643686
C	3.433590	3.753035	0.136021
C	3.332100	1.233651	-1.567803
C	2.789464	1.452104	-2.853376
C	3.626195	1.576696	-3.974528
C	5.019515	1.482181	-3.829967
C	5.573259	1.261912	-2.557474
C	-2.331857	5.148917	0.070468
C	4.739325	1.139237	-1.433941
C	3.251490	0.370739	1.195935
C	3.368154	0.938060	2.487151
C	4.125117	0.299710	3.483973
C	4.783871	-0.909463	3.207792
C	4.679868	-1.478559	1.928237
C	3.919176	-0.849001	0.929458
C	-1.154738	-2.981152	-0.783085
C	-0.905164	-3.635533	-2.011350
C	-1.913265	-4.386699	-2.639358

C	-3.253654	5.455448	1.085863
C	-3.180252	-4.511532	-2.046994
C	-3.440361	-3.866416	-0.825702
C	-2.442816	-3.096603	-0.203842
C	0.090336	-2.482086	1.776330
C	-0.448787	-3.740128	2.140292
C	-0.420781	-4.173450	3.476712
C	0.156330	-3.366703	4.471190
C	0.712388	-2.125621	4.119179
C	0.679620	-1.685474	2.785196
C	1.671594	-2.813091	-0.570431
C	-3.892453	4.415069	1.777705
C	2.180857	-3.933586	0.125782
C	3.321680	-4.609708	-0.337264
C	3.971283	-4.181397	-1.507489
C	3.472060	-3.073458	-2.211385
C	2.334613	-2.388505	-1.746960
C	-3.620792	3.074103	1.452970
C	-3.339785	0.092033	1.244121
C	-4.742326	-0.067977	1.135572
C	-5.469791	-0.688470	2.164583
H	-3.364056	-1.333773	-1.558804
H	-4.732896	-1.596319	-3.607566
H	-5.670388	0.422256	-4.770689
H	-5.217843	2.703735	-3.843500
H	-3.839505	2.972081	-1.790317
H	-2.664311	-2.586191	0.737533
H	-4.425039	-3.950371	-0.354833
H	-3.959185	-5.109033	-2.531074
H	-1.699441	-4.882464	-3.591721
H	0.081118	-3.559687	-2.476295
H	1.692851	-4.268794	1.044476
H	3.702084	-5.472035	0.220187
H	4.860977	-4.708004	-1.867635
H	3.968917	-2.726766	-3.123075
H	1.954520	-1.529500	-2.308120
H	-1.605080	-0.269444	2.492520
H	-2.892901	-1.365015	4.320193
H	-5.379939	-1.639187	4.115590
H	-6.553767	-0.806877	2.065719
H	-5.258062	0.291720	0.240863
H	-4.135153	2.273860	1.990883
H	-1.300494	3.581752	-1.011733
H	-1.821790	5.950757	-0.472883
H	-3.468250	6.498933	1.337583
H	-4.608860	4.642000	2.573988
H	4.190933	3.361389	-0.548342
H	4.424306	5.666912	0.347768
H	2.704459	6.588878	1.919846
H	0.732593	5.177353	2.562625
H	0.479153	2.884309	1.624913
H	1.705488	1.498666	-2.980469
H	5.177151	0.959761	-0.448046
H	6.658669	1.184494	-2.436015
H	3.183228	1.737321	-4.962488
H	5.671127	1.574994	-4.704571
H	3.840305	-1.308844	-0.058115
H	2.879778	1.891735	2.705932
H	4.209614	0.759664	4.474161
H	5.376731	-1.403837	3.983723
H	5.183055	-2.422557	1.698595
H	-0.906069	-4.375005	1.376527
H	1.120936	-0.720380	2.521110
H	1.183493	-1.494791	4.879584
H	0.179908	-3.706952	5.511452
H	-0.850568	-5.146025	3.737933
H	-0.073561	0.593673	1.256161
O	0.367499	-0.648026	-3.333848
C	-0.415710	-0.139021	-2.522516
H	-1.514400	-0.227476	-2.684549
H	-0.128467	2.109762	-0.282397
H	-0.064065	0.978450	-2.041072

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Complex 20-perp

Ru	-0.071796	0.518396	-0.267889
P	-2.365385	0.980084	-0.022078
P	2.200947	1.135120	-0.059319
P	0.124662	-1.896142	-0.011521
H	-0.061539	0.444160	1.384405
C	-0.391611	-0.048065	-2.337575
H	-0.135010	1.964908	0.378964
H	-0.046310	1.670180	-1.417634
C	-2.704948	2.745952	0.508146
C	-3.472464	0.903742	-1.522917
C	2.379055	2.888239	0.602880
C	3.328760	1.266219	-1.539024
C	3.307696	0.265349	1.175730
C	-1.203457	-2.923724	-0.829498
C	0.096959	-2.574443	1.728698
C	1.629946	-2.788013	-0.675924
C	-3.393413	0.072050	1.240005
O	0.408473	-0.318065	-3.232619
H	-1.481375	-0.085556	-2.609834
C	-2.771369	-0.389884	2.421296
C	-3.769309	-0.359202	-2.095349
C	-3.931340	2.068977	-2.177696
C	-1.929030	3.806951	-0.017216
C	1.551209	3.337029	1.661402
C	3.371906	3.767105	0.113761
C	2.756234	1.573616	-2.792737
C	4.737921	1.163266	-1.439606
C	3.472190	0.765675	2.489106
C	3.959908	-0.942634	0.827776
C	-0.984554	-3.518881	-2.093000
C	-2.480521	-3.052561	-0.230328
C	-0.438881	-3.850303	2.029918
C	0.706456	-1.836431	2.768490
C	2.139265	-3.958947	-0.068552
C	2.265899	-2.293170	-1.839087
C	-3.775230	3.062276	1.376197
C	-4.786587	-0.122204	1.081589
C	-3.522475	-1.030535	3.421020
C	-4.517972	-0.446856	-3.279806
C	-4.674474	1.974638	-3.367548
C	1.717291	4.618068	2.213199
C	3.525902	5.054586	0.656908
C	3.570119	1.766509	-3.921796
C	5.547580	1.354222	-2.571080
C	-2.218169	5.141195	0.314219
C	4.254041	0.072767	3.428708
C	4.745862	-1.627029	1.769282
C	-2.013720	-4.226321	-2.737403
C	-3.499726	-3.777103	-0.870882
C	-0.388295	-4.357388	3.339542
C	0.764384	-2.351513	4.074086
C	-4.054199	4.396880	1.716462
C	3.255222	-4.619021	-0.609006
C	3.378444	-2.962142	-2.380502
C	-5.533839	-0.766064	2.082252
H	-3.430519	-1.275070	-1.602883
H	-3.710555	3.051981	-1.753493
H	-2.677555	-2.588092	0.739586
H	-0.005050	-3.433717	-2.571167
H	1.670721	-4.345138	0.840443
H	1.885711	-1.391289	-2.329702
H	-1.691317	-0.259544	2.539089
H	-5.279011	0.224968	0.168904
H	-4.389575	2.259075	1.790895
H	-1.086032	3.582250	-0.677428
H	4.025785	3.443842	-0.699902
H	0.761350	2.682717	2.042879
H	1.669820	1.630764	-2.884779
H	5.196702	0.930143	-0.474848
H	3.851624	-1.350422	-0.179563
H	3.004891	1.713258	2.769924
H	-0.912957	-4.439663	1.240375
H	1.138864	-0.855599	2.549408
C	-4.904541	-1.220199	3.254103
C	-4.969467	0.718792	-3.921030

C	2.703152	5.482931	1.710016
C	4.965618	1.655727	-3.814590
C	4.893182	-1.125437	3.072596
C	-3.279004	5.439693	1.185225
C	-3.270956	-4.363970	-2.127246
C	0.210876	-3.609074	4.365871
C	3.877636	-4.122685	-1.767510
H	-4.735365	-1.432502	-3.702354
H	-5.025766	2.888462	-3.857547
H	-4.476622	-3.870526	-0.386203
H	-1.824467	-4.677523	-3.716679
H	3.637558	-5.521770	-0.121396
H	3.856050	-2.561073	-3.279981
H	-3.018822	-1.391965	4.322785
H	-6.610391	-0.910978	1.944902
H	-1.603090	5.944589	-0.103533
H	-4.881345	4.618179	2.398770
H	4.294657	5.720958	0.252147
H	1.064128	4.940497	3.030530
H	6.635335	1.269541	-2.478795
H	3.106725	1.993677	-4.887093
H	4.374153	0.483138	4.436892
H	5.235498	-2.560298	1.475434
H	1.251004	-1.765758	4.860343
H	-0.818594	-5.340961	3.554458
H	-5.546243	0.647966	-4.848591
H	-4.066930	-4.926531	-2.625192
H	4.747371	-4.637704	-2.188041
H	-5.488356	-1.723264	4.031448
H	-3.497669	6.479133	1.449977
H	2.825583	6.484868	2.133629
H	5.598506	1.801907	-4.695831
H	5.505843	-1.662328	3.803645
H	0.251522	-4.006672	5.385028

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Complex 20

Ru	-0.000759	0.487871	0.129758
P	2.276820	1.080846	0.031477
P	-2.289991	1.071899	0.061245
P	0.015166	-1.945336	-0.004505
C	2.455455	2.810522	-0.667684
C	5.303477	-1.074481	-2.849877
C	3.923108	-1.103266	-3.107224
C	3.028360	-0.470046	-2.227295
C	3.275587	1.231750	1.595148
C	3.160719	0.222916	2.579327
C	3.931388	0.281850	3.751967
C	4.825552	1.343975	3.960671
C	4.949514	2.351622	2.989503
C	4.181524	2.297777	1.814457
C	-2.622114	2.857128	-0.411863
C	1.949500	3.908277	0.071909
C	-1.608757	3.696725	-0.918227
C	-1.903229	5.012816	-1.319118
C	-3.210403	5.509788	-1.214897
C	-4.228522	4.683749	-0.704920
C	-3.939326	3.369914	-0.309607
C	-3.372501	0.998194	1.577060
C	-2.855924	1.542255	2.777108
C	-3.633782	1.565556	3.944246
C	-4.940287	1.048004	3.934293
C	-5.466843	0.513365	2.747885
C	2.033426	5.213405	-0.435317
C	-4.691719	0.489853	1.575126
C	-3.330524	0.244632	-1.250701
C	-3.588048	0.891442	-2.483125
C	-4.287524	0.230011	-3.506960
C	-4.753715	-1.080300	-3.313917
C	-4.501570	-1.734239	-2.096043
C	-3.786726	-1.085603	-1.075762
C	1.368317	-2.804863	0.951067
C	1.096069	-3.427224	2.190692
C	2.131460	-4.013295	2.938187
C	2.602685	5.445120	-1.701316
C	3.450801	-3.998231	2.457539
C	3.734063	-3.381237	1.227759
C	2.705078	-2.780926	0.483229
C	0.216976	-2.686655	-1.714348
C	1.035986	-3.806274	-1.991290
C	1.116047	-4.331402	-3.293374
C	0.369391	-3.760647	-4.336815
C	-0.467470	-2.663956	-4.069073
C	-0.543493	-2.131394	-2.771991
C	-1.439308	-2.986595	0.564078
C	3.095313	4.364735	-2.448138
C	-1.759467	-4.214530	-0.059240
C	-2.852466	-4.979358	0.381286
C	-3.642101	-4.532429	1.454233
C	-3.328438	-3.318294	2.087445
C	-2.237025	-2.548754	1.646910
C	3.032419	3.056881	-1.932176
C	3.502030	0.205017	-1.079742
C	4.893954	0.229174	-0.831489
C	5.785728	-0.408612	-1.709704
H	2.463556	-0.605599	2.433748
H	3.823145	-0.506752	4.502614
H	5.421177	1.389172	4.877971
H	5.643310	3.184138	3.145028
H	4.272027	3.091089	1.067095
H	2.943623	-2.286506	-0.461672
H	4.759170	-3.352798	0.845410
H	4.254424	-4.462137	3.038256
H	1.900251	-4.486579	3.898002
H	0.073374	-3.442456	2.573126
H	-1.156788	-4.570422	-0.898823
H	-3.084404	-5.926793	-0.116305
H	-4.494682	-5.128310	1.795910
H	-3.934428	-2.956528	2.924022
H	-1.969930	-1.618521	2.155166
H	1.953368	-0.520822	-2.420453
H	3.531980	-1.632602	-3.981273
H	6.000110	-1.573774	-3.530703
H	6.860179	-0.385699	-1.500460
H	5.275136	0.740100	0.057391
H	3.438646	2.225316	-2.513890
H	1.483681	3.731697	1.047202
H	1.648460	6.049326	0.157507
H	2.662017	6.463035	-2.099245
H	3.540281	4.534163	-3.433995
H	-4.735395	2.736991	0.093356
H	-5.250655	5.064616	-0.611777
H	-3.437359	6.535508	-1.522682
H	-1.096856	5.644500	-1.704850
H	-0.583240	3.323605	-0.982066
H	-1.838616	1.945618	2.796724
H	-5.110510	0.071423	0.655916
H	-6.486585	0.115004	2.728849
H	-3.214739	1.985717	4.864053
H	-5.544466	1.063961	4.846818
H	-3.567602	-1.618672	-0.147419
H	-3.252957	1.921141	-2.634641
H	-4.478018	0.749142	-4.452059
H	-5.307397	-1.590816	-4.108179
H	-4.846976	-2.760092	-1.935644
H	1.621381	-4.258949	-1.186535
H	-1.213801	-1.288829	-2.572907
H	-1.070711	-2.221525	-4.868299
H	0.431558	-4.172621	-5.349065
H	1.762277	-5.193718	-3.487905
H	-0.107585	0.306444	-1.676673
O	-0.223382	-0.639812	2.863945
C	0.058905	0.333459	2.147597
H	0.419263	1.257316	2.697014
H	0.035298	1.147092	-1.540089
H	0.027228	2.062634	0.487319

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Complex 21

Ru	-0.010320	0.444185	-0.302563
P	-2.269629	1.022811	-0.084036
P	2.253240	1.105297	-0.092356
P	0.058223	-1.932090	0.008796
C	-2.528141	2.775587	0.535912
C	-5.072866	-1.146888	3.001755
C	-3.701808	-0.985310	3.262473
C	-2.876300	-0.348139	2.320966
C	-3.335223	1.051166	-1.614303
C	-3.228064	-0.012578	-2.540486
C	-4.037134	-0.039757	-3.687975
C	-4.960044	0.991102	-3.929708
C	-5.075798	2.051543	-3.015701
C	-4.271118	2.082527	-1.864405
C	2.502893	2.909392	0.345040
C	-1.979478	3.856251	-0.198044
C	1.461417	3.666434	0.921679
C	1.678595	4.998640	1.315562
C	2.935863	5.594430	1.131498
C	3.980666	4.850481	0.554413
C	3.769186	3.517882	0.169685
C	3.395130	1.008034	-1.564315
C	2.917041	1.496324	-2.803182
C	3.737198	1.484591	-3.941107
C	5.047641	0.983334	-3.862789
C	5.535357	0.501437	-2.637715
C	-2.161958	5.179965	0.228750
C	4.718053	0.515188	-1.493853
C	3.275829	0.355036	1.280375
C	3.550058	1.075094	2.467786
C	4.253818	0.471235	3.524004
C	4.705290	-0.853092	3.408812
C	4.438106	-1.578085	2.235142
C	3.721719	-0.986789	1.182691
C	-1.285105	-2.913142	-0.840220
C	-1.042942	-3.526614	-2.091155
C	-2.080865	-4.179586	-2.777520
C	-2.878258	5.450784	1.409437
C	-3.370284	-4.240323	-2.224298
C	-3.621314	-3.634631	-0.981570
C	-2.591512	-2.969505	-0.296411
C	-0.117643	-2.484050	1.783622
C	-0.725869	-3.701661	2.171504
C	-0.803859	-4.060550	3.527836
C	-0.274877	-3.214287	4.517389
C	0.336385	-2.005111	4.144275
C	0.413299	-1.641918	2.789054
C	1.534638	-2.977414	-0.497549
C	-3.418903	4.389467	2.150006
C	1.918258	-4.135225	0.216620
C	3.027637	-4.895172	-0.189732
C	3.770266	-4.513343	-1.319959
C	3.397083	-3.366680	-2.040417
C	2.290761	-2.600008	-1.632840
C	-3.255568	3.061950	1.712490
C	-3.410240	0.140218	1.106653
C	-4.792030	-0.023234	0.856869
C	-5.614828	-0.665674	1.797598
H	-2.508868	-0.817350	-2.365711
H	-3.937903	-0.870695	-4.392876
H	-5.584711	0.969904	-4.828369
H	-5.792371	2.859167	-3.197173
H	-4.360384	2.913653	-1.159313
H	-2.802673	-2.488667	0.662108
H	-4.623153	-3.668431	-0.541982
H	-4.175184	-4.756104	-2.757548
H	-1.874568	-4.648170	-3.745409
H	-0.041462	-3.490213	-2.527132
H	1.356973	-4.434084	1.105812
H	3.310716	-5.786699	0.379771
H	4.635633	-5.105168	-1.635520
H	3.970780	-3.054110	-2.918709
H	1.993705	-1.710235	-2.195947
H	-1.805739	-0.252941	2.523985
H	-3.262392	-1.369367	4.187752
H	-5.714978	-1.650053	3.731533
H	-6.682354	-0.788849	1.587789
H	-5.219293	0.351413	-0.077448
H	-3.696908	2.244550	2.287750
H	-1.399429	3.650579	-1.103546
H	-1.737596	6.000157	-0.359058
H	-3.012714	6.483608	1.746150
H	-3.978655	4.588529	3.069651
H	4.585653	2.944911	-0.279869
H	4.962974	5.309055	0.401543
H	3.102108	6.634309	1.430528
H	0.852640	5.567384	1.753863
H	0.472250	3.213085	1.037493
H	1.895634	1.882497	-2.875032
H	5.105998	0.136944	-0.544270
H	6.557327	0.115082	-2.565945
H	3.347784	1.862953	-4.891569
H	5.684796	0.970110	-4.752662
H	3.497478	-1.570960	0.287222
H	3.224563	2.114834	2.557518
H	4.458517	1.045877	4.433382
H	5.259279	-1.319746	4.229403
H	4.773393	-2.614817	2.134977
H	-1.153117	-4.356992	1.406748
H	0.900807	-0.703303	2.502383
H	0.761387	-1.343266	4.905723
H	-0.334566	-3.498044	5.573057
H	-1.280121	-5.004900	3.811443
O	0.302250	-0.601932	-2.955545
C	-0.083418	0.326106	-2.236769
H	-0.558298	1.216963	-2.734790
H	-0.064787	2.046045	-0.553866

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Complex 22

Ru	0.019913	0.437683	-0.365245
P	-2.211118	1.054979	-0.031264
P	2.266250	1.026500	-0.045544
P	-0.023498	-1.936909	-0.004616
C	-3.204671	0.305234	1.358678
C	-5.264184	0.753598	-3.583794
C	-4.252469	-0.206815	-3.425630
C	-3.336791	-0.103951	-2.365912
C	-2.384773	2.865220	0.410866
C	-1.925011	3.841933	-0.505739
C	-2.036952	5.207921	-0.210620
C	-2.597321	5.623879	1.011487
C	-3.049670	4.665348	1.929967
C	-2.952629	3.293406	1.629701
C	2.507670	2.711609	0.729747
C	-2.534438	-0.112814	2.530525
C	1.459662	3.378379	1.397549
C	1.675346	4.638323	1.984970
C	2.936605	5.248216	1.909617
C	3.988571	4.593148	1.244444
C	3.777325	3.335673	0.660068
C	3.300767	1.274398	-1.579721
C	2.722387	2.011920	-2.640122
C	3.445855	2.263301	-3.814847
C	4.758737	1.780247	-3.953486
C	5.345980	1.053703	-2.905960
C	-3.252734	-0.649414	3.612644
C	4.626440	0.805500	-1.723395
C	3.409701	0.029776	1.041616
C	3.802646	0.492540	2.319317
C	4.612077	-0.301668	3.149766
C	5.050243	-1.563041	2.716201
C	4.665900	-2.033436	1.449621
C	3.847069	-1.250270	0.620788
C	-1.526774	-2.827334	-0.665733
C	-1.513643	-3.418483	-1.950617
C	-2.676659	-4.005487	-2.478395
C	-4.650006	-0.777380	3.536781
C	-3.865552	-4.018674	-1.730966
C	-3.888747	-3.434670	-0.453354
C	-2.733320	-2.837743	0.075705

C	0.074098	-2.619454	1.727987
C	-0.524795	-3.845176	2.109561
C	-0.383954	-4.330787	3.420452
C	0.359412	-3.606700	4.367624
C	0.960737	-2.392372	3.998412
C	0.817112	-1.899217	2.690839
C	1.288055	-2.973697	-0.857865
C	-5.326625	-0.365655	2.375412
C	1.645805	-4.261548	-0.396835
C	2.602807	-5.028578	-1.081017
C	3.214208	-4.526587	-2.243170
C	2.869573	-3.248775	-2.711635
C	1.918961	-2.475515	-2.021058
C	-4.611208	0.173247	1.293156
C	-3.423689	0.963060	-1.444692
C	-4.449171	1.925393	-1.611301
C	-5.361362	1.819839	-2.673950
H	-1.470217	3.523380	-1.449159
H	-1.679443	5.948816	-0.932798
H	-2.678831	6.690661	1.242828
H	-3.487715	4.979142	2.883124
H	-3.319158	2.553271	2.345459
H	-2.766507	-2.378125	1.066919
H	-4.810955	-3.431917	0.135908
H	-4.768949	-4.480851	-2.140926
H	-2.645912	-4.462760	-3.472830
H	-0.588258	-3.429806	-2.533280
H	1.187267	-4.655140	0.514599
H	2.871455	-6.020690	-0.703598
H	3.958877	-5.126343	-2.776158
H	3.345727	-2.840442	-3.608765
H	1.679811	-1.468801	-2.373373
H	-2.549162	-0.853862	-2.256358
H	-4.166569	-1.041644	-4.127551
H	-5.972034	0.674719	-4.415049
H	-6.144739	2.575376	-2.792715
H	-4.519238	2.765190	-0.914182
H	-5.141554	0.484180	0.388588
H	-1.444027	-0.030093	2.573857
H	-2.713385	-0.979640	4.505700
H	-5.209086	-1.201843	4.376754
H	-6.415013	-0.465218	2.309087
H	4.595800	2.835854	0.133429
H	4.974129	5.064687	1.174783
H	3.100567	6.232560	2.359922
H	0.844265	5.143188	2.487259
H	0.472703	2.910318	1.439461
H	1.699082	2.384879	-2.535961
H	5.092827	0.240064	-0.911891
H	6.370285	0.678984	-3.003255
H	2.979890	2.832849	-4.625233
H	5.320315	1.971404	-4.873381
H	3.535736	-1.639756	-0.351713
H	3.484686	1.482327	2.656885
H	4.908030	0.075496	4.134266
H	5.684673	-2.177957	3.362194
H	4.990848	-3.019211	1.103218
H	-1.122790	-4.405507	1.384688
H	1.278363	-0.948773	2.407941
H	1.549609	-1.823563	4.724932
H	0.468794	-3.987911	5.388064
H	-0.859918	-5.276029	3.701400
H	0.057415	2.045326	-0.535739
H	0.027448	0.747673	1.280286
C	-0.043603	0.303567	-2.261839
O	-0.104228	0.302517	-3.440823

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TS[9-9perp]

Ru	0.066410	0.288220	-0.461161
P	-2.108358	1.053490	-0.101133
P	2.281958	0.987095	-0.080670
P	-0.042079	-2.081156	-0.029696
C	-2.182494	2.908694	0.167455
C	-4.368669	-0.336274	3.780670
C	-2.966165	-0.250352	3.760093
C	-2.301190	0.158264	2.591741
C	-3.425829	0.885823	-1.408378
C	-3.464395	-0.283733	-2.200860
C	-4.461994	-0.448546	-3.175467
C	-5.429416	0.548945	-3.376329
C	-5.398440	1.718298	-2.597957
C	-4.402781	1.888514	-1.622141
C	2.806030	2.290296	-1.318696
C	-1.619926	3.764506	-0.811305
C	2.405653	3.636518	-1.161534
C	2.692886	4.588164	-2.153263
C	3.380214	4.212991	-3.319866
C	3.787064	2.879495	-3.484884
C	3.506358	1.924603	-2.492924
C	3.849960	-0.032357	-0.031326
C	3.774307	-1.419719	0.196274
C	4.939369	-2.201708	0.279546
C	6.200300	-1.603595	0.141423
C	6.292745	-0.218644	-0.087119
C	-1.672518	5.158042	-0.662384
C	5.130634	0.562831	-0.176522
C	2.448629	1.942938	1.524505
C	1.370842	2.755417	1.956167
C	1.471160	3.514760	3.132808
C	2.637608	3.462497	3.913619
C	3.705782	2.648157	3.506365
C	3.616626	1.899017	2.320338
C	-1.670046	-2.932819	-0.385399
C	-1.889739	-3.650789	-1.583370
C	-3.149559	-4.208216	-1.862858
C	-2.280507	5.724971	0.472891
C	-4.205863	-4.064156	-0.949527
C	-3.997451	-3.356561	0.246363
C	-2.743673	-2.791738	0.527344
C	0.273269	-2.658372	1.714369
C	-0.174004	-3.918559	2.183175
C	0.120839	-4.339991	3.489620
C	0.865434	-3.513356	4.349412
C	1.308863	-2.260179	3.898130
C	1.013890	-1.833679	2.591808
C	1.076084	-3.227192	-1.003234
C	-2.842151	4.889140	1.449102
C	1.740174	-4.341914	-0.442698
C	2.556086	-5.162843	-1.240546
C	2.713662	-4.889249	-2.609368
C	2.053762	-3.787250	-3.178885
C	1.246136	-2.956691	-2.384280
C	-2.802568	3.489923	1.294889
C	-3.028453	0.491415	1.425929
C	-4.439994	0.407989	1.460615
C	-5.102727	-0.005975	2.628703
H	-2.702345	-1.053120	-2.065068
H	-4.474530	-1.361244	-3.778859
H	-6.202869	0.419013	-4.140222
H	-6.147019	2.502464	-2.751119
H	-4.376020	2.806038	-1.027833
H	-2.597528	-2.238340	1.458306
H	-4.813234	-3.232446	0.964996
H	-5.185857	-4.500797	-1.166321
H	-3.298117	-4.765451	-2.793809
H	-1.069057	-3.783786	-2.292678
H	1.617127	-4.566287	0.620635
H	3.063132	-6.022957	-0.790323
H	3.347407	-5.531800	-3.228929
H	2.168059	-3.569962	-4.246274
H	0.719399	-2.098560	-2.817516
H	-1.207398	0.199534	2.569543
H	-2.382722	-0.514557	4.647768
H	-4.886494	-0.663380	4.687979
H	-6.195753	-0.071229	2.636012
H	-5.015327	0.658127	0.564938
H	-3.254744	2.847699	2.055040
H	-1.128265	3.328639	-1.687405
H	-1.237086	5.801290	-1.433929
H	-2.315303	6.812517	0.592288
H	-3.319679	5.320624	2.334938

H	3.843774	0.891675	-2.624459
H	4.329671	2.577553	-4.386582
H	3.601643	4.955892	-4.092374
H	2.382338	5.628110	-2.008656
H	1.872940	3.943433	-0.256367
H	2.797994	-1.896108	0.286967
H	5.208403	1.636691	-0.369224
H	7.273380	0.254840	-0.201303
H	4.849010	-3.280456	0.436510
H	7.108745	-2.211127	0.202700
H	4.457045	1.271023	2.014773
H	0.444930	2.772575	1.374630
H	0.626264	4.139968	3.439359
H	2.710369	4.047160	4.836229
H	4.616383	2.591170	4.111813
H	-0.768916	-4.557030	1.523563
H	1.347324	-0.849731	2.246890
H	1.885172	-1.606263	4.560856
H	1.093557	-3.844395	5.367633
H	-0.235347	-5.314963	3.837934
H	0.120871	0.565885	1.107861
O	-0.433503	-0.296837	-2.554215
C	0.635009	0.432017	-2.620202
H	0.563121	1.493243	-2.926442
H	0.132530	1.889153	-0.653434
H	1.613273	-0.057345	-2.815942

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TS[9perp-19]

Ru	-0.017305	-0.402684	-0.327342
P	2.196260	-1.063727	-0.059440
P	-2.250136	-1.073211	-0.119580
P	-0.028623	1.989303	0.048559
C	2.456749	-2.831693	0.509481
C	4.944108	0.775867	3.280871
C	3.556164	0.654832	3.463423
C	2.751875	0.129985	2.438836
C	3.234092	-1.039675	-1.603811
C	3.817136	0.172674	-2.050705
C	4.467533	0.233397	-3.294289
C	4.525404	-0.900558	-4.122263
C	3.928773	-2.100065	-3.700837
C	3.288390	-2.172238	-2.451879
C	-2.425458	-2.482546	1.099445
C	1.396820	-3.593066	1.042262
C	-1.720009	-2.447234	2.324692
C	-1.867223	-3.476351	3.269851
C	-2.714461	-4.565072	3.001278
C	-3.418766	-4.613546	1.786977
C	-3.281738	-3.578374	0.846235
C	-2.976616	-1.851327	-1.650383
C	-2.126076	-2.557861	-2.531923
C	-2.643057	-3.179009	-3.679338
C	-4.015569	-3.101118	-3.968680
C	-4.870454	-2.399564	-3.103039
C	1.621822	-4.892583	1.531526
C	-4.357207	-1.778736	-1.951762
C	-3.685795	-0.023925	0.455694
C	-4.456530	-0.342719	1.598722
C	-5.518152	0.488076	1.997343
C	-5.830541	1.641309	1.260238
C	-5.072736	1.965998	0.121990
C	-4.007787	1.143567	-0.274935
C	1.489110	2.916971	-0.544855
C	1.489109	3.605738	-1.780821
C	2.663035	4.202036	-2.273047
C	2.906405	-5.453124	1.485611
C	3.856127	4.134776	-1.535785
C	3.867874	3.461027	-0.302571
C	2.700369	2.851764	0.186954
C	-0.111534	2.481592	1.848974
C	0.556894	3.609823	2.381275
C	0.424094	3.945389	3.739694
C	-0.389096	3.172424	4.585005
C	-1.077901	2.065171	4.062506
C	-0.941188	1.721598	2.707549
C	-1.319253	3.187430	-0.629834
C	3.972772	-4.701829	0.958923
C	-1.811537	4.267828	0.137885
C	-2.725153	5.183622	-0.410758
C	-3.160978	5.041499	-1.738280
C	-2.680694	3.972511	-2.512881
C	-1.773169	3.048730	-1.964884
C	3.754236	-3.400489	0.484748
C	3.322084	-0.286302	1.213978
C	4.720304	-0.165200	1.042879
C	5.521723	0.366303	2.067551
H	3.762004	1.070325	-1.426669
H	4.918282	1.177071	-3.616673
H	5.027197	-0.847495	-5.093431
H	3.964543	-2.986955	-4.341886
H	2.841371	-3.115324	-2.122717
H	2.732663	2.320897	1.140664
H	4.788217	3.398431	0.286304
H	4.767194	4.608973	-1.914198
H	2.636183	4.732179	-3.230813
H	0.559265	3.698820	-2.348442
H	-1.481402	4.393678	1.171906
H	-3.094539	6.010732	0.204498
H	-3.868144	5.759525	-2.166359
H	-3.013503	3.847865	-3.548806
H	-1.418299	2.210355	-2.574107
H	1.667667	0.065381	2.574780
H	3.091485	0.981142	4.399007
H	5.570765	1.189380	4.077199
H	6.602289	0.457622	1.915553
H	5.179793	-0.467167	0.097901
H	4.594117	-2.822013	0.090608
H	0.391588	-3.165773	1.071452
H	0.781291	-5.458858	1.944953
H	3.081083	-6.467097	1.859286
H	4.980028	-5.129392	0.922018
H	-3.839158	-3.618032	-0.093688
H	-4.081047	-5.457606	1.568864
H	-2.824266	-5.370644	3.734303
H	-1.311133	-3.429793	4.211879
H	-1.041463	-1.611462	2.524257
H	-1.055020	-2.611824	-2.310572
H	-5.027194	-1.227068	-1.286615
H	-5.940994	-2.331799	-3.322276
H	-1.968499	-3.717640	-4.352687
H	-4.415907	-3.580606	-4.867572
H	-3.409297	1.421331	-1.145387
H	-4.231420	-1.246477	2.170772
H	-6.105147	0.225854	2.883808
H	-6.657411	2.286993	1.572740
H	-5.292259	2.869579	-0.454068
H	1.189064	4.221328	1.730943
H	-1.490344	0.867595	2.300966
H	-1.730858	1.468026	4.707651
H	-0.492394	3.436906	5.642207
H	0.955167	4.817520	4.135107
H	0.030047	-0.389708	1.240158
O	-0.618284	0.452277	-3.121733
C	0.506742	0.150273	-2.691739
H	1.396339	0.814018	-2.780067
H	-0.048070	-2.023159	-0.487357
H	0.708932	-0.909265	-2.340139

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TS[19-20perp]

Ru	-0.077551	0.518710	-0.308927
P	-2.365927	0.976718	-0.035043
P	2.187633	1.142769	-0.076974
P	0.134163	-1.894630	-0.007016
C	-2.691166	2.759295	0.446416
C	-4.859421	-1.126226	3.336525
C	-3.466671	-0.987034	3.455534
C	-2.727710	-0.375030	2.428691
C	-3.505843	0.850047	-1.510248
C	-3.778197	-0.433015	-2.048573
C	-4.560810	-0.570350	-3.205536

C	-5.073892	0.566308	-3.852874
C	-4.805424	1.842014	-3.332454
C	-4.026964	1.985836	-2.170267
C	2.367394	2.903338	0.562399
C	-1.989651	3.798859	-0.212368
C	1.483846	3.394791	1.553990
C	1.653529	4.679464	2.097054
C	2.699563	5.503958	1.651219
C	3.578716	5.032397	0.663833
C	3.419875	3.742104	0.129945
C	3.328611	1.244255	-1.549997
C	2.769710	1.524920	-2.816027
C	3.594158	1.693203	-3.941132
C	4.988420	1.583195	-3.818420
C	5.557405	1.305439	-2.563652
C	-2.252869	5.145357	0.086005
C	4.736721	1.138851	-1.436171
C	3.277119	0.291620	1.183625
C	3.417928	0.813692	2.491315
C	4.186176	0.137876	3.454150
C	4.833719	-1.064455	3.127397
C	4.708522	-1.587647	1.830368
C	3.936684	-0.920197	0.865195
C	-1.189425	-2.945608	-0.803475
C	-0.973694	-3.546759	-2.064835
C	-1.999311	-4.270783	-2.696186
C	-3.209290	5.479601	1.059733
C	-3.249873	-4.419960	-2.074914
C	-3.475815	-3.827035	-0.820899
C	-2.460682	-3.084892	-0.193938
C	0.109256	-2.541475	1.744582
C	-0.409821	-3.819620	2.066465
C	-0.358218	-4.303077	3.384785
C	0.224668	-3.528306	4.400956
C	0.761446	-2.268354	4.089447
C	0.702879	-1.777069	2.774508
C	1.643446	-2.793512	-0.654129
C	-3.906493	4.459471	1.725047
C	2.163256	-3.948640	-0.025806
C	3.284461	-4.609047	-0.554981
C	3.902049	-4.128832	-1.722819
C	3.392707	-2.984040	-2.356655
C	2.274929	-2.314784	-1.826624
C	-3.656971	3.110602	1.415795
C	-3.372920	0.106137	1.268087
C	-4.777192	-0.036789	1.158364
C	-5.512398	-0.650562	2.185977
H	-3.391273	-1.326357	-1.550062
H	-4.757346	-1.571420	-3.601102
H	-5.677945	0.457714	-4.759193
H	-5.205501	2.733253	-3.826782
H	-3.827578	2.983888	-1.771521
H	-2.656108	-2.615926	0.774426
H	-4.447822	-3.929369	-0.328078
H	-4.042557	-4.996266	-2.562284
H	-1.812341	-4.726161	-3.673976
H	0.000634	-3.452591	-2.551728
H	1.699649	-4.321554	0.891165
H	3.674907	-5.499348	-0.051137
H	4.776000	-4.643975	-2.134377
H	3.866374	-2.595662	-3.263768
H	1.885994	-1.425678	-2.333266
H	-1.640978	-0.279903	2.511126
H	-2.945104	-1.365128	4.340100
H	-5.434139	-1.606595	4.134791
H	-6.597718	-0.755624	2.086828
H	-5.287595	0.329224	0.263037
H	-4.214595	2.325641	1.933156
H	-1.220701	3.548016	-0.949696
H	-1.698040	5.931346	-0.436247
H	-3.406098	6.529300	1.299849
H	-4.650811	4.708581	2.488396
H	4.115751	3.385272	-0.633649
H	4.394607	5.667606	0.303664
H	2.824871	6.508764	2.067184
H	0.955260	5.036621	2.860896
H	0.648644	2.770946	1.886576
H	1.684343	1.579976	-2.922752
H	5.185871	0.921016	-0.463269
H	6.643948	1.219105	-2.459373
H	3.140094	1.900180	-4.915372
H	5.629949	1.710198	-4.696324
H	3.844962	-1.343783	-0.137279
H	2.941880	1.763600	2.749584
H	4.289057	0.564228	4.457582
H	5.435504	-1.588047	3.876859
H	5.204552	-2.524639	1.560026
H	-0.871512	-4.430266	1.285773
H	1.123615	-0.794934	2.540397
H	1.236332	-1.661763	4.867011
H	0.266277	-3.907621	5.427021
H	-0.774736	-5.289218	3.614595
H	-0.066886	0.511550	1.345501
O	0.389367	-0.387905	-3.258945
C	-0.404628	-0.055674	-2.378227
H	-1.496028	-0.081129	-2.636044
H	-0.146198	2.038658	0.144713
H	-0.051266	1.472312	-1.640320

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TS[20-21]

Ru	-0.013162	0.455973	-0.261065
P	-2.276801	1.046112	-0.071303
P	2.254339	1.096240	-0.068815
P	0.041291	-1.938346	0.001325
C	-2.486340	2.761348	0.657741
C	-5.293588	-1.197045	2.752970
C	-3.918083	-1.181792	3.036689
C	-3.027005	-0.521520	2.173046
C	-3.281153	1.202471	-1.634360
C	-3.178773	0.178988	-2.605771
C	-3.945423	0.234218	-3.780794
C	-4.821006	1.308919	-4.006491
C	-4.932401	2.329594	-3.047970
C	-4.171042	2.277541	-1.867831
C	2.582388	2.914264	0.252986
C	-1.992881	3.880922	-0.058282
C	1.556290	3.800803	0.637384
C	1.843688	5.147463	0.925483
C	3.157587	5.628367	0.827528
C	4.189921	4.754146	0.441588
C	3.906922	3.409701	0.160997
C	3.427525	0.879391	-1.504163
C	3.005006	1.357761	-2.767239
C	3.849743	1.272178	-3.883606
C	5.130863	0.708062	-3.758979
C	5.564192	0.236965	-2.509478
C	-2.121228	5.177367	0.461731
C	4.721342	0.322755	-1.387321
C	3.199630	0.382320	1.372234
C	3.428090	1.141170	2.545043
C	4.058524	0.561738	3.659654
C	4.481695	-0.776504	3.617858
C	4.259913	-1.539635	2.458830
C	3.615134	-0.972542	1.348250
C	-1.267513	-2.867720	-0.955734
C	-0.966864	-3.471566	-2.198118
C	-1.977317	-4.090281	-2.953809
C	-2.718942	5.379819	1.719630
C	-3.298703	-4.125361	-2.479487
C	-3.608647	-3.529749	-1.245322
C	-2.604952	-2.899695	-0.491451
C	-0.221836	-2.597449	1.731970
C	-0.889153	-3.812630	2.016317
C	-1.020612	-4.262648	3.341191
C	-0.484686	-3.513075	4.402591
C	0.188447	-2.309824	4.131507
C	0.318546	-1.855880	2.808222
C	1.532753	-2.978479	-0.472986
C	-3.197754	4.278616	2.444264
C	1.898206	-4.144851	0.237659
C	3.020899	-4.897119	-0.145882
C	3.795173	-4.499786	-1.249178

C	3.439458	-3.345819	-1.966536
C	2.319707	-2.587137	-1.581712
C	-3.093620	2.979159	1.913750
C	-3.500016	0.137342	1.015700
C	-4.887089	0.118042	0.741479
C	-5.774924	-0.547252	1.603302
H	-2.496302	-0.659600	-2.444444
H	-3.849715	-0.566398	-4.520445
H	-5.412447	1.352201	-4.926539
H	-5.612918	3.170606	-3.216083
H	-4.255911	3.078818	-1.128416
H	-2.860644	-2.428696	0.460841
H	-4.635131	-3.544609	-0.865575
H	-4.082528	-4.613991	-3.066991
H	-1.724708	-4.551234	-3.914344
H	0.058889	-3.453459	-2.573733
H	1.307985	-4.459279	1.102168
H	3.288729	-5.795665	0.419958
H	4.671027	-5.085614	-1.546478
H	4.037164	-3.019941	-2.823418
H	2.034171	-1.692842	-2.142426
H	-1.955618	-0.544092	2.389780
H	-3.525420	-1.697758	3.917857
H	-5.986727	-1.717867	3.421084
H	-6.845501	-0.557803	1.373987
H	-5.268030	0.618446	-0.153442
H	-3.491755	2.130716	2.476137
H	-1.506386	3.728522	-1.027281
H	-1.750488	6.030303	-0.115968
H	-2.810653	6.391051	2.128166
H	-3.664660	4.424876	3.423600
H	4.714468	2.737979	-0.144458
H	5.217974	5.120593	0.356136
H	3.379149	6.677872	1.046213
H	1.027656	5.814165	1.221649
H	0.527530	3.434767	0.696761
H	2.008874	1.797663	-2.874839
H	5.069054	-0.046239	-0.418718
H	6.564106	-0.195935	-2.401195
H	3.503296	1.644368	-4.852932
H	5.788242	0.639445	-4.631431
H	3.423090	-1.583884	0.463134
H	3.126553	2.191735	2.577378
H	4.228587	1.165404	4.557271
H	4.979760	-1.223788	4.483818
H	4.575482	-2.586522	2.415597
H	-1.317461	-4.396020	1.196294
H	0.852009	-0.923048	2.600971
H	0.619630	-1.722475	4.948551
H	-0.586970	-3.867170	5.433369
H	-1.542987	-5.203611	3.543086
H	0.262142	1.393470	2.738018
O	0.332922	-0.603677	-2.914636
C	-0.058721	0.324709	-2.198885
H	-0.515666	1.220366	-2.705910
H	-0.354074	1.660504	2.395883
H	-0.087766	2.055541	-0.524089

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TS[21-22]

Ru	-0.030733	0.439586	-0.388276
P	-2.289616	1.008549	-0.044480
P	2.253398	0.940496	-0.043874
P	-0.046736	-1.829466	-0.119840
C	-2.492788	2.849934	-0.319521
C	-3.833768	0.431286	4.340493
C	-2.620897	1.092424	4.079863
C	-2.171626	1.249497	2.760246
C	-3.677236	0.454516	-1.148646
C	-3.428619	-0.448222	-2.202438
C	-4.455406	-0.785962	-3.102738
C	-5.734485	-0.229140	-2.958536
C	-5.989628	0.681584	-1.916307
C	-4.967358	1.029901	-1.022860
C	2.661723	2.755990	-0.270630
C	-2.365474	3.335998	-1.644332
C	1.657897	3.722784	-0.497116
C	1.996181	5.077401	-0.672252
C	3.336158	5.486553	-0.616948
C	4.345146	4.532446	-0.393539
C	4.012752	3.180320	-0.229875
C	3.628555	0.254684	-1.105178
C	3.413112	0.201471	-2.501580
C	4.449948	-0.168369	-3.372038
C	5.715689	-0.503497	-2.863177
C	5.937880	-0.468351	-1.477581
C	-2.433616	4.712006	-1.911299
C	4.905805	-0.087839	-0.602963
C	2.887836	0.646798	1.675404
C	2.904241	1.690275	2.629275
C	3.321242	1.442675	3.947415
C	3.736307	0.155671	4.329228
C	3.716850	-0.889275	3.390389
C	3.286560	-0.651937	2.075215
C	-1.464967	-2.888410	-0.736862
C	-1.376318	-3.688190	-1.898050
C	-2.488959	-4.422396	-2.345330
C	-2.636883	5.626170	-0.862739
C	-3.700516	-4.377849	-1.636939
C	-3.796180	-3.592889	-0.475379
C	-2.692226	-2.851468	-0.029581
C	-0.101751	-2.353579	1.674400
C	-0.381757	-3.692321	2.047462
C	-0.398575	-4.065588	3.399509
C	-0.142725	-3.109252	4.399762
C	0.128689	-1.781146	4.039903
C	0.148506	-1.404822	2.684935
C	1.392679	-2.842229	-0.749993
C	-2.781022	5.153335	0.451344
C	2.137495	-3.729063	0.062409
C	3.197888	-4.475889	-0.480020
C	3.522658	-4.358982	-1.840706
C	2.795014	-3.475471	-2.655139
C	1.746301	-2.712863	-2.116296
C	-2.711122	3.775610	0.723383
C	-2.947918	0.775248	1.673457
C	-4.161563	0.104191	1.948214
C	-4.595567	-0.070353	3.273854
H	-2.431339	-0.875640	-2.328077
H	-4.245659	-1.489797	-3.913370
H	-6.531460	-0.493665	-3.660853
H	-6.981576	1.132438	-1.810394
H	-5.155653	1.768589	-0.237530
H	-2.774716	-2.248522	0.881046
H	-4.735341	-3.555002	0.085930
H	-4.563236	-4.955745	-1.982935
H	-2.399771	-5.042061	-3.243886
H	-0.429543	-3.753547	-2.440984
H	1.876214	-3.844205	1.117968
H	3.764784	-5.156613	0.164027
H	4.344816	-4.945594	-2.262869
H	3.054426	-3.363053	-3.712571
H	1.204597	-1.998374	-2.746081
H	-1.203104	1.719691	2.556176
H	-2.012855	1.472733	4.907148
H	-4.176276	0.297778	5.371364
H	-5.535126	-0.597364	3.469271
H	-4.768578	-0.275377	1.121644
H	-2.830359	3.419319	1.750116
H	-2.224713	2.632010	-2.471841
H	-2.335404	5.067752	-2.942071
H	-2.693834	6.699056	-1.071597
H	-2.955719	5.856503	1.272336
H	4.806112	2.441800	-0.085674
H	5.394910	4.840387	-0.354400
H	3.597133	6.541045	-0.751829
H	1.199473	5.806554	-0.849600
H	0.607992	3.416217	-0.521845
H	2.426578	0.441352	-2.908526
H	5.091711	-0.060820	0.474457
H	6.919735	-0.732735	-1.071334
H	4.263986	-0.197318	-4.450577

H	6.523508	-0.793190	-3.542669
H	3.253056	-1.478097	1.357177
H	2.598152	2.697857	2.333075
H	3.334127	2.262720	4.672913
H	4.071286	-0.032639	5.354106
H	4.024795	-1.897942	3.683128
H	-0.594344	-4.433853	1.271893
H	0.356499	-0.369288	2.396130
H	0.330426	-1.030649	4.810055
H	-0.160642	-3.401536	5.454741
H	-0.618685	-5.102451	3.673954
H	-0.004797	1.816856	0.597171
O	-0.038552	-0.171229	-3.354531
C	-0.051320	0.442544	-2.297020
H	-0.073689	1.613027	-2.286354

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Complex 13H

Ru	0.005793	-0.027950	-0.323319
P	-2.316490	0.102926	-0.047799
P	2.323326	0.081723	-0.043931
C	-3.185793	1.657489	-0.576490
C	-3.905780	-0.601599	4.302921
C	-4.598284	0.272102	3.448809
C	-4.132288	0.500506	2.143089
C	-3.271113	-1.189991	-0.987062
C	-3.197725	-1.189674	-2.401749
C	-3.855542	-2.175250	-3.152230
C	-4.585287	-3.186167	-2.501274
C	-4.656110	-3.201652	-1.099607
C	-4.005738	-2.209440	-0.344623
C	3.014443	1.760329	0.362845
C	-2.508503	2.895946	-0.517958
C	2.286490	2.605194	1.232184
C	2.804069	3.853579	1.610183
C	4.049061	4.282078	1.118451
C	4.777860	3.454230	0.249596
C	4.268025	2.198767	-0.124438
C	3.344368	-0.400888	-1.526149
C	3.223157	0.358318	-2.716456
C	3.912458	-0.020640	-3.877300
C	4.722447	-1.171096	-3.874568
C	4.845534	-1.932442	-2.702497
C	-3.166355	4.085779	-0.870737
C	4.166056	-1.549358	-1.531917
C	3.099196	-0.956287	1.289395
C	4.373260	-0.652710	1.825595
C	4.945365	-1.479740	2.804610
C	4.254731	-2.617549	3.258556
C	2.988070	-2.923275	2.735905
C	2.407363	-2.096338	1.757884
C	-4.506817	4.054941	-1.289199
C	-5.189254	2.828349	-1.356369
C	-4.536317	1.636416	-1.002913
C	-2.960669	-0.139970	1.679103
C	-2.266436	-1.013566	2.548960
C	-2.741411	-1.244736	3.850163
H	-2.628036	-0.405066	-2.913110
H	-3.795362	-2.156713	-4.245139
H	-5.092635	-3.959548	-3.086316
H	-5.219201	-3.987640	-0.586399
H	-4.064912	-2.225493	0.746712
H	-4.673008	1.188524	1.486670
H	-5.501652	0.782431	3.797933
H	-4.269004	-0.776285	5.320703
H	-2.193364	-1.922966	4.511992
H	-1.355100	-1.502134	2.194615
H	-5.065471	0.681305	-1.069437
H	-1.457816	2.910231	-0.211311
H	-2.626515	5.037051	-0.824270
H	-5.017068	4.982273	-1.568277
H	-6.231916	2.797471	-1.688580
H	4.834511	1.561502	-0.809704
H	5.745917	3.783901	-0.141193
H	4.447347	5.259360	1.408816
H	2.229409	4.495021	2.285975
H	1.308367	2.277559	1.596795
H	2.589855	1.252935	-2.724930
H	4.279473	-2.136590	-0.616667
H	5.475315	-2.827847	-2.692356
H	3.815962	0.581229	-4.786709
H	5.253980	-1.469557	-4.783450
H	1.409766	-2.316054	1.354299
H	4.905845	0.240843	1.486685
H	5.928821	-1.232469	3.217189
H	4.702874	-3.259479	4.023934
H	2.442705	-3.803757	3.091115
H	0.427890	0.281132	-1.986943
H	0.054102	0.241724	1.274134
O	-0.301050	-2.156130	0.211173
C	0.031053	-2.129588	-1.048404
H	-0.753682	-2.269529	-1.817699
H	-0.466991	0.278013	-1.974663
H	1.061610	-2.417626	-1.345918
H	0.087423	1.572974	-0.309771

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Complex 23-perp

Ru	0.009828	-0.522902	0.537995
P	-2.250666	-0.078327	0.109594
P	2.204043	-0.042204	0.079961
C	-2.593623	1.617863	-0.568036
C	-5.325606	-0.265672	3.632151
C	-4.074492	-0.891739	3.749491
C	-3.150639	-0.832852	2.691510
C	-3.007372	-1.184237	-1.175965
C	-2.286986	-1.394292	-2.377995
C	-2.790995	-2.248854	-3.370062
C	-4.010659	-2.919827	-3.169609
C	-4.725183	-2.728821	-1.976349
C	-4.230386	-1.863878	-0.984921
C	2.561598	1.417618	-1.022357
C	-2.107502	2.735950	0.151479
C	1.592032	2.425837	-1.210969
C	1.874790	3.545451	-2.012855
C	3.123717	3.668306	-2.641151
C	4.094655	2.666671	-2.464702
C	3.818253	1.551772	-1.659138
C	3.087106	-1.418146	-0.812325
C	2.316508	-2.239697	-1.668044
C	2.916719	-3.283755	-2.389399
C	4.295991	-3.522470	-2.266152
C	5.070939	-2.716608	-1.415522
C	-2.347636	4.038842	-0.309710
C	4.473894	-1.671279	-0.690680
C	3.345211	0.320262	1.504345
C	3.633559	1.657319	1.863032
C	4.397692	1.939689	3.007075
C	4.888429	0.895233	3.807328
C	4.610870	-0.437345	3.459150
C	3.841913	-0.725838	2.320284
C	-3.067961	4.246264	-1.500013
C	-3.552419	3.144407	-2.221224
C	-3.322916	1.836418	-1.756666
C	-3.478059	-0.145753	1.500993
C	-4.739944	0.488662	1.393289
C	-5.657478	0.425351	2.453082
H	-1.326520	-0.885902	-2.519748
H	-2.227762	-2.396639	-4.297188
H	-4.398246	-3.594059	-3.939820
H	-5.671453	-3.254180	-1.812210
H	-4.791353	-1.715213	-0.058244
H	-2.171598	-1.317300	2.770687
H	-3.809909	-1.426584	4.667348
H	-6.041622	-0.309736	4.459185
H	-6.629157	0.921188	2.360980
H	-4.992719	1.042988	0.484137
H	-3.703177	0.982002	-2.323493
H	-1.540708	2.574897	1.074879
H	-1.971423	4.893625	0.261642
H	-3.250643	5.263303	-1.861004
H	-4.114819	3.297689	-3.147891

H	4.573025	0.768972	-1.542105
H	5.067504	2.750478	-2.959562
H	3.339755	4.536730	-3.271558
H	1.107406	4.313609	-2.150699
H	0.609744	2.317259	-0.742355
H	1.238107	-2.054445	-1.751694
H	5.079383	-1.063528	-0.011299
H	6.144422	-2.904250	-1.310453
H	2.304894	-3.913569	-3.043149
H	4.764437	-4.338051	-2.825869
H	3.637686	-1.767382	2.053704
H	3.262221	2.475662	1.238982
H	4.612893	2.980446	3.269717
H	5.485422	1.117538	4.697173
H	4.992745	-1.257509	4.075654
H	0.019134	0.879411	1.226218
O	-0.482932	-2.133512	1.784133
C	0.829039	-1.982300	1.913362
H	1.489846	-2.731655	1.431064
H	1.226328	-1.516613	2.836005
H	-0.001829	0.323295	-0.823558

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Complex 23

Ru	-0.013787	-0.245511	0.093347
P	2.310494	0.056875	-0.026182
P	-2.282748	0.052646	-0.001303
C	3.013518	1.767056	-0.217338
C	4.604006	-2.284756	-3.361945
C	3.321501	-1.763640	-3.601236
C	2.638844	-1.077850	-2.584724
C	3.092804	-0.530032	1.551198
C	2.859567	-1.873710	1.940995
C	3.367611	-2.353765	3.157339
C	4.102278	-1.501757	4.001903
C	4.330596	-0.168138	3.625713
C	3.830163	0.319405	2.405844
C	-2.910610	1.780296	-0.280902
C	2.271095	2.883382	0.229548
C	-2.184613	2.627486	-1.148902
C	-2.653281	3.918339	-1.436906
C	-3.844846	4.385065	-0.854780
C	-4.567215	3.555181	0.017443
C	-4.106571	2.257682	0.302044
C	-3.245584	-0.465176	1.503377
C	-2.896809	0.135027	2.739721
C	-3.513430	-0.274659	3.930825
C	-4.478272	-1.298083	3.910094
C	-4.825116	-1.904950	2.692920
C	2.804457	4.179173	0.134333
C	-4.215566	-1.491961	1.494442
C	-3.148196	-0.860414	-1.375756
C	-4.495544	-0.582235	-1.709474
C	-5.133996	-1.289447	-2.739707
C	-4.434473	-2.277825	-3.454728
C	-3.093930	-2.551598	-3.140935
C	-2.449664	-1.847106	-2.108557
C	4.080752	4.378307	-0.417192
C	4.824323	3.276454	-0.873533
C	4.297188	1.979011	-0.773539
C	3.235587	-0.898123	-1.316628
C	4.522962	-1.434139	-1.081535
C	5.201627	-2.122657	-2.100846
H	2.272021	-2.520962	1.277853
H	3.186588	-3.393867	3.447248
H	4.493973	-1.877244	4.952605
H	4.902624	0.497195	4.280493
H	4.013720	1.356903	2.112699
H	1.627268	-0.696506	-2.757358
H	2.845209	-1.899994	-4.577250
H	5.133100	-2.824600	-4.153598
H	6.196242	-2.536730	-1.906703
H	4.982696	-1.324462	-0.094666
H	4.874037	1.124549	-1.139227
H	1.266614	2.723211	0.635216
H	2.215472	5.033501	0.482988
H	4.492476	5.389333	-0.498341
H	5.816028	3.425936	-1.312287
H	-4.664701	1.619701	0.993931
H	-5.490423	3.916582	0.481875
H	-4.204720	5.394890	-1.075826
H	-2.081849	4.563749	-2.111799
H	-1.243624	2.269113	-1.578220
H	-2.136958	0.924785	2.759188
H	-4.500406	-1.958413	0.547047
H	-5.574483	-2.702788	2.670888
H	-3.237727	0.202325	4.876783
H	-4.954193	-1.621862	4.840940
H	-1.398862	-2.054033	-1.874973
H	-5.034464	0.204324	-1.172227
H	-6.175394	-1.063280	-2.990207
H	-4.932676	-2.826084	-4.260647
H	-2.540942	-3.312932	-3.700537
H	-0.114541	0.072961	-1.430872
O	0.487703	-2.414876	-0.234049
C	-0.500051	-2.263684	0.605456
H	-0.295301	-2.274513	1.708831
H	-1.512182	-2.628210	0.333875
H	-0.142472	1.319150	0.425489

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Complex 24

C	5.131472	-1.170201	-2.838739
C	4.741878	-2.487023	-3.137373
C	3.624992	-3.050111	-2.497610
C	2.894314	-2.301783	-1.559801
C	3.282983	-0.977438	-1.249955
C	4.407051	-0.416757	-1.900497
P	2.308131	-0.033281	0.018505
C	3.265396	-0.362830	1.576535
C	2.659705	-0.052769	2.817878
C	3.343633	-0.284099	4.021574
C	4.634540	-0.839313	4.003494
C	5.241313	-1.158887	2.777588
C	4.563883	-0.920969	1.569770
Ru	-0.020027	-0.382399	0.142358
C	-0.477080	-2.226029	0.909090
O	0.163292	-2.986170	0.129956
P	-2.272311	0.010631	-0.000833
C	-3.099982	-0.720106	-1.499443
C	-4.218952	-0.126429	-2.127003
C	-4.809475	-0.730932	-3.249129
C	-4.290090	-1.933057	-3.758732
C	-3.173573	-2.527989	-3.147953
C	-2.578077	-1.925025	-2.027647
C	2.787432	1.721145	-0.370104
C	2.166446	2.373678	-1.461648
C	2.516923	3.689930	-1.796945
C	3.484302	4.377972	-1.043241
C	4.104110	3.740747	0.043003
C	3.762666	2.418108	0.376895
C	-2.829234	1.782199	-0.046264
C	-1.954485	2.784969	-0.518348
C	-2.378241	4.122251	-0.588858
C	-3.677066	4.475326	-0.188046
C	-4.552425	3.487087	0.293075
C	-4.132992	2.148829	0.367990
C	-3.332466	-0.653182	1.380634
C	-2.920493	-0.383636	2.708979
C	-3.655710	-0.877290	3.796864
C	-4.807547	-1.653646	3.575765
C	-5.220256	-1.932694	2.263270
C	-4.488998	-1.435604	1.169158
H	1.645341	0.360592	2.828509
H	2.863615	-0.038155	4.974128
H	5.163414	-1.027890	4.943016
H	6.244035	-1.597576	2.758504
H	5.036899	-1.175376	0.616939
H	2.015688	-2.730907	-1.065014
H	3.314644	-4.073681	-2.730996
H	5.305775	-3.070952	-3.871922

H	5.997831	-0.725733	-3.339096
H	4.704433	0.611885	-1.676569
H	4.250233	1.924425	1.222129
H	1.403163	1.840412	-2.038232
H	2.031006	4.180188	-2.646755
H	3.751655	5.407333	-1.302058
H	4.857985	4.270111	0.634467
H	-4.809287	1.386545	0.766851
H	-5.561387	3.758129	0.620121
H	-4.003507	5.518794	-0.240134
H	-1.685832	4.889569	-0.949305
H	-0.936591	2.508795	-0.806689
H	-2.013028	0.207861	2.877747
H	-4.812799	-1.654516	0.147638
H	-6.113359	-2.540454	2.085911
H	-3.327642	-0.659708	4.818417
H	-5.377290	-2.043388	4.425107
H	-1.698003	-2.385579	-1.564851
H	-4.614461	0.818828	-1.743575
H	-5.672223	-0.257814	-3.729100
H	-4.749361	-2.400195	-4.635735
H	-2.756515	-3.458296	-3.546440
H	-0.100065	0.407471	-1.261952
H	0.103205	-1.448785	1.676593
H	-1.433961	-2.560610	1.369077
H	-0.081431	0.966674	0.949416

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Complex 25

Ru	0.009297	-0.208875	0.209183
P	2.323236	0.022588	0.061902
P	-2.308473	0.023548	0.051789
C	2.952462	1.608973	-0.677145
C	4.191892	-3.220217	-2.753359
C	3.078505	-2.461559	-3.155131
C	2.540420	-1.491251	-2.297037
C	3.357034	-0.055836	1.608821
C	2.805161	-0.593348	2.790823
C	3.575673	-0.689466	3.962029
C	4.906857	-0.243857	3.967401
C	5.464513	0.305746	2.799454
C	4.696715	0.403045	1.628556
C	-3.338423	-0.683580	1.435046
C	2.400001	2.835345	-0.240994
C	-2.835399	-0.619206	2.755400
C	-3.583788	-1.124106	3.830449
C	-4.839986	-1.711492	3.601712
C	-5.346131	-1.788632	2.293907
C	-4.603568	-1.275965	1.216363
C	-3.124429	-0.731767	-1.440227
C	-2.562257	-1.899456	-2.005232
C	-3.167332	-2.513834	-3.113704
C	-4.334459	-1.967967	-3.673708
C	-4.895557	-0.802202	-3.125525
C	2.878367	4.052395	-0.748833
C	-4.295207	-0.184819	-2.015382
C	-2.939181	1.770887	-0.030018
C	-4.102632	2.181368	0.660096
C	-4.567741	3.503442	0.547276
C	-3.882967	4.426485	-0.258966
C	-2.726732	4.026555	-0.951227
C	-2.253493	2.710419	-0.835791
C	3.908907	4.063611	-1.705250
C	4.460162	2.851676	-2.149329
C	3.989154	1.629726	-1.637042
C	3.120369	-1.256066	-1.025599
C	4.235946	-2.026927	-0.629764
C	4.766130	-3.003625	-1.490675
H	1.758238	-0.911195	2.783972
H	3.131127	-1.105269	4.872000
H	5.506228	-0.313952	4.880590
H	6.497819	0.667128	2.802171
H	5.127662	0.851425	0.728246
H	1.657395	-0.916096	-2.596354
H	2.620750	-2.631636	-4.134829
H	4.605843	-3.982625	-3.420853
H	5.629718	-3.595410	-1.170511
H	4.689724	-1.859037	0.350775
H	4.414690	0.687412	-1.993849
H	1.581902	2.827923	0.486634
H	2.440087	4.993677	-0.401796
H	4.275911	5.013873	-2.105712
H	5.258130	2.852253	-2.898839
H	-4.998665	-1.344008	0.198646
H	-6.320378	-2.252096	2.108117
H	-5.418945	-2.113397	4.439200
H	-3.181731	-1.064564	4.847098
H	-1.845442	-0.181029	2.925422
H	-1.643332	-2.314639	-1.578737
H	-4.724727	0.731826	-1.599635
H	-5.798864	-0.367317	-3.565337
H	-2.720328	-3.416709	-3.541916
H	-4.802276	-2.445488	-4.540552
H	-1.342818	2.399790	-1.357979
H	-4.639025	1.466260	1.290369
H	-5.466200	3.809297	1.092915
H	-4.246162	5.455531	-0.345125
H	-2.186566	4.741951	-1.579694
H	-0.003554	0.198248	1.762759
H	-0.009784	1.339273	0.516929
C	-0.017055	-1.988082	1.064453
O	0.013430	-2.616315	-0.013481
H	0.010849	0.521162	-1.301139
H	-0.066795	-2.532075	2.034389

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Complex 26b-trans

Ru	0.003093	-0.054877	0.084986
P	-2.336328	0.003770	0.014879
P	2.341253	0.007098	0.028878
H	0.000528	-0.122936	-1.590640
H	0.009109	1.621208	-0.481354
C	0.008074	-1.906236	0.290058
H	-0.004135	1.682780	0.387332
C	-3.015106	1.733214	0.050571
C	-3.190184	-0.690108	-1.483039
C	3.188295	-1.165837	-1.144224
C	3.287283	-0.260740	1.606765
C	3.004793	1.658430	-0.508752
C	-3.265405	-0.814125	1.406679
H	0.000327	0.172693	1.746469
O	0.011012	-3.075190	0.429719
C	-2.704767	-0.790151	2.705148
C	-2.564881	-1.707855	-2.234969
C	-4.474891	-0.239739	-1.873703
C	-2.722104	2.598458	-1.032463
C	2.586699	-1.425154	-2.398851
C	4.416619	-1.793812	-0.835948
C	2.695726	-0.986402	2.662954
C	4.606392	0.229998	1.765305
C	3.613846	1.852421	-1.767145
C	2.820182	2.773653	0.344924
C	-3.754143	2.231722	1.145036
C	-4.517895	-1.442024	1.216416
C	-3.390557	-1.362721	3.788689
C	-3.214868	-2.277164	-3.342147
C	-5.118215	-0.807030	-2.985846
C	3.210383	-2.273825	-3.327509
C	5.031001	-2.651573	-1.763412
C	3.412885	-1.234536	3.845174
C	5.317037	-0.014635	2.951203
C	-3.160061	3.930578	-1.015383
C	4.025210	3.136540	-2.165950
C	3.235827	4.051593	-0.056304
C	-4.185848	3.570123	1.159254
C	-5.195829	-2.021955	2.301089
H	-1.557033	-2.029707	-1.958391
H	-4.959232	0.566811	-1.314797
H	-1.715503	-0.340116	2.843069
H	-4.955444	-1.486362	0.215323
H	-3.989691	1.571187	1.984204
H	-2.154464	2.219630	-1.889396

H	4.886063	-1.618086	0.135569
H	1.614187	-0.972755	-2.621256
H	1.661685	-1.327736	2.557323
H	5.065180	0.816191	0.963334
H	2.356197	2.632698	1.327202
H	3.763550	0.997545	-2.432683
C	-4.636960	-1.979342	3.589054
C	-4.491532	-1.829247	-3.718899
C	4.433374	-2.888833	-3.011968
C	4.723317	-0.751231	3.990905
C	3.837427	4.236229	-1.314385
C	-3.890676	4.420288	0.082471
H	-2.717027	-3.066153	-3.914788
H	-6.108188	-0.445848	-3.282242
H	-2.942218	-1.337172	4.787167
H	-6.160774	-2.511945	2.136216
H	-2.930391	4.587500	-1.860429
H	-4.756959	3.944292	2.014905
H	5.977114	-3.137908	-1.505141
H	2.731698	-2.463194	-4.293771
H	6.333765	0.374881	3.064846
H	2.941149	-1.799052	4.655768
H	4.496197	3.272985	-3.144676
H	3.090864	4.904319	0.614684
H	-4.994176	-2.269090	-4.586035
H	-5.166131	-2.434716	4.432195
H	-4.228547	5.461218	0.095340
H	4.913549	-3.558943	-3.732105
H	5.278632	-0.939488	4.915182
H	4.159354	5.234541	-1.626712

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Complex 26a

C	5.154342	-2.472948	-1.812693
C	4.669398	-2.570779	-3.126273
C	3.488459	-1.898135	-3.485299
C	2.793617	-1.135337	-2.534601
C	3.277412	-1.023371	-1.209197
C	4.467020	-1.701513	-0.859172
P	2.325068	0.017400	0.007900
C	3.246496	-0.332999	1.589396
C	2.735805	-1.283022	2.501417
C	3.439494	-1.595062	3.676360
C	4.657174	-0.955833	3.960925
C	5.170469	-0.001727	3.066153
C	4.472355	0.307950	1.887497
Ru	0.000505	-0.236278	0.005689
C	0.001276	-2.177081	-0.006773
O	0.001279	-3.345794	-0.014007
P	-2.324010	0.015648	-0.005086
C	-2.963326	1.719164	0.390475
C	-4.103041	1.914889	1.204374
C	-4.590090	3.210851	1.449028
C	-3.953015	4.324901	0.880396
C	-2.821049	4.140852	0.067833
C	-2.326751	2.849629	-0.172180
C	2.961956	1.720196	-0.393521
C	2.320372	2.851579	0.161349
C	2.811614	4.142991	-0.084081
C	3.945155	4.325997	-0.894636
C	4.587130	3.210841	-1.455705
C	4.103334	1.914768	-1.205382
C	-3.279382	-1.022330	1.212148
C	-2.800162	-1.127118	2.539832
C	-3.496704	-1.887080	3.491526
C	-4.674600	-2.564385	3.131254
C	-5.154647	-2.474159	1.815337
C	-4.465750	-1.705402	0.860785
C	-3.241275	-0.337055	-1.588473
C	-2.721873	-1.277075	-2.505809
C	-3.423878	-1.590743	-3.681416
C	-4.648603	-0.963121	-3.961235
C	-5.170630	-0.018699	-3.061201
C	-4.474180	0.292564	-1.882066
H	1.773623	-1.759588	2.293076
H	3.028920	-2.332906	4.372987
H	5.200942	-1.194313	4.880442
H	6.114194	0.507295	3.286576
H	4.870488	1.057801	1.197725
H	1.859399	-0.633911	-2.807126
H	3.100951	-1.974089	-4.506355
H	5.204937	-3.173421	-3.866568
H	6.069797	-2.998889	-1.523445
H	4.852457	-1.626252	0.161052
H	4.605913	1.050890	-1.649205
H	1.425057	2.711546	0.774948
H	2.303290	5.007591	0.354764
H	4.323079	5.334246	-1.091284
H	5.467193	3.345339	-2.092730
H	-4.847501	-1.636032	-0.161226
H	-6.067582	-3.003934	1.525123
H	-5.211501	-3.164721	3.872435
H	-3.112876	-1.957176	4.514391
H	-1.868206	-0.622197	2.813603
H	-1.754660	-1.744753	-2.301009
H	-4.879078	1.035306	-1.188519
H	-6.119925	0.481474	-3.277911
H	-3.006571	-2.320977	-4.382046
H	-5.191182	-1.203023	-4.881081
H	-1.432927	2.709345	-0.787959
H	-4.602153	1.051938	1.653829
H	-5.468994	3.346057	2.087499
H	-4.333515	5.333064	1.072476
H	-2.316588	5.004592	-0.377133
H	-0.003127	1.104370	-0.913683
H	-0.029093	-0.524549	1.630660
H	0.002480	1.078768	0.961393
H	0.030899	-0.495214	-1.624401

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Complex 26b-cis

Ru	0.015802	-0.246217	0.210566
P	-2.297158	0.019792	0.028657
P	2.321324	0.040437	0.033854
C	-3.235850	0.112994	1.635067
C	-4.582677	-3.349563	-2.291733
C	-3.300559	-2.940978	-2.696177
C	-2.622294	-1.939694	-1.983952
C	-2.936268	1.534311	-0.852512
C	-2.292081	2.779389	-0.672109
C	-2.788140	3.937945	-1.290619
C	-3.929325	3.869070	-2.107641
C	-4.574857	2.636738	-2.298537
C	-4.086657	1.477012	-1.673010
C	2.946987	1.272191	-1.213739
C	-4.180583	1.126336	1.911368
C	2.052204	2.076824	-1.948993
C	2.535045	2.995504	-2.897879
C	3.914527	3.121233	-3.121149
C	4.815536	2.317472	-2.399549
C	4.337551	1.395278	-1.457027
C	3.351039	-1.435964	-0.443082
C	2.910137	-2.230868	-1.527238
C	3.664930	-3.332989	-1.955092
C	4.866233	-3.662934	-1.303731
C	5.310382	-2.883370	-0.224292
C	-4.839600	1.165609	3.153054
C	4.561319	-1.773457	0.203457
C	3.144002	0.596360	1.604155
C	3.746721	1.865590	1.744322
C	4.273156	2.271419	2.983652
C	4.212049	1.415493	4.093820
C	3.613554	0.148915	3.966091
C	3.076149	-0.255317	2.735424
C	-4.572011	0.192263	4.128028
C	-3.637680	-0.824470	3.861285
C	-2.970558	-0.861335	2.627980
C	-3.222005	-1.327548	-0.859685
C	-4.513882	-1.743217	-0.462100
C	-5.186709	-2.750705	-1.173894
H	-1.386620	2.823909	-0.058435
H	-2.276421	4.893825	-1.138707

H	-4.310558	4.771099	-2.596730
H	-5.461626	2.573428	-2.937283
H	-4.595414	0.521222	-1.824649
H	-1.615463	-1.630482	-2.282003
H	-2.821572	-3.408651	-3.562158
H	-5.106951	-4.136638	-2.842763
H	-6.183550	-3.068063	-0.851583
H	-4.986194	-1.282218	0.409943
H	-2.235206	-1.648112	2.428147
H	-4.395834	1.886492	1.155597
H	-5.564484	1.960827	3.354536
H	-5.086156	0.225056	5.093655
H	-3.423832	-1.587624	4.616441
H	5.041071	0.754506	-0.916872
H	5.892265	2.402575	-2.577647
H	4.289702	3.836032	-3.860446
H	1.826668	3.608517	-3.464300
H	0.978853	1.965620	-1.772978
H	1.966749	-1.980940	-2.023816
H	4.908125	-1.177020	1.051790
H	6.242963	-3.137192	0.290002
H	3.309698	-3.940216	-2.793750
H	5.450174	-4.527604	-1.634318
H	2.597737	-1.236925	2.644387
H	3.807552	2.533532	0.880662
H	4.733151	3.260424	3.076868
H	4.624582	1.732514	5.056649
H	3.560737	-0.523808	4.828160
H	0.008579	-0.220518	-1.404527
H	0.056985	1.400461	0.020766
C	-0.002918	-2.165034	0.204928
O	-0.011530	-3.339702	0.196607
H	-0.000270	0.430492	1.856927
H	0.047814	-0.409829	2.009707

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Complex 27

Ru	-0.000649	-0.305034	-0.291269
P	-2.292852	0.015204	-0.156587
P	2.289350	-0.004252	-0.158027
C	-2.761857	0.245428	1.630634
C	-5.142913	-3.423486	-1.570079
C	-4.161748	-3.654863	-0.589828
C	-3.327828	-2.610036	-0.166401
C	-3.022403	1.531920	-0.940660
C	-2.324549	2.192279	-1.974433
C	-2.873621	3.331253	-2.587381
C	-4.117899	3.827832	-2.166135
C	-4.816189	3.182834	-1.130069
C	-4.274281	2.039934	-0.521890
C	3.092671	1.538276	-0.819794
C	-1.916668	1.041970	2.442386
C	2.321965	2.704154	-1.024559
C	2.923557	3.882587	-1.496838
C	4.299383	3.910160	-1.776732
C	5.074437	2.753498	-1.584561
C	4.477493	1.574307	-1.111186
C	3.436427	-1.315480	-0.797581
C	3.148124	-1.914962	-2.044913
C	4.000798	-2.895689	-2.574710
C	5.145778	-3.294867	-1.864126
C	5.436827	-2.710621	-0.620527
C	-2.210407	1.234549	3.801446
C	4.589193	-1.724409	-0.088306
C	2.719811	0.045831	1.649710
C	3.397580	1.128713	2.252618
C	3.617844	1.142506	3.640625
C	3.163682	0.081314	4.441090
C	2.486363	-1.000580	3.851682
C	2.262328	-1.019694	2.466541
C	-3.348419	0.636950	4.369629
C	-4.192316	-0.155275	3.573874
C	-3.902841	-0.353324	2.213283
C	-3.474148	-1.309146	-0.706961
C	-4.462800	-1.086716	-1.691260
C	-5.287817	-2.140901	-2.120918

H	-1.343216	1.812668	-2.274973
H	-2.323256	3.834024	-3.389114
H	-4.541340	4.719693	-2.638955
H	-5.781725	3.572423	-0.792189
H	-4.813755	1.544978	0.291546
H	-2.551871	-2.801201	0.581642
H	-4.036408	-4.654402	-0.161876
H	-5.786083	-4.242709	-1.906265
H	-6.045901	-1.954732	-2.888476
H	-4.587809	-0.087679	-2.117291
H	-4.552445	-0.985669	1.601490
H	-1.030263	1.506686	1.995278
H	-1.545562	1.849790	4.416061
H	-3.575399	0.786440	5.429929
H	-5.079605	-0.623734	4.012061
H	5.081831	0.671962	-0.980645
H	6.145746	2.765764	-1.809313
H	4.766184	4.827018	-2.150671
H	2.311990	4.777273	-1.652144
H	1.247827	2.665104	-0.815265
H	2.243909	-1.617749	-2.586256
H	4.811099	-1.277916	0.885562
H	6.323330	-3.024213	-0.059967
H	3.763465	-3.356397	-3.538703
H	5.804910	-4.065695	-2.275597
H	1.736089	-1.864131	2.007159
H	3.750974	1.956783	1.632093
H	4.146804	1.985923	4.096089
H	3.335888	0.096505	5.521873
H	2.129639	-1.830330	4.470157
H	0.005658	-0.046627	-1.829161
H	-0.055494	1.361307	-0.118850
C	0.015437	-2.170620	-0.665083
O	0.022487	-3.314709	-0.951462

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TS[13H-23perp]

Ru	0.025399	-0.536417	-0.023394
P	-2.266115	-0.023053	-0.086383
P	2.266937	-0.040146	-0.079140
C	-2.904377	1.378768	-1.124891
C	-3.739115	0.941586	4.250626
C	-4.101300	1.803823	3.203789
C	-3.687505	1.531124	1.887434
C	-3.415296	-1.392767	-0.596715
C	-3.119762	-2.114082	-1.776193
C	-3.968141	-3.142445	-2.212758
C	-5.118734	-3.469158	-1.474175
C	-5.416777	-2.764365	-0.297054
C	-4.570992	-1.730936	0.141757
C	2.775647	1.642871	-0.690490
C	-2.032624	2.375903	-1.612565
C	1.934399	2.742979	-0.408894
C	2.316393	4.044489	-0.770476
C	3.538840	4.265751	-1.426689
C	4.382627	3.179842	-1.711289
C	4.009802	1.877247	-1.339608
C	3.318544	-1.187760	-1.088087
C	3.333881	-1.055942	-2.498516
C	4.005400	-1.996933	-3.293467
C	4.658056	-3.091039	-2.699041
C	4.635129	-3.240100	-1.303008
C	-2.529589	3.448801	-2.371813
C	3.970853	-2.297727	-0.499928
C	3.132970	-0.023509	1.572786
C	4.542865	0.041097	1.670097
C	5.165769	0.103619	2.925916
C	4.392212	0.115781	4.099974
C	2.991962	0.068205	4.013449
C	2.364597	-0.002414	2.757704
C	-3.901645	3.538451	-2.654992
C	-4.778885	2.547780	-2.180284
C	-4.286255	1.474231	-1.422660
C	-2.900521	0.392879	1.609117
C	-2.532032	-0.468154	2.673265
C	-2.956024	-0.195881	3.982894

H	-2.214136	-1.874502	-2.342321
H	-3.725398	-3.694954	-3.126053
H	-5.776699	-4.275872	-1.812391
H	-6.307556	-3.019437	0.286004
H	-4.797507	-1.192239	1.066069
H	-3.977117	2.203061	1.074584
H	-4.707922	2.692178	3.407269
H	-4.062885	1.155986	5.274133
H	-2.670415	-0.871355	4.795975
H	-1.908897	-1.343489	2.454509
H	-4.968701	0.693237	-1.073761
H	-0.961083	2.292002	-1.408309
H	-1.838561	4.209222	-2.749290
H	-4.286441	4.371886	-3.251167
H	-5.848199	2.605688	-2.407137
H	4.671420	1.037359	-1.570406
H	5.336250	3.344517	-2.223214
H	3.832759	5.279933	-1.714848
H	1.655508	4.886567	-0.540697
H	0.978259	2.563812	0.092703
H	2.812809	-0.215855	-2.968772
H	3.969549	-2.412166	0.588212
H	5.138045	-4.091384	-0.833039
H	4.014780	-1.877415	-4.381546
H	5.178280	-3.825064	-3.321982
H	1.271837	-0.034850	2.680249
H	5.151096	0.042643	0.761020
H	6.257732	0.149231	2.988173
H	4.881449	0.167264	5.077744
H	2.382343	0.085421	4.922597
H	0.131651	-1.264132	-2.490446
H	0.033392	0.688645	0.944974
O	-0.608593	-2.385947	0.775376
C	0.709673	-2.403205	0.877566
H	1.289390	-3.018241	0.159489
H	0.193858	-1.775125	-3.053848
H	1.174036	-2.273931	1.875040
H	0.115683	0.596401	-1.147041

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TS[23perp-23]

Ru	0.033258	-0.534458	-0.133642
P	2.321608	-0.008569	-0.105720
P	-2.205917	-0.073361	-0.074111
C	2.743973	1.793202	-0.094990
C	5.524513	-1.857322	-2.977272
C	4.350740	-2.561133	-2.660899
C	3.391048	-1.992432	-1.806617
C	2.880905	-0.585964	1.563790
C	2.228166	-0.058843	2.708798
C	2.536819	-0.546221	3.988414
C	3.490257	-1.567961	4.143086
C	4.137675	-2.099330	3.014852
C	3.836829	-1.613566	1.731718
C	-2.696179	1.605608	-0.725124
C	1.991735	2.678029	-0.899808
C	-1.978849	2.753607	-0.314689
C	-2.353677	4.029521	-0.762812
C	-3.442862	4.181642	-1.638052
C	-4.158313	3.049702	-2.058389
C	-3.792408	1.770576	-1.603168
C	-3.052060	-0.071709	1.586293
C	-2.560382	-0.933346	2.593280
C	-3.174331	-0.985391	3.855129
C	-4.285369	-0.170712	4.129711
C	-4.777589	0.697456	3.140200
C	2.316002	4.043290	-0.946727
C	-4.166712	0.750039	1.876064
C	-3.328292	-1.174685	-1.073644
C	-2.837362	-1.668218	-2.306943
C	-3.638375	-2.493840	-3.111112
C	-4.932960	-2.847052	-2.692536
C	-5.424091	-2.373373	-1.464787
C	-4.628586	-1.540334	-0.659025
C	3.386488	4.542071	-0.185096
C	4.133711	3.671971	0.626522
C	3.818004	2.303662	0.670876
C	3.606931	-0.708320	-1.250388
C	4.787458	-0.003231	-1.582551
C	5.739452	-0.576538	-2.440303
H	1.482537	0.733987	2.585111
H	2.031270	-0.126798	4.864238
H	3.727958	-1.948716	5.141333
H	4.882038	-2.893442	3.131895
H	4.339001	-2.029422	0.853658
H	2.460323	-2.519088	-1.574586
H	4.171831	-3.553584	-3.087079
H	6.267132	-2.301180	-3.648198
H	6.647411	-0.019116	-2.692365
H	4.953235	0.998730	-1.176605
H	4.392398	1.628369	1.312664
H	1.143171	2.288292	-1.470828
H	1.725986	4.717849	-1.575168
H	3.634170	5.607717	-0.218895
H	4.962613	4.057730	1.228497
H	-4.354773	0.894046	-1.935785
H	-5.004791	3.156839	-2.744356
H	-3.728704	5.176806	-1.993228
H	-1.787456	4.906091	-0.431563
H	-1.113123	2.637364	0.344751
H	-1.683842	-1.556357	2.382171
H	-4.543641	1.438826	1.113856
H	-5.637217	1.340824	3.353850
H	-2.780282	-1.657455	4.624245
H	-4.762179	-0.206470	5.114314
H	-5.013654	-1.176021	0.297996
H	-1.814509	-1.421061	-2.612396
H	-3.244348	-2.871124	-4.060120
H	-5.553162	-3.497304	-3.317541
H	-6.428295	-2.652680	-1.129878
H	-0.087481	0.023936	-1.585191
O	0.486493	-2.553643	-0.951472
C	-0.451142	-2.627179	-0.048041
H	-0.177823	-2.931484	0.997208
H	-1.479025	-2.899870	-0.356114
H	-0.044390	0.945944	0.499064

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TS[23-24]

Ru	-0.015454	-0.424159	0.121763
P	2.313344	-0.068989	-0.001561
P	-2.259777	0.000672	-0.020366
C	2.760743	1.607477	-0.668725
C	5.041768	-2.902815	-2.531464
C	3.825129	-3.365531	-2.004015
C	3.005551	-2.504907	-1.253920
C	3.159196	-0.074270	1.651732
C	2.476811	0.505087	2.749972
C	3.062328	0.519971	4.025227
C	4.330105	-0.053316	4.224962
C	5.011074	-0.639285	3.145101
C	4.432117	-0.649701	1.864711
C	-2.787325	1.764392	-0.264303
C	2.217821	2.006697	-1.913756
C	-1.910100	2.679364	-0.886269
C	-2.315663	4.003004	-1.122815
C	-3.597312	4.429827	-0.737959
C	-4.472818	3.531118	-0.105268
C	-4.072154	2.206466	0.133972
C	-3.274649	-0.474299	1.467733
C	-2.887692	0.059393	2.722315
C	-3.561366	-0.315542	3.893901
C	-4.623594	-1.235890	3.833705
C	-5.012263	-1.773443	2.596701
C	2.534950	3.259185	-2.459732
C	-4.344163	-1.395272	1.417717
C	-3.151548	-0.883312	-1.395268
C	-4.331269	-0.377717	-1.989507
C	-4.979290	-1.094065	-3.008524
C	-4.457858	-2.322846	-3.448402
C	-3.281269	-2.829554	-2.872718
C	-2.626161	-2.114993	-1.854799

C	3.391604	4.135038	-1.769107
C	3.933686	3.749183	-0.533525
C	3.625050	2.490852	0.013893
C	3.404650	-1.168790	-1.023194
C	4.629450	-0.707938	-1.562793
C	5.442902	-1.573318	-2.311373
H	1.482947	0.938270	2.591757
H	2.525063	0.974191	4.863869
H	4.783406	-0.047670	5.221185
H	5.996071	-1.092024	3.297207
H	4.963525	-1.107817	1.025717
H	2.048575	-2.850162	-0.848599
H	3.505639	-4.397751	-2.179699
H	5.675664	-3.574266	-3.119630
H	6.387042	-1.207482	-2.727632
H	4.934193	0.331084	-1.404339
H	4.050763	2.195756	0.976910
H	1.541142	1.329211	-2.445762
H	2.110493	3.552366	-3.425369
H	3.633773	5.114262	-2.193940
H	4.601662	4.425525	0.009451
H	-4.745988	1.514569	0.648154
H	-5.466939	3.862947	0.211018
H	-3.909872	5.462911	-0.920073
H	-1.622508	4.702935	-1.599950
H	-0.903306	2.349771	-1.157493
H	-2.053596	0.768715	2.769605
H	-4.654543	-1.810057	0.454686
H	-5.838251	-2.489950	2.544107
H	-3.255801	0.108442	4.855911
H	-5.144096	-1.532634	4.749591
H	-1.698276	-2.508789	-1.423582
H	-4.728952	0.588482	-1.665295
H	-5.888644	-0.688160	-3.463425
H	-4.962591	-2.878483	-4.245207
H	-2.861914	-3.779475	-3.219479
H	-0.087456	0.086254	-1.377589
O	0.109649	-2.884551	0.081018
C	-0.562791	-2.232822	0.949706
H	-0.020442	-1.637097	1.807224
H	-1.579775	-2.565260	1.251590
H	-0.031606	1.080981	0.618792

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TS[24-25]

Ru	-0.024526	-0.402303	0.252461
P	2.303364	-0.045809	0.048985
P	-2.269451	0.008322	0.026700
C	2.761724	1.667225	-0.516577
C	4.556708	-2.815098	-2.977277
C	3.468021	-3.299402	-2.233339
C	2.787996	-2.453478	-1.341836
C	3.365445	-0.236048	1.564024
C	2.822977	0.101383	2.825595
C	3.602360	-0.006101	3.988616
C	4.928163	-0.464160	3.909080
C	5.474515	-0.810599	2.661897
C	4.701124	-0.694191	1.495059
C	-2.782379	1.789584	-0.092678
C	2.187927	2.172550	-1.708293
C	-1.881271	2.752232	-0.597954
C	-2.274675	4.094361	-0.726919
C	-3.569215	4.491370	-0.353776
C	-4.470498	3.543367	0.159301
C	-4.081046	2.200795	0.294627
C	-3.377518	-0.587301	1.403325
C	-2.972620	-0.319577	2.733723
C	-3.747095	-0.761665	3.816933
C	-4.931683	-1.484558	3.588855
C	-5.337637	-1.762108	2.273955
C	2.520749	3.454437	-2.170101
C	-4.567162	-1.316556	1.184612
C	-3.084948	-0.755968	-1.461415
C	-4.191673	-0.166955	-2.113849
C	-4.783467	-0.798287	-3.220607
C	-4.277742	-2.022599	-3.689068
C	-3.173127	-2.613313	-3.052758
C	-2.577350	-1.983397	-1.947850
C	3.417953	4.257584	-1.443367
C	3.986954	3.768224	-0.257678
C	3.667532	2.477995	0.201818
C	3.197773	-1.109208	-1.182551
C	4.290694	-0.627263	-1.941137
C	4.965194	-1.478422	-2.832044
H	1.781699	0.433646	2.886501
H	3.169047	0.259631	4.958071
H	5.531844	-0.556853	4.817394
H	6.504464	-1.175233	2.595028
H	5.127586	-0.968491	0.525918
H	1.928351	-2.824766	-0.772779
H	3.140148	-4.337528	-2.348448
H	5.082626	-3.475480	-3.674162
H	5.808269	-1.094408	-3.415335
H	4.603275	0.416261	-1.840264
H	4.122485	2.098874	1.120563
H	1.472690	1.553601	-2.260122
H	2.074627	3.828220	-3.097416
H	3.670256	5.260816	-1.801072
H	4.686038	4.387095	0.313869
H	-4.776466	1.469643	0.718025
H	-5.476276	3.849551	0.464441
H	-3.872604	5.538432	-0.452782
H	-1.562524	4.830312	-1.113318
H	-0.869623	2.440408	-0.872219
H	-2.039321	0.229049	2.906903
H	-4.885850	-1.536278	0.161612
H	-6.256130	-2.329030	2.091047
H	-3.423107	-0.546597	4.840342
H	-5.531798	-1.834782	4.434519
H	-1.706784	-2.439196	-1.463738
H	-4.576255	0.795067	-1.762387
H	-5.636609	-0.328720	-3.720753
H	-4.738037	-2.510835	-4.553905
H	-2.766758	-3.561279	-3.419271
H	-0.067646	0.315117	-1.257382
O	0.052648	-3.021532	0.464708
C	-0.486226	-2.123162	1.136123
H	0.206053	-0.827771	1.854826
H	-1.267706	-2.370929	1.890200
H	-0.125583	0.958201	1.026046

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TS[25-26btrans]

Ru	-0.006750	0.007080	-0.004600
P	-2.344880	0.018577	-0.046992
P	2.330616	0.051084	-0.073250
C	-3.105686	1.555643	-0.771927
C	-3.912058	-0.022435	4.362287
C	-2.940371	0.904048	3.944615
C	-2.505503	0.911438	2.610593
C	-3.321285	-1.288906	-0.928332
C	-2.692103	-2.483535	-1.344080
C	-3.432364	-3.473108	-2.015444
C	-4.797186	-3.280663	-2.279948
C	-5.430265	-2.092371	-1.872975
C	-4.698378	-1.100474	-1.203681
C	3.237461	-1.367138	-0.845782
C	-2.761052	1.907664	-2.099354
C	2.554946	-2.240374	-1.719395
C	3.237359	-3.303109	-2.335968
C	4.602960	-3.505928	-2.083307
C	5.290097	-2.647925	-1.205482
C	4.612914	-1.586455	-0.587037
C	3.127314	0.117214	1.611592
C	2.998758	-1.015568	2.454067
C	3.516813	-0.994568	3.757375
C	4.162854	0.155928	4.243157
C	4.296779	1.282124	3.415755
C	-3.296023	3.060123	-2.692112
C	3.784606	1.265757	2.106805
C	3.076349	1.525923	-0.928941
C	4.077361	1.403109	-1.918347

C	4.590361	2.543695	-2.559433
C	4.120523	3.821164	-2.215834
C	3.125321	3.956338	-1.232731
C	2.600049	2.819321	-0.599134
C	-4.178877	3.882513	-1.969041
C	-4.528207	3.541811	-0.653458
C	-3.999077	2.382984	-0.056784
C	-3.046133	-0.002284	1.670934
C	-4.019068	-0.930009	2.102516
C	-4.446714	-0.938162	3.441529
H	-1.632054	-2.644054	-1.125669
H	-2.934400	-4.395986	-2.329275
H	-5.368806	-4.052272	-2.805590
H	-6.492926	-1.935127	-2.083565
H	-5.187101	-0.167796	-0.905387
H	-1.741091	1.628046	2.286267
H	-2.515813	1.617002	4.658552
H	-4.246276	-0.033399	5.404399
H	-5.199144	-1.664881	3.764089
H	-4.439609	-1.642795	1.387600
H	-4.274153	2.122612	0.969126
H	-2.073943	1.270409	-2.666793
H	-3.022048	3.317823	-3.720149
H	-4.591629	4.784250	-2.431968
H	-5.217382	4.175278	-0.085746
H	5.143547	-0.926306	0.105971
H	6.352973	-2.809029	-0.999096
H	5.131727	-4.337169	-2.560523
H	2.693365	-3.979744	-3.002254
H	1.483569	-2.098631	-1.882725
H	2.499426	-1.916610	2.081978
H	3.902266	2.142652	1.463945
H	4.807456	2.177565	3.784719
H	3.414353	-1.879150	4.393919
H	4.562853	0.171579	5.261804
H	1.801105	2.929059	0.141864
H	4.452559	0.411179	-2.183760
H	5.360264	2.429807	-3.329289
H	4.522991	4.708271	-2.714719
H	2.748341	4.948277	-0.963793
H	-0.023324	-0.623391	-1.444675
H	-0.000227	1.245912	-1.268926
C	0.053952	-1.843103	0.676829
H	0.039487	-1.718556	1.834423
H	-0.066302	1.829479	-0.675786
O	0.110293	-2.995606	0.246234

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TS[26btrans-26a]

Ru	-0.000111	-0.157742	0.027977
P	-2.334014	-0.003756	-0.008406
P	2.333838	0.007199	0.010707
H	0.011862	-0.361144	-1.625732
H	-0.007031	1.314455	-0.689113
C	0.014160	-2.079980	0.160154
H	-0.010457	1.376026	0.592932
C	-2.975972	1.728889	0.207794
C	-3.243448	-0.517601	-1.548648
C	3.246946	-1.125147	-1.153124
C	3.260788	-0.260769	1.604191
C	2.986358	1.677432	-0.484202
C	-3.276072	-0.923920	1.311641
H	-0.013222	-0.168121	1.693680
O	0.024292	-3.246722	0.248535
C	-2.719065	-1.018278	2.608754
C	-2.695381	-1.505360	-2.395558
C	-4.503024	0.040821	-1.874688
C	-2.601517	2.716667	-0.735378
C	2.714992	-1.341863	-2.446754
C	4.451268	-1.772914	-0.795463
C	2.703845	-1.066614	2.620567
C	4.539544	0.311460	1.808450
C	3.873716	1.853803	-1.568211
C	2.568207	2.813879	0.249301
C	-3.797795	2.098412	1.294348
C	-4.539588	-1.510933	1.070347
C	-3.416071	-1.667434	3.640152
C	-3.397042	-1.938359	-3.532908
C	-5.198857	-0.390710	-3.015632
C	3.380957	-2.171111	-3.362589
C	5.108117	-2.612270	-1.711490
C	3.413987	-1.308786	3.808324
C	5.243629	0.072606	2.999557
C	-3.041630	4.040304	-0.591406
C	4.324084	3.140133	-1.916614
C	3.025766	4.093239	-0.097008
C	-4.230365	3.428982	1.438490
C	-5.229450	-2.168161	2.102672
H	-1.706091	-1.912769	-2.168021
H	-4.928025	0.823253	-1.238895
H	-1.725206	-0.595562	2.789431
H	-4.978412	-1.458403	0.070373
H	-4.095769	1.344778	2.028255
H	-1.962773	2.441762	-1.581491
H	4.870702	-1.623138	0.202826
H	1.762280	-0.872536	-2.713037
H	1.700456	-1.480179	2.482691
H	4.972612	0.954489	1.036656
H	1.879845	2.690729	1.091975
H	4.206831	0.984641	-2.142148
C	-4.672517	-2.244045	3.389733
C	-4.649206	-1.383730	-3.844085
C	4.578346	-2.809323	-2.996768
C	4.683952	-0.740760	3.999799
C	3.902976	4.260014	-1.183685
C	-3.855382	4.400352	0.498269
H	-2.958676	-2.704816	-4.180007
H	-6.169270	0.053467	-3.259164
H	-2.969980	-1.730990	4.637943
H	-6.202935	-2.624559	1.896778
H	-2.746291	4.792532	-1.329829
H	-4.864049	3.701582	2.288484
H	6.034792	-3.114233	-1.415447
H	2.956082	-2.327324	-4.359420
H	6.228673	0.526608	3.147663
H	2.967992	-1.935166	4.587449
H	5.007585	3.261650	-2.763046
H	2.693907	4.961842	0.480698
H	-5.191894	-1.717740	-4.734016
H	-5.211103	-2.758242	4.192041
H	-4.193958	5.434996	0.611380
H	5.091146	-3.464688	-3.707863
H	5.233390	-0.923904	4.928596
H	4.254665	5.259936	-1.456391

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TS[26a-26bcis]

Ru	0.004147	-0.260390	-0.066781
P	-2.320414	0.003745	-0.017760
P	2.324578	0.006738	-0.008339
H	0.011095	-0.500393	-1.704360
H	0.000156	0.887424	-1.221946
C	0.005356	-2.200334	-0.026527
H	0.019273	1.187009	0.680671
C	-2.943215	1.726152	0.316627
C	-3.275020	-0.411268	-1.563642
C	3.348578	-1.139513	-1.063957
C	3.177853	-0.163287	1.637236
C	2.952179	1.671836	-0.559927
C	-3.255393	-0.974194	1.262933
H	-0.012837	-0.455465	1.571619
O	0.012029	-3.368415	0.029937
C	-2.716121	-1.086392	2.566063
C	-2.820154	-1.454005	-2.401899
C	-4.465112	0.270866	-1.909739
C	-2.289166	2.831026	-0.275297
C	2.845129	-1.558114	-2.317504
C	4.627373	-1.589344	-0.660141
C	2.681808	-1.081294	2.589524
C	4.343441	0.577342	1.945285
C	4.017292	1.806263	-1.478537
C	2.358127	2.841134	-0.028773

C	-4.089281	1.958236	1.111751
C	-4.496552	-1.591318	0.983821
C	-3.406932	-1.788114	3.565750
C	-3.543116	-1.813973	-3.550773
C	-5.182729	-0.087487	-3.062994
C	3.605303	-2.395307	-3.149638
C	5.381990	-2.432767	-1.492519
C	3.342549	-1.264291	3.814788
C	4.997785	0.396870	3.175300
C	-2.774733	4.133838	-0.083559
C	4.472853	3.081073	-1.859707
C	2.822486	4.110572	-0.403565
C	-4.566883	3.265616	1.308673
C	-5.180622	-2.300760	1.986201
H	-1.886907	-1.968435	-2.155554
H	-4.820959	1.089751	-1.277935
H	-1.742391	-0.634335	2.780850
H	-4.922973	-1.519291	-0.020421
H	-4.600354	1.113982	1.582941
H	-1.388583	2.662318	-0.873510
H	5.027160	-1.283309	0.310668
H	1.845980	-1.234318	-2.626067
H	1.763444	-1.634339	2.371452
H	4.727083	1.302393	1.221632
H	1.520513	2.746376	0.669651
H	4.485809	0.912008	-1.898072
C	-4.640096	-2.398017	3.278299
C	-4.725063	-1.131776	-3.883635
C	4.874892	-2.835047	-2.738773
C	4.500761	-0.526172	4.110457
C	3.879523	4.233828	-1.322664
C	-3.913554	4.354467	0.710031
H	-3.176173	-2.623631	-4.189567
H	-6.098402	0.454017	-3.321147
H	-2.975537	-1.865742	4.568941
H	-6.136787	-2.779729	1.752308
H	-2.257350	4.978148	-0.550451
H	-5.450352	3.429995	1.933859
H	6.366889	-2.777906	-1.162083
H	3.199573	-2.710920	-4.116166
H	5.894340	0.982183	3.403227
H	2.944975	-1.979078	4.542351
H	5.294008	3.168477	-2.578339
H	2.353698	5.005078	0.019115
H	-5.283734	-1.408333	-4.783329
H	-5.173348	-2.952730	4.056766
H	-4.286498	5.371812	0.864925
H	5.463273	-3.494632	-3.384376
H	5.010033	-0.664323	5.069415
H	4.235524	5.225111	-1.620510

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TS[26bcis-27]

Ru	0.013709	-0.295663	0.060212
P	-2.289148	0.007286	-0.048044
P	2.311117	0.012239	-0.035501
C	-3.085224	0.114136	1.631906
C	-4.780661	-3.325384	-2.198180
C	-3.471209	-3.027266	-2.609982
C	-2.732082	-2.035384	-1.946175
C	-2.953104	1.537122	-0.885182
C	-2.250312	2.758556	-0.770992
C	-2.756878	3.931468	-1.354020
C	-3.963467	3.899584	-2.072840
C	-4.664348	2.689321	-2.202170
C	-4.167388	1.516652	-1.609751
C	2.952544	1.315688	-1.199187
C	-3.658989	1.305921	2.126740
C	2.056498	2.103536	-1.952074
C	2.541433	3.072731	-2.847880
C	3.922922	3.268243	-2.997310
C	4.824522	2.484626	-2.254562
C	4.344947	1.510578	-1.366606
C	3.399803	-1.418031	-0.517328
C	2.956667	-2.262116	-1.561679
C	3.751466	-3.333181	-1.997224
C	4.995189	-3.582280	-1.392110
C	5.442448	-2.753318	-0.350666
C	-4.164386	1.358547	3.437389
C	4.653434	-1.674763	0.083578
C	3.022156	0.529617	1.599580
C	3.402627	1.864896	1.862020
C	3.827215	2.243435	3.147826
C	3.880116	1.297627	4.185258
C	3.501441	-0.033107	3.935990
C	3.067483	-0.415590	2.656325
C	-4.108728	0.225918	4.265385
C	-3.542208	-0.967084	3.781870
C	-3.027634	-1.022269	2.478581
C	-3.296627	-1.323660	-0.864265
C	-4.616714	-1.629844	-0.457397
C	-5.351053	-2.627119	-1.120541
H	-1.292520	2.766761	-0.239807
H	-2.200447	4.869070	-1.253708
H	-4.352412	4.812222	-2.535519
H	-5.601202	2.653843	-2.767419
H	-4.718375	0.578148	-1.716391
H	-1.704248	-1.813186	-2.249293
H	-3.018373	-3.574039	-3.443011
H	-5.353153	-4.104490	-2.711202
H	-6.369069	-2.859898	-0.792247
H	-5.058810	-1.093489	0.387465
H	-2.582783	-1.950692	2.104868
H	-3.708580	2.189528	1.484468
H	-4.605763	2.288934	3.808904
H	-4.503846	0.271150	5.284992
H	-3.496620	-1.854171	4.421546
H	5.050827	0.887383	-0.809684
H	5.903400	2.627147	-2.373047
H	4.299648	4.023310	-3.694617
H	1.833891	3.672163	-3.429815
H	0.982194	1.946032	-1.821692
H	1.977912	-2.078223	-2.016892
H	5.001285	-1.041322	0.904742
H	6.407865	-2.945579	0.128550
H	3.393706	-3.980348	-2.804314
H	5.610149	-4.423303	-1.727379
H	2.764968	-1.451400	2.467511
H	3.371495	2.603205	1.055781
H	4.119276	3.281505	3.336133
H	4.212960	1.595246	5.184386
H	3.539744	-0.776020	4.739168
H	0.015205	-0.334755	-1.500438
H	0.087519	1.381645	0.046572
C	-0.024656	-2.196184	0.134629
O	-0.045615	-3.372466	0.227097
H	0.298610	-0.393683	3.333776
H	-0.435726	-0.486400	3.190967

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TS[27-22]

Ru	1.426214	0.354949	-0.350168
P	0.982039	2.615002	-0.034493
P	2.364100	-1.739968	-0.031328
P	-2.923996	-0.672086	0.095793
C	-0.326495	2.938901	1.248406
C	-0.590189	5.161489	-3.639574
C	-1.202033	3.944917	-3.289539
C	-0.719255	3.199162	-2.204073
C	2.405980	3.632199	0.599525
C	3.718462	3.336537	0.165789
C	4.806183	4.110394	0.600664
C	4.600030	5.185412	1.481649
C	3.301357	5.484507	1.925274
C	2.210292	4.715953	1.485691
C	4.086680	-1.794830	0.680329
C	-0.469171	2.024186	2.317811
C	4.622519	-0.677235	1.356856
C	5.914559	-0.729484	1.908532
C	6.688505	-1.894319	1.788348
C	6.167859	-3.010802	1.110681
C	4.878537	-2.962638	0.558841

C	2.577764	-2.858586	-1.501052
C	3.032957	-2.280996	-2.709194
C	3.249058	-3.078980	-3.842737
C	3.007651	-4.462606	-3.789422
C	2.550036	-5.045664	-2.596757
C	-1.451058	2.225384	3.301406
C	2.338346	-4.251219	-1.456475
C	1.419882	-2.819475	1.150816
C	1.933757	-3.185864	2.415058
C	1.155309	-3.948018	3.303255
C	-0.139074	-4.356140	2.941175
C	-0.660954	-3.994425	1.686325
C	0.108930	-3.225816	0.799012
C	-4.093193	0.437039	-0.837038
C	-5.062547	-0.035161	-1.752001
C	-5.901437	0.867399	-2.427554
C	-2.299660	3.343048	3.232465
C	-5.787677	2.248436	-2.196326
C	-4.826197	2.727349	-1.290106
C	-3.979079	1.831760	-0.618512
C	-3.882951	-0.951801	1.668133
C	-5.262952	-0.674823	1.801677
C	-5.916170	-0.893929	3.026301
C	-5.204028	-1.394762	4.129106
C	-3.831975	-1.672974	4.005806
C	-3.171528	-1.447802	2.787318
C	-3.192594	-2.290551	-0.785857
C	-2.167514	4.258251	2.173819
C	-4.073070	-3.298613	-0.328920
C	-4.190945	-4.511509	-1.030590
C	-3.438755	-4.732157	-2.196423
C	-2.562017	-3.736087	-2.660360
C	-2.431908	-2.526867	-1.958691
C	-1.191561	4.057084	1.182334
C	0.378173	3.668187	-1.442938
C	0.983630	4.894522	-1.798350
C	0.501843	5.632532	-2.893765
H	3.879898	2.485467	-0.503446
H	5.815861	3.867383	0.254448
H	5.449385	5.784304	1.825361
H	3.134340	6.316000	2.617480
H	1.201883	4.947485	1.841122
H	-3.226622	2.214251	0.079861
H	-4.726502	3.802499	-1.110764
H	-6.441594	2.949569	-2.724728
H	-6.645794	0.489220	-3.136173
H	-5.149198	-1.109841	-1.938788
H	-4.664007	-3.127808	0.576096
H	-4.876681	-5.283825	-0.666135
H	-3.532006	-5.677834	-2.739719
H	-1.968092	-3.901579	-3.564852
H	-1.738497	-1.759616	-2.321566
H	-1.190740	2.245791	-1.944867
H	-2.054115	3.568866	-3.864073
H	-0.961645	5.736646	-4.493652
H	0.984382	6.577913	-3.162422
H	1.831840	5.269803	-1.219550
H	-1.101575	4.759803	0.348332
H	0.196293	1.154695	2.362054
H	-1.563085	1.499451	4.112352
H	-3.068577	3.495215	3.996259
H	-2.828444	5.129241	2.115685
H	4.487913	-3.828307	0.015454
H	6.768387	-3.920144	1.006031
H	7.696187	-1.932350	2.214536
H	6.314441	0.147046	2.428710
H	4.013791	0.228666	1.439320
H	3.204482	-1.200559	-2.754707
H	1.970535	-4.708364	-0.533310
H	2.354992	-6.121978	-2.550297
H	3.598093	-2.616808	-4.771526
H	3.170810	-5.082508	-4.676656
H	-0.309914	-2.949781	-0.173981
H	2.945545	-2.881192	2.695850
H	1.567348	-4.228306	4.278204
H	-0.739946	-4.955443	3.632589
H	-1.668504	-4.301736	1.390425
H	-5.817992	-0.277563	0.946287
H	-2.102038	-1.664694	2.693768
H	-3.271480	-2.061667	4.862344
H	-5.714948	-1.563234	5.082557
H	-6.984689	-0.672398	3.118535
H	2.777055	0.762523	-1.011378
H	2.070514	0.612235	1.183587
C	0.699779	0.098612	-2.085441
O	0.244319	-0.069162	-3.162636

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Complex 28

Ru	-0.020940	-0.241702	-0.030235
P	-2.281508	0.014851	-0.046188
P	2.254019	0.020870	-0.044490
C	-2.988061	1.750004	0.066029
C	-4.488901	-1.970827	3.612698
C	-3.296340	-1.243147	3.775253
C	-2.665841	-0.661370	2.665020
C	-3.298697	-0.626171	-1.494740
C	-2.760865	-1.693106	-2.249069
C	-3.485257	-2.256923	-3.312869
C	-4.753036	-1.753987	-3.650351
C	-5.291826	-0.680511	-2.920564
C	-4.572137	-0.121753	-1.849810
C	3.314286	-0.897881	-1.293825
C	-2.294297	2.814789	-0.551777
C	2.727000	-1.308912	-2.509205
C	3.490975	-1.968327	-3.486358
C	4.851702	-2.235561	-3.260326
C	5.444435	-1.846405	-2.046798
C	4.682122	-1.184038	-1.069603
C	3.214000	-0.399458	1.510244
C	3.039371	-1.698611	2.051025
C	3.705866	-2.068809	3.229301
C	4.544999	-1.154067	3.891953
C	4.717023	0.136770	3.367501
C	-2.814665	4.118495	-0.529196
C	4.058620	0.512581	2.181939
C	2.884341	1.770510	-0.331482
C	4.070113	2.059096	-1.045391
C	4.506564	3.385789	-1.211156
C	3.771218	4.446717	-0.658803
C	2.589481	4.173603	0.051991
C	2.145736	2.850592	0.207699
C	-4.032307	4.384780	0.121207
C	-4.724125	3.338824	0.753263
C	-4.207467	2.031062	0.726239
C	-3.226261	-0.783305	1.369115
C	-4.425356	-1.516336	1.218513
C	-5.048360	-2.108732	2.332575
H	-1.748973	-2.038626	-2.006243
H	-3.049961	-3.083417	-3.885310
H	-5.314089	-2.187778	-4.485497
H	-6.272467	-0.271123	-3.188266
H	-4.988943	0.724351	-1.294650
H	-1.717227	-0.123809	2.775156
H	-2.846066	-1.139352	4.768498
H	-4.972669	-2.436007	4.478517
H	-5.971898	-2.682261	2.195109
H	-4.867345	-1.625673	0.223913
H	-4.740784	1.222289	1.235457
H	-1.328140	2.597870	-1.021362
H	-2.260068	4.930343	-1.012639
H	-4.433798	5.403862	0.144732
H	-5.666111	3.539016	1.276105
H	5.139617	-0.898919	-0.117137
H	6.500758	-2.066444	-1.855404
H	5.445095	-2.756736	-4.019818
H	3.016238	-2.286057	-4.421373
H	1.653592	-1.129880	-2.648098
H	2.371775	-2.401203	1.527131
H	4.196512	1.519375	1.777448
H	5.365572	0.857397	3.878710
H	3.563056	-3.077014	3.634431
H	5.058963	-1.445760	4.814856

H	1.207560	2.623855	0.726355
H	4.647500	1.238688	-1.481332
H	5.423483	3.586957	-1.776568
H	4.111646	5.480144	-0.787972
H	2.001705	4.993637	0.479414
H	-0.013294	-0.916931	-1.542802
H	-0.014075	1.027231	-1.061361
C	-0.057503	-2.340538	0.325396
O	0.876605	-3.178269	0.341675
H	-0.006761	-1.395667	1.280509
H	-1.106202	-2.758600	0.289163
H	-0.022641	0.972448	1.143629

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Complex 29a-perp

Ru	0.013907	-0.125936	0.022126
P	2.288674	0.035524	0.005819
P	-2.269606	0.046251	0.013663
C	3.059439	1.668762	-0.507882
C	4.651548	-2.831191	-2.903772
C	3.370003	-2.353254	-3.226932
C	2.682074	-1.513278	-2.336232
C	3.242246	-0.236039	1.606243
C	2.709355	-1.140755	2.552089
C	3.400207	-1.424849	3.741668
C	4.628669	-0.798888	4.014091
C	5.161827	0.115460	3.090292
C	4.476289	0.392918	1.894168
C	-3.269492	-0.853533	1.322950
C	2.442139	2.865075	-0.073121
C	-2.725842	-0.966951	2.621989
C	-3.451345	-1.588976	3.650430
C	-4.728897	-2.117302	3.397311
C	-5.275241	-2.022444	2.106695
C	-4.552897	-1.394093	1.076992
C	-3.203775	-0.497132	-1.518587
C	-2.947137	-1.802791	-2.007456
C	-3.581113	-2.261394	-3.172191
C	-4.467272	-1.425789	-3.877043
C	-4.721615	-0.128687	-3.405326
C	2.996695	4.114572	-0.390331
C	-4.098383	0.332382	-2.230368
C	-3.015049	1.763470	0.220718
C	-4.301106	1.974475	0.771425
C	-4.836893	3.270141	0.871617
C	-4.100684	4.376901	0.416300
C	-2.822280	4.180125	-0.132617
C	-2.281678	2.886796	-0.224131
C	4.171125	4.194117	-1.159726
C	4.786716	3.015020	-1.608851
C	4.238440	1.760851	-1.282627
C	3.267699	-1.128409	-1.107621
C	4.555965	-1.620264	-0.791210
C	5.240702	-2.465558	-1.681986
H	1.728285	-1.584594	2.351089
H	2.969677	-2.129083	4.462102
H	5.162443	-1.014206	4.946303
H	6.111784	0.619433	3.301144
H	4.890855	1.112211	1.181218
H	1.666009	-1.165923	-2.558181
H	2.895578	-2.644434	-4.170524
H	5.183745	-3.493743	-3.595247
H	6.234430	-2.843146	-1.415964
H	5.015150	-1.344421	0.162712
H	4.721024	0.845364	-1.637530
H	1.507361	2.786872	0.492840
H	2.503155	5.029419	-0.044010
H	4.598410	5.170248	-1.414586
H	5.695974	3.066506	-2.218262
H	-4.974459	-1.335854	0.069049
H	-6.264431	-2.444314	1.895995
H	-5.290668	-2.610566	4.198245
H	-3.010358	-1.672497	4.650030
H	-1.711745	-0.589525	2.795116
H	-2.246954	-2.439702	-1.449361
H	-4.304938	1.342441	-1.865574
H	-5.406900	0.531388	-3.949238
H	-3.374474	-3.274642	-3.534779
H	-4.953360	-1.783967	-4.791581
H	-1.274792	2.718147	-0.621041
H	-4.876732	1.116749	1.131955
H	-5.831246	3.413147	1.309391
H	-4.518390	5.386770	0.495519
H	-2.236297	5.036863	-0.483735
H	-0.010789	-0.611381	1.609664
H	0.039511	1.246187	0.957202
C	0.044946	-2.237569	0.083739
O	-0.881486	-3.058088	0.002673
H	-0.064997	-0.709838	-1.521070
H	1.079283	-2.704292	0.211961
H	0.030510	1.142149	-1.042267

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Complex 29a

Ru	0.003650	0.003172	0.060341
P	2.289778	0.063924	0.009164
P	-2.285631	0.087456	0.020156
H	0.018138	-0.021026	1.721774
H	0.033394	1.514735	0.704797
C	-0.061696	-2.092478	0.452301
H	-0.011767	-0.609522	-1.470522
H	-0.001471	1.155914	-1.103102
C	3.097375	1.580394	-0.758960
C	3.246357	0.027585	1.626300
C	-3.248790	-0.799257	1.365887
C	-3.175113	-0.593660	-1.483288
C	-3.107423	1.777244	0.124290
C	3.229406	-1.285100	-0.903076
O	-0.371101	-3.042724	-0.286656
H	0.224985	-2.413017	1.512525
C	2.579547	-1.944508	-1.970749
C	2.732663	-0.763344	2.679741
C	4.458241	0.725990	1.835602
C	2.522406	2.846230	-0.498491
C	-2.677091	-0.888079	2.655562
C	-4.520738	-1.379876	1.148909
C	-2.656302	-1.775571	-2.066023
C	-4.321132	0.004356	-2.055724
C	-4.352746	1.993176	0.759290
C	-2.459696	2.879258	-0.479361
C	4.254875	1.520780	-1.568314
C	4.551324	-1.671140	-0.574258
C	3.241188	-2.942453	-2.705129
C	3.421626	-0.870130	3.898239
C	5.141850	0.627054	3.061056
C	-3.364802	-1.522240	3.702822
C	-5.205328	-2.018778	2.197423
C	-3.283536	-2.344634	-3.186567
C	-4.937524	-0.564045	-3.185762
C	3.096704	4.016749	-1.018085
C	-4.934008	3.273740	0.784617
C	-3.046569	4.154561	-0.463460
C	4.821955	2.694103	-2.099184
C	5.210344	-2.671763	-1.308800
H	1.773993	-1.273343	2.534469
H	4.856679	1.358319	1.036063
H	1.537986	-1.679123	-2.182828
H	5.057429	-1.193869	0.270630
H	4.706437	0.548931	-1.788251
H	1.601374	2.885010	0.093746
H	-4.963728	-1.341534	0.148979
H	-1.672478	-0.473373	2.803051
H	-1.758777	-2.240693	-1.630290
H	-4.722562	0.924202	-1.619616
H	-1.475954	2.715895	-0.933147
H	-4.859730	1.154056	1.245230
C	4.558550	-3.306216	-2.380112
C	4.628549	-0.175573	4.092857
C	-4.631391	-2.088308	3.477905
C	-4.421028	-1.741010	-3.751486
C	-4.285411	4.356887	0.169322
C	4.248225	3.945002	-1.821938

H	3.007918	-1.490130	4.701205
H	6.074802	1.182630	3.208477
H	2.715611	-3.447576	-3.522647
H	6.232015	-2.960541	-1.037405
H	2.635139	4.987165	-0.803840
H	5.713165	2.625886	-2.733178
H	-6.185856	-2.470322	2.009230
H	-2.902365	-1.585172	4.694110
H	-5.818666	-0.081687	-3.623912
H	-2.872247	-3.261541	-3.623399
H	-5.894734	3.422632	1.290297
H	-2.527268	4.994876	-0.937580
H	5.160555	-0.252402	5.047497
H	5.070267	-4.090778	-2.948484
H	4.689589	4.858254	-2.236100
H	-5.162944	-2.592146	4.292697
H	-4.899978	-2.183226	-4.632470
H	-4.738119	5.354382	0.190326

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Complex 29b-trans

Ru	0.001132	0.084009	-0.024097
P	2.292085	0.051092	-0.004882
P	-2.286600	0.067601	-0.011394
C	3.123098	1.558209	-0.749992
C	4.501436	-3.348067	-2.406548
C	3.188058	-2.964030	-2.722890
C	2.544345	-1.959216	-1.981188
C	3.221762	0.008040	1.628127
C	2.612255	-0.631127	2.730605
C	3.279450	-0.728176	3.962523
C	4.559832	-0.170085	4.120536
C	5.167564	0.490554	3.039939
C	4.505207	0.579088	1.802599
C	-3.170516	-0.586388	1.513419
C	2.770261	2.832416	-0.239869
C	-2.514731	-0.474898	2.761486
C	-3.132323	-0.929815	3.938517
C	-4.408606	-1.514482	3.887520
C	-5.064593	-1.645363	2.651041
C	-4.451232	-1.186293	1.473012
C	-3.225681	-0.871107	-1.336885
C	-2.646473	-2.050688	-1.861919
C	-3.324671	-2.795111	-2.842015
C	-4.575506	-2.369699	-3.323321
C	-5.153774	-1.194556	-2.815843
C	3.322737	4.000477	-0.785431
C	-4.485378	-0.452117	-1.826117
C	-3.125407	1.735098	-0.187417
C	-4.074182	2.233544	0.732462
C	-4.636950	3.511803	0.560819
C	-4.268762	4.306104	-0.536438
C	-3.327604	3.818451	-1.461476
C	-2.757267	2.548919	-1.287115
C	4.230359	3.921990	-1.857715
C	4.583032	2.666010	-2.375583
C	4.038151	1.491708	-1.823812
C	3.211078	-1.313903	-0.914756
C	4.527356	-1.722223	-0.593117
C	5.168061	-2.728382	-1.335130
H	1.596385	-1.023051	2.612822
H	2.790903	-1.231819	4.803916
H	5.076351	-0.239054	5.084244
H	6.157665	0.944695	3.159731
H	4.974354	1.111106	0.968782
H	1.506214	-1.669357	-2.184691
H	2.650746	-3.458451	-3.539574
H	4.999391	-4.137105	-2.981243
H	6.186862	-3.033192	-1.070367
H	5.043619	-1.261041	0.253909
H	4.320791	0.514834	-2.226201
H	2.046017	2.893288	0.579526
H	3.037784	4.976265	-0.376648
H	4.655320	4.835568	-2.287539
H	5.285553	2.594335	-3.213506
H	-4.959128	-1.303278	0.511060
H	-6.054888	-2.111737	2.600745
H	-4.886215	-1.877490	4.804411
H	-2.606795	-0.837564	4.895607
H	-1.507410	-0.037315	2.771268
H	-1.660988	-2.370010	-1.497477
H	-4.932431	0.469670	-1.440381
H	-6.124042	-0.850493	-3.191793
H	-2.865024	-3.708433	-3.235756
H	-5.094877	-2.948427	-4.095460
H	-2.008273	2.175386	-1.993885
H	-4.368494	1.614883	1.585063
H	-5.366263	3.884031	1.289085
H	-4.708316	5.300546	-0.670095
H	-3.030892	4.432434	-2.319058
H	0.029224	0.497334	1.616676
H	0.013573	1.808160	-0.067621
C	-0.074261	-1.876967	0.631078
O	-0.131879	-2.939669	-0.008274
H	-0.019894	-0.561545	-1.571480
H	-0.100882	-2.007186	1.768592
H	0.030268	1.516302	-0.986711

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Complex 30

Ru	0.023736	-0.376450	0.013235
P	-2.245460	-0.104650	0.013286
P	2.290629	-0.127025	0.006998
C	-2.667240	1.723032	0.093458
C	-4.854068	-1.747355	3.569470
C	-3.462080	-1.599251	3.695019
C	-2.701531	-1.116014	2.617635
C	-3.310413	-0.594440	-1.453753
C	-3.091575	-1.863144	-2.043237
C	-3.849978	-2.269317	-3.152543
C	-4.831182	-1.420458	-3.696213
C	-5.052237	-0.158338	-3.122525
C	-4.297787	0.252340	-2.007990
C	3.331950	-0.896078	-1.359599
C	-1.879844	2.599864	-0.693998
C	2.707585	-1.068112	-2.618271
C	3.409250	-1.637816	-3.692685
C	4.739510	-2.060933	-3.526983
C	5.363716	-1.914483	-2.277035
C	4.666666	-1.336398	-1.200811
C	3.339177	-0.583153	1.499024
C	2.844715	-1.581416	2.367508
C	3.585193	-1.979040	3.493153
C	4.820794	-1.372239	3.778206
C	5.310777	-0.359511	2.935888
C	-2.108124	3.984657	-0.670978
C	4.575528	0.032745	1.803407
C	2.777866	1.672753	-0.149253
C	3.818529	2.142109	-0.981910
C	4.107794	3.516785	-1.057973
C	3.364222	4.439026	-0.303847
C	2.322808	3.983243	0.524765
C	2.028827	2.613079	0.599943
C	-3.120384	4.521484	0.144928
C	-3.902168	3.664263	0.936344
C	-3.679973	2.275302	0.910351
C	-3.323778	-0.766213	1.399767
C	-4.723354	-0.932319	1.277403
C	-5.482709	-1.416389	2.356736
H	-2.323514	-2.514535	-1.608004
H	-3.668403	-3.254049	-3.597909
H	-5.416823	-1.740092	-4.565627
H	-5.810316	0.512905	-3.542247
H	-4.466546	1.240763	-1.569840
H	-1.610579	-1.009628	2.680371
H	-2.962413	-1.871621	4.631476
H	-5.445951	-2.130482	4.408376
H	-6.565652	-1.543469	2.246174
H	-5.211163	-0.697505	0.325946
H	-4.290724	1.610591	1.528820
H	-1.080926	2.172807	-1.313274
H	-1.487236	4.645052	-1.286170

H	-3.294301	5.602994	0.166922
H	-4.688780	4.075324	1.579303
H	5.153940	-1.239502	-0.226039
H	6.395262	-2.255964	-2.134147
H	5.282313	-2.515387	-4.363282
H	2.907431	-1.765292	-4.658295
H	1.654241	-0.771690	-2.711750
H	1.853561	-2.000914	2.160016
H	4.946566	0.838292	1.161065
H	6.262607	0.132986	3.164948
H	3.187392	-2.754127	4.157489
H	5.392632	-1.676175	4.661979
H	1.205687	2.251205	1.228705
H	4.391830	1.425685	-1.578288
H	4.914838	3.865899	-1.711973
H	3.589464	5.509330	-0.365632
H	1.729758	4.696117	1.107735
H	-0.037617	-0.100231	-1.664242
C	-0.013788	-2.279859	-0.052851
O	-0.981420	-3.070490	-0.055151
H	0.022702	-0.212288	1.706095
H	1.023988	-2.734590	-0.107416

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Complex 31

C	5.245332	-2.413297	-1.679642
C	4.635836	-2.800281	-2.884151
C	3.330414	-2.365881	-3.173864
C	2.639233	-1.547359	-2.267167
C	3.247601	-1.139128	-1.056433
C	4.557943	-1.587125	-0.771947
P	2.251649	-0.019111	0.075245
C	3.304828	-0.137427	1.631003
C	2.854284	-0.997650	2.657254
C	3.607929	-1.171105	3.829442
C	4.816404	-0.474719	4.003787
C	5.265349	0.400203	3.000104
C	4.516958	0.567499	1.821282
Ru	0.003721	-0.386688	0.181456
C	0.058258	-2.255290	-0.081136
O	0.106973	-3.445609	-0.124375
P	-2.256178	-0.047462	0.069003
C	-2.810337	1.727519	-0.202223
C	-3.970944	2.277566	0.387550
C	-4.349643	3.607206	0.124409
C	-3.579929	4.402953	-0.738635
C	-2.421985	3.866033	-1.329842
C	-2.035846	2.544203	-1.059072
C	2.857164	1.643513	-0.562106
C	2.115254	2.807661	-0.261311
C	2.559545	4.071510	-0.681159
C	3.748844	4.195640	-1.420291
C	4.489025	3.045673	-1.739033
C	4.049080	1.779436	-1.313068
C	-3.354137	-0.486980	1.536665
C	-2.772651	-0.455073	2.823698
C	-3.542557	-0.735219	3.964366
C	-4.902254	-1.068117	3.837574
C	-5.487576	-1.122768	2.561422
C	-4.720983	-0.833509	1.418539
C	-3.266014	-0.868101	-1.292097
C	-2.932228	-2.184227	-1.686517
C	-3.674649	-2.847230	-2.676832
C	-4.756678	-2.204476	-3.302664
C	-5.090821	-0.892338	-2.931000
C	-4.353837	-0.229161	-1.933390
H	1.881806	-1.487561	2.524816
H	3.241929	-1.842807	4.613962
H	5.399461	-0.603171	4.922571
H	6.197443	0.960461	3.135752
H	4.863213	1.262082	1.048991
H	1.608481	-1.227946	-2.460658
H	2.840978	-2.675424	-4.103795
H	5.170695	-3.446724	-3.588760
H	6.257360	-2.758344	-1.439606
H	5.032981	-1.293688	0.168896
H	4.623572	0.885883	-1.575931
H	1.170129	2.687738	0.281215
H	1.966938	4.960368	-0.437796
H	4.090973	5.181372	-1.754599
H	5.409982	3.129287	-2.327064
H	-5.178276	-0.890319	0.425751
H	-6.542856	-1.397530	2.451913
H	-5.499870	-1.296722	4.727089
H	-3.073527	-0.706443	4.954308
H	-1.697688	-0.243253	2.893463
H	-2.069739	-2.675024	-1.227620
H	-4.613519	0.796334	-1.654401
H	-5.924999	-0.377169	-3.420724
H	-3.396122	-3.866230	-2.966932
H	-5.329290	-2.719916	-4.081575
H	-1.116540	2.121387	-1.479640
H	-4.572313	1.662023	1.063161
H	-5.246784	4.019025	0.600286
H	-3.874167	5.438428	-0.943039
H	-1.808211	4.481675	-1.996692
H	0.009873	-0.623633	1.837766
H	-0.020923	1.192616	0.742259
H	-0.009816	0.210014	-1.407245

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TS[13-28]

Ru	-0.031451	-0.439202	-0.122659
P	-2.258759	-0.067906	-0.047758
P	2.245114	-0.079369	-0.046802
C	-2.823678	1.687595	0.312725
C	-4.574915	-2.398363	3.338038
C	-3.308340	-1.830391	3.564130
C	-2.650958	-1.136383	2.536778
C	-3.347081	-0.394359	-1.555112
C	-2.864707	-1.306042	-2.519684
C	-3.632895	-1.627471	-3.651740
C	-4.890979	-1.032277	-3.844580
C	-5.374306	-0.106875	-2.903078
C	-4.608744	0.211078	-1.767636
C	3.414492	-0.866748	-1.290339
C	-2.091550	2.763931	-0.238412
C	2.877721	-1.286423	-2.527271
C	3.702951	-1.861099	-3.507868
C	5.075789	-2.037144	-3.263842
C	5.618975	-1.638277	-2.030547
C	4.795683	-1.056565	-1.050625
C	3.218601	-0.394728	1.530261
C	2.937919	-1.568652	2.270474
C	3.639205	-1.844857	3.455523
C	4.624601	-0.958585	3.924911
C	4.907211	0.211585	3.201547
C	-2.495393	4.091111	-0.023717
C	4.208663	0.492806	2.013498
C	2.695694	1.728675	-0.296074
C	3.766750	2.172484	-1.103756
C	4.037895	3.546357	-1.246759
C	3.251200	4.496107	-0.576148
C	2.184063	4.066454	0.233560
C	1.903755	2.697911	0.366839
C	-3.631931	4.368788	0.756606
C	-4.360265	3.309749	1.321633
C	-3.961817	1.978943	1.099867
C	-3.255581	-0.981381	1.263833
C	-4.526208	-1.563061	1.047512
C	-5.178048	-2.266884	2.076888
H	-1.857316	-1.717927	-2.374786
H	-3.240270	-2.335300	-4.390339
H	-5.487195	-1.276942	-4.730721
H	-6.346374	0.375537	-3.056451
H	-4.978838	0.949353	-1.048786
H	-1.648844	-0.716607	2.689849
H	-2.822357	-1.938757	4.540029
H	-5.082864	-2.949436	4.137096
H	-6.160294	-2.714973	1.888297
H	-5.002312	-1.466463	0.067179
H	-4.523796	1.156069	1.552335

H	-1.185731	2.541224	-0.813106
H	-1.912654	4.910392	-0.458936
H	-3.941120	5.405248	0.930865
H	-5.239446	3.516620	1.942300
H	5.218600	-0.762600	-0.084891
H	6.685478	-1.786320	-1.826059
H	5.717578	-2.494197	-4.025386
H	3.268081	-2.185463	-4.460026
H	1.795370	-1.179862	-2.678147
H	2.164223	-2.248934	1.890145
H	4.422314	1.412738	1.460887
H	5.668725	0.912463	3.562315
H	3.409493	-2.757987	4.016357
H	5.166232	-1.176130	4.852502
H	1.054445	2.349195	0.965811
H	4.386161	1.436573	-1.624879
H	4.867304	3.870739	-1.885446
H	3.463190	5.565308	-0.687770
H	1.559525	4.799060	0.756747
H	0.027870	-0.979849	-1.701650
H	-0.016630	0.755988	-1.144595
C	-0.090469	-2.712266	-0.125440
O	1.048247	-3.022025	0.357837
H	-0.919455	-2.446322	0.600941
H	-0.451831	-3.187618	-1.067903
H	-0.014572	0.346884	1.406921

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TS[28-29aperp]

Ru	-0.019995	-0.230819	-0.005579
P	-2.283118	0.017134	-0.034391
P	2.256831	0.019746	-0.033782
C	-3.000480	1.746900	0.102014
C	-4.566385	-2.031234	3.544340
C	-3.354843	-1.343927	3.738206
C	-2.698030	-0.746623	2.651417
C	-3.276064	-0.599469	-1.509773
C	-2.740947	-1.673088	-2.256953
C	-3.451092	-2.219042	-3.339307
C	-4.701557	-1.691671	-3.703298
C	-5.237260	-0.612156	-2.980543
C	-4.532139	-0.071250	-1.890904
C	3.299716	-0.903015	-1.295377
C	-2.305106	2.826322	-0.488241
C	2.709290	-1.277686	-2.521174
C	3.462793	-1.935153	-3.507611
C	4.816449	-2.236343	-3.281517
C	5.412457	-1.881851	-2.059150
C	4.660600	-1.221293	-1.072553
C	3.232385	-0.404979	1.510858
C	3.049102	-1.698986	2.060382
C	3.726594	-2.072761	3.231154
C	4.585745	-1.165667	3.878466
C	4.767212	0.120271	3.345455
C	-2.832513	4.126787	-0.448555
C	4.098057	0.498771	2.166676
C	2.901865	1.764107	-0.325973
C	4.095455	2.038998	-1.032353
C	4.546190	3.360827	-1.198707
C	3.817865	4.430543	-0.653897
C	2.628988	4.170942	0.049868
C	2.170969	2.852794	0.205563
C	-4.059020	4.375434	0.191920
C	-4.753045	3.314641	0.796257
C	-4.229515	2.010047	0.751745
C	-3.250154	-0.813606	1.348611
C	-4.468379	-1.507031	1.165910
C	-5.118262	-2.114287	2.256118
H	-1.742150	-2.040149	-1.994507
H	-3.017913	-3.050937	-3.905481
H	-5.251021	-2.111537	-4.553108
H	-6.204160	-0.183944	-3.267998
H	-4.947030	0.778466	-1.339879
H	-1.734903	-0.241525	2.785171
H	-2.910550	-1.283604	4.737734
H	-5.070917	-2.508072	4.391794
H	-6.056392	-2.656849	2.093903
H	-4.903215	-1.574548	0.164413
H	-4.766162	1.189499	1.237887
H	-1.332600	2.621537	-0.950298
H	-2.276461	4.949783	-0.911054
H	-4.466100	5.391908	0.229014
H	-5.702570	3.500355	1.310748
H	5.120768	-0.961350	-0.114296
H	6.463334	-2.126981	-1.868297
H	5.401565	-2.755880	-4.048500
H	2.985423	-2.223909	-4.450640
H	1.641609	-1.071034	-2.663100
H	2.367539	-2.394881	1.548249
H	4.244363	1.501386	1.755007
H	5.431507	0.835057	3.844483
H	3.576613	-3.077293	3.642686
H	5.107917	-1.459562	4.796037
H	1.226927	2.636995	0.717943
H	4.667786	1.211764	-1.462054
H	5.468851	3.551337	-1.758444
H	4.169474	5.460177	-0.783393
H	2.046757	4.997859	0.471621
H	-0.008523	-0.876150	-1.529271
H	-0.017860	1.064996	-1.030927
C	-0.065868	-2.310873	0.314452
O	0.856613	-3.149580	0.356525
H	0.008261	-1.203235	1.381612
H	-1.117179	-2.733201	0.350749
H	-0.028265	1.010644	1.126880

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TS[29aperp-29a]

Ru	0.006230	-0.017057	0.063756
P	2.291168	0.059700	0.013803
P	-2.284291	0.077512	0.020513
H	0.011883	-0.059303	1.725116
H	0.034096	1.495279	0.710993
C	-0.024861	-2.115340	0.456229
H	-0.019246	-0.646294	-1.457790
H	-0.002238	1.128201	-1.108695
C	3.096769	1.576309	-0.754628
C	3.247274	0.028485	1.632578
C	-3.260830	-0.784612	1.372972
C	-3.176146	-0.607635	-1.479689
C	-3.093303	1.775075	0.107887
C	3.234774	-1.282928	-0.906364
O	-0.452857	-3.063210	-0.224250
H	0.430899	-2.442633	1.453200
C	2.613534	-1.879076	-2.027751
C	2.705166	-0.712349	2.707625
C	4.487142	0.682924	1.822222
C	2.504455	2.839557	-0.523862
C	-2.706279	-0.845577	2.671590
C	-4.531490	-1.366131	1.152407
C	-2.681686	-1.813173	-2.035055
C	-4.296900	0.011994	-2.078123
C	-4.344191	2.002904	0.727867
C	-2.432958	2.869134	-0.496443
C	4.275360	1.517490	-1.533486
C	4.528047	-1.723724	-0.537420
C	3.275202	-2.869362	-2.771695
C	3.392568	-0.814809	3.927797
C	5.169577	0.588362	3.048379
C	-3.408916	-1.455234	3.723449
C	-5.230925	-1.981060	2.205673
C	-3.307635	-2.382473	-3.156118
C	-4.911950	-0.557557	-3.208391
C	3.082056	4.009059	-1.042371
C	-4.917939	3.286995	0.738191
C	-3.012229	4.148082	-0.495431
C	4.846621	2.689564	-2.062300
C	5.186351	-2.719130	-1.280558
H	1.724322	-1.183035	2.576880
H	4.907973	1.280003	1.007126
H	1.591188	-1.572232	-2.275584
H	5.012991	-1.293754	0.344270

H	4.738863	0.546644	-1.732636
H	1.568447	2.876502	0.044594
H	-4.962297	-1.346961	0.146687
H	-1.702575	-0.430835	2.823794
H	-1.806124	-2.297061	-1.573102
H	-4.680145	0.948541	-1.662017
H	-1.446283	2.696174	-0.939977
H	-4.861946	1.170212	1.213432
C	4.563980	-3.290770	-2.402843
C	4.627102	-0.165655	4.102088
C	-4.673782	-2.023908	3.494494
C	-4.419370	-1.756751	-3.747990
C	-4.256347	4.362189	0.122704
C	4.254938	3.938445	-1.814610
H	2.955388	-1.395314	4.747698
H	6.124144	1.110200	3.179847
H	2.771831	-3.324124	-3.631682
H	6.184736	-3.052430	-0.975570
H	2.606630	4.977734	-0.851880
H	5.754588	2.622056	-2.672120
H	-6.210050	-2.434438	2.014628
H	-2.959867	-1.496829	4.721992
H	-5.773298	-0.058741	-3.667007
H	-2.915853	-3.317516	-3.572083
H	-5.883346	3.444901	1.232074
H	-2.483065	4.981830	-0.970251
H	5.158160	-0.238499	5.057580
H	5.074828	-4.070991	-2.977855
H	4.699291	4.850774	-2.227581
H	-5.216907	-2.508746	4.313179
H	-4.897114	-2.199650	-4.629345
H	-4.703398	5.362417	0.131942

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TS[29a-29btrans]

Ru	0.000575	0.093485	0.094476
P	2.290238	0.063817	0.027216
P	-2.288517	0.076144	0.028555
C	3.111301	1.595918	-0.682172
C	4.411205	-3.241724	-2.575056
C	3.086505	-2.852432	-2.831428
C	2.466443	-1.875507	-2.034250
C	3.281570	-0.064325	1.619614
C	2.728919	-0.808955	2.685712
C	3.436554	-0.976018	3.886804
C	4.701894	-0.385512	4.050829
C	5.254596	0.374532	3.006817
C	4.551925	0.532611	1.798760
C	-3.233711	-0.753942	1.424340
C	2.739954	2.855455	-0.150857
C	-2.615198	-0.838373	2.692364
C	-3.281608	-1.434306	3.776312
C	-4.571991	-1.964180	3.609114
C	-5.192695	-1.898485	2.349588
C	-4.529237	-1.300017	1.265211
C	-3.174757	-0.697609	-1.434062
C	-2.599806	-1.842191	-2.035577
C	-3.238322	-2.467309	-3.119715
C	-4.444526	-1.955549	-3.629847
C	-5.016789	-0.812732	-3.047650
C	3.303374	4.039012	-0.650074
C	-4.388145	-0.189304	-1.954582
C	-3.128245	1.754207	0.018564
C	-4.156464	2.118642	0.916068
C	-4.724307	3.405529	0.873327
C	-4.282052	4.343555	-0.072637
C	-3.262086	3.990530	-0.974768
C	-2.686683	2.712170	-0.926979
C	4.240445	3.991050	-1.698321
C	4.610623	2.749994	-2.239106
C	4.055100	1.560210	-1.732695
C	3.167701	-1.265201	-0.969274
C	4.496308	-1.678907	-0.708865
C	5.113571	-2.655789	-1.507534
H	1.723207	-1.226139	2.564698
H	2.991626	-1.558878	4.700818
H	5.249441	-0.507887	4.991861
H	6.233622	0.850733	3.132138
H	4.980598	1.135691	0.992130
H	1.422025	-1.586056	-2.195789
H	2.521448	-3.321007	-3.644446
H	4.890710	-4.008546	-3.193700
H	6.142360	-2.964279	-1.289915
H	5.041116	-1.242580	0.133533
H	4.351593	0.595447	-2.153950
H	1.989878	2.892874	0.646348
H	3.003062	5.003091	-0.224832
H	4.673577	4.916632	-2.092983
H	5.334729	2.701827	-3.060169
H	-5.008487	-1.267429	0.282146
H	-6.193621	-2.321153	2.207258
H	-5.087963	-2.436598	4.452404
H	-2.783738	-1.494327	4.750564
H	-1.595887	-0.440849	2.788629
H	-1.647293	-2.228959	-1.647317
H	-4.830735	0.707745	-1.510150
H	-5.951322	-0.400440	-3.444862
H	-2.782172	-3.355108	-3.571799
H	-4.933320	-2.441635	-4.481780
H	-1.874503	2.443909	-1.611209
H	-4.509615	1.388604	1.649857
H	-5.515405	3.671480	1.583407
H	-4.724930	5.344960	-0.105999
H	-2.906662	4.716678	-1.714257
H	0.007855	0.214641	1.776383
H	0.008501	1.759128	0.365599
C	-0.047452	-1.958315	0.480460
O	-0.178252	-2.924870	-0.289270
H	-0.004329	-0.337667	-1.523007
H	0.044983	-2.247737	1.583367
H	0.011040	1.589658	-0.684931

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TS[29btrans-30]

Ru	-0.031521	-0.240523	-0.092268
P	-2.307204	-0.055117	-0.041708
P	2.263104	-0.068357	-0.045786
C	-2.986151	1.685029	-0.189958
C	-4.346394	-1.389835	4.000577
C	-3.062321	-0.819718	3.977195
C	-2.475987	-0.443415	2.757190
C	-3.385350	-0.915993	-1.320182
C	-2.820104	-2.009291	-2.012826
C	-3.573325	-2.718614	-2.963619
C	-4.895579	-2.337209	-3.248470
C	-5.462623	-1.238114	-2.580350
C	-4.714856	-0.532806	-1.621106
C	3.353493	-1.166831	-1.107501
C	-3.048409	2.304287	-1.462051
C	2.747307	-1.890641	-2.156112
C	3.518498	-2.712013	-2.995600
C	4.904571	-2.826122	-2.794999
C	5.516952	-2.120466	-1.744387
C	4.746849	-1.298877	-0.903859
C	3.221982	-0.156101	1.568086
C	2.887865	-1.168388	2.499642
C	3.570293	-1.261821	3.722953
C	4.593905	-0.351552	4.041385
C	4.934210	0.655841	3.124941
C	-3.444385	3.645263	-1.586820
C	4.254224	0.753786	1.896967
C	2.824378	1.626249	-0.622580
C	3.749079	1.839003	-1.669294
C	4.068607	3.143010	-2.090614
C	3.476863	4.253680	-1.468576
C	2.554348	4.055330	-0.424845
C	2.225946	2.756394	-0.009777
C	-3.781373	4.394085	-0.445930
C	-3.721015	3.790660	0.821150
C	-3.328528	2.447713	0.949801
C	-3.175456	-0.611346	1.536972
C	-4.462246	-1.195281	1.573790

C	-5.040564	-1.583425	2.794813
H	-1.769033	-2.253231	-1.814755
H	-3.119351	-3.563982	-3.492531
H	-5.478812	-2.885815	-3.996338
H	-6.487475	-0.925024	-2.809952
H	-5.152157	0.334349	-1.115692
H	-1.454444	-0.044527	2.713287
H	-2.502910	-0.682495	4.909246
H	-4.797881	-1.695151	4.951067
H	-6.035642	-2.042644	2.801030
H	-5.006164	-1.361601	0.639568
H	-3.285123	1.981185	1.938448
H	-2.777270	1.728107	-2.352069
H	-3.485047	4.107505	-2.579290
H	-4.087036	5.441223	-0.544550
H	-3.982420	4.365661	1.716465
H	5.221258	-0.767754	-0.072644
H	6.595272	-2.215519	-1.573351
H	5.505122	-3.470780	-3.446666
H	3.031368	-3.272465	-3.801445
H	1.659994	-1.795626	-2.277124
H	2.098322	-1.880601	2.232391
H	4.514018	1.551743	1.195276
H	5.728242	1.372763	3.363479
H	3.297386	-2.051420	4.432261
H	5.121570	-0.426269	4.998987
H	1.483085	2.592867	0.778993
H	4.219805	0.977385	-2.151304
H	4.784465	3.287307	-2.907795
H	3.726386	5.268369	-1.797834
H	2.078924	4.914751	0.060592
H	-0.016053	-0.749122	-1.712954
H	-0.020515	1.366340	-1.967498
C	-0.045092	-2.038540	0.559593
O	0.909393	-2.806742	0.815406
H	0.037101	0.629574	1.370312
H	-1.082622	-2.458554	0.740569
H	-0.066763	2.128957	-2.012841

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TS[30-31]

Ru	-0.000724	-0.489613	0.334657
P	2.270213	-0.081206	0.054119
P	-2.202890	-0.108046	0.081975
C	2.615545	1.667675	-0.510928
C	4.738948	-2.616059	-3.046653
C	3.334326	-2.629329	-3.056273
C	2.611947	-1.863684	-2.124476
C	3.425312	-0.203537	1.524188
C	3.640608	-1.484414	2.093964
C	4.420232	-1.632126	3.250326
C	4.997793	-0.506868	3.865664
C	4.789053	0.767298	3.312018
C	4.011907	0.919807	2.150976
C	-3.382976	-0.298502	1.535979
C	1.908979	2.719279	0.126992
C	-2.858161	-0.114807	2.836211
C	-3.685326	-0.233167	3.964725
C	-5.047595	-0.546998	3.815242
C	-5.577208	-0.747713	2.529521
C	-4.752155	-0.625961	1.397198
C	-3.183564	-1.020739	-1.233960
C	-2.889674	-2.388594	-1.451674
C	-3.599981	-3.121258	-2.417155
C	-4.603943	-2.504571	-3.184597
C	-4.896570	-1.145991	-2.982999
C	2.111662	4.054231	-0.256762
C	-4.192500	-0.408755	-2.013391
C	-2.614269	1.661044	-0.412131
C	-3.770696	2.360271	0.002316
C	-3.989934	3.687594	-0.410469
C	-3.062053	4.331073	-1.246242
C	-1.906755	3.644810	-1.661660
C	-1.681384	2.324282	-1.242417
C	3.005338	4.365378	-1.297473
C	3.698383	3.331452	-1.948139
C	3.511361	1.994707	-1.555508
C	3.287589	-1.070217	-1.172984
C	4.703817	-1.069088	-1.165317
C	5.422914	-1.834659	-2.098024
H	3.183404	-2.363479	1.626146
H	4.573198	-2.630151	3.675613
H	5.603004	-0.623382	4.771025
H	5.235386	1.650377	3.783250
H	3.851702	1.915314	1.726577
H	1.514629	-1.874833	-2.094104
H	2.794541	-3.245030	-3.784047
H	5.300999	-3.218391	-3.768986
H	6.518517	-1.827215	-2.079680
H	5.235725	-0.476080	-0.414479
H	4.057846	1.195684	-2.064452
H	1.174134	2.458542	0.899313
H	1.552729	4.850067	0.247184
H	3.151724	5.406339	-1.605890
H	4.389346	3.562687	-2.766712
H	-5.163992	-0.799768	0.398043
H	-6.634837	-1.007143	2.405456
H	-5.690616	-0.646209	4.696884
H	-3.260729	-0.089795	4.964632
H	-1.787306	0.105648	2.930858
H	-2.096750	-2.863170	-0.857833
H	-4.413713	0.653246	-1.868420
H	-5.669828	-0.653829	-3.583993
H	-3.360301	-4.179216	-2.572498
H	-5.151393	-3.078855	-3.940631
H	-0.766910	1.787427	-1.525299
H	-4.491218	1.864802	0.661030
H	-4.886719	4.220014	-0.073201
H	-3.232619	5.365657	-1.564402
H	-1.168878	4.142017	-2.300499
H	-0.038437	0.691966	1.603532
C	-0.028545	-2.336736	0.784238
O	-0.630839	-3.403961	0.637334
H	-0.081025	-0.999594	-1.228770
H	0.752539	-2.230958	1.637421

ETHANOL

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13H'

Ru	-0.019850	-0.216450	-0.312289
P	-2.327543	0.093065	-0.080410
P	2.284934	0.072068	-0.046837
C	-3.108896	1.545105	-0.941208
C	-3.883155	0.515644	4.318149
C	-4.529907	1.218243	3.288233
C	-4.073927	1.107405	1.963868
C	-3.386628	-1.314905	-0.687261
C	-3.390992	-1.616366	-2.072046
C	-4.111669	-2.714742	-2.562457
C	-4.827154	-3.540614	-1.676158
C	-4.822139	-3.256410	-0.302020
C	-4.110683	-2.148332	0.192164
C	2.817716	1.856546	0.069204
C	-2.371303	2.738360	-1.111094
C	2.049129	2.752272	0.848993
C	2.448379	4.088918	1.001200
C	3.613892	4.556603	0.369536
C	4.381230	3.678939	-0.411971
C	3.989893	2.336182	-0.558792
C	3.395075	-0.529246	-1.418594
C	3.109060	-0.113165	-2.742365
C	3.880314	-0.572954	-3.819306
C	4.943548	-1.466784	-3.595618
C	5.234500	-1.887590	-2.289151
C	-2.963228	3.863746	-1.707332
C	4.470042	-1.419740	-1.204759
C	3.125854	-0.615924	1.464786
C	4.393008	-0.143567	1.886839
C	5.012504	-0.688803	3.021766
C	4.374248	-1.706369	3.753505

C	3.113326	-2.172509	3.350041
C	2.487948	-1.630739	2.212842
C	-4.296989	3.813438	-2.145268
C	-5.039375	2.631566	-1.984565
C	-4.453160	1.504449	-1.385539
C	-2.957844	0.296772	1.657188
C	-2.308477	-0.402675	2.702028
C	-2.774873	-0.296342	4.022561
H	-2.828335	-0.979888	-2.764632
H	-4.111461	-2.929758	-3.635870
H	-5.383215	-4.402618	-2.057677
H	-5.375825	-3.895497	0.393201
H	-4.113854	-1.928855	1.263043
H	-4.577605	1.660785	1.166307
H	-5.389394	1.857792	3.513433
H	-4.238597	0.604740	5.349721
H	-2.263525	-0.843178	4.821288
H	-1.442661	-1.026644	2.462969
H	-5.031554	0.582702	-1.273633
H	-1.325780	2.767331	-0.788755
H	-2.376375	4.779041	-1.835110
H	-4.755002	4.689820	-2.614638
H	-6.077741	2.583892	-2.328175
H	4.588674	1.660867	-1.176316
H	5.287820	4.035702	-0.911463
H	3.919403	5.601464	0.483707
H	1.843198	4.767448	1.611082
H	1.130235	2.392762	1.321946
H	2.278960	0.579585	-2.921578
H	4.711223	-1.740541	-0.187624
H	6.060491	-2.582602	-2.106906
H	3.650190	-0.235465	-4.835052
H	5.539861	-1.831925	-4.437517
H	1.496730	-1.977939	1.897122
H	4.881068	0.665514	1.334943
H	5.990102	-0.312811	3.340385
H	4.857803	-2.126666	4.641286
H	2.606401	-2.956665	3.921935
H	0.409570	-0.547163	-1.977194
H	0.018966	0.481394	1.152818
O	-0.290168	-2.131049	0.826455
C	-0.189630	-2.485809	-0.417896
C	1.004252	-3.288450	-0.909381
H	-0.463309	-0.356075	-1.991726
H	0.088489	1.302442	-0.792684
H	0.834099	-4.355835	-0.661846
H	1.116910	-3.215485	-2.003666
H	1.943894	-2.974459	-0.429647
H	-1.129313	-2.650931	-0.986451

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Complex 23'

Ru	0.024052	-0.486750	-0.050705
P	2.251337	0.039642	-0.034320
P	-2.293602	-0.045315	-0.039764
C	2.709722	1.785560	0.409815
C	4.499021	-0.678883	-4.085593
C	3.253918	-1.278631	-3.838483
C	2.582039	-1.042645	-2.625854
C	3.310398	-0.926324	1.156283
C	3.003138	-0.836665	2.537136
C	3.689044	-1.624794	3.472548
C	4.683799	-2.524008	3.045513
C	4.992496	-2.623736	1.680110
C	4.313029	-1.829346	0.738275
C	-2.680873	1.771510	-0.170732
C	1.812419	2.837213	0.119823
C	-2.139322	2.498726	-1.257631
C	-2.423656	3.863433	-1.413411
C	-3.245342	4.525594	-0.483557
C	-3.785875	3.814131	0.598356
C	-3.511643	2.443012	0.752583
C	-3.150906	-0.511864	1.543717
C	-2.520223	-0.183824	2.770334
C	-3.108017	-0.541468	3.993403
C	-4.327078	-1.242108	4.012316
C	-4.956615	-1.580161	2.803773
C	2.166409	4.168349	0.392738
C	-4.375635	-1.216150	1.576527
C	-3.446480	-0.728090	-1.326564
C	-4.694946	-0.117809	-1.599608
C	-5.561646	-0.671870	-2.553988
C	-5.190539	-1.836560	-3.249681
C	-3.950682	-2.442788	-2.991479
C	-3.077998	-1.893759	-2.035462
C	3.414004	4.466996	0.965112
C	4.306998	3.427260	1.273021
C	3.959721	2.093895	0.998967
C	3.159857	-0.205009	-1.642896
C	4.411176	0.401101	-1.905312
C	5.074995	0.164604	-3.119186
H	2.223835	-0.141712	2.869167
H	3.447362	-1.538679	4.536905
H	5.214433	-3.142498	3.776032
H	5.767420	-3.319109	1.341632
H	4.567697	-1.898654	-0.323096
H	1.602205	-1.501541	-2.442088
H	2.794513	-1.927633	-4.591003
H	5.017286	-0.859582	-5.032822
H	6.039599	0.644572	-3.313678
H	4.852514	1.076789	-1.166736
H	4.647737	1.285215	1.263473
H	0.828434	2.600633	-0.294322
H	1.457824	4.971394	0.166756
H	3.685108	5.505230	1.181117
H	5.274252	3.651648	1.734173
H	-3.936524	1.893355	1.597102
H	-4.427222	4.322172	1.325765
H	-3.461698	5.591779	-0.603991
H	-2.000808	4.411178	-2.261810
H	-1.489702	1.986064	-1.975287
H	-1.564622	0.351335	2.753515
H	-4.873072	-1.474561	0.637594
H	-5.904214	-2.128235	2.811927
H	-2.611613	-0.274728	4.931953
H	-4.781685	-1.525548	4.966727
H	-2.099264	-2.344570	-1.839663
H	-4.976867	0.797849	-1.070488
H	-6.523463	-0.190971	-2.759408
H	-5.866223	-2.264775	-3.997192
H	-3.653257	-3.343068	-3.538887
H	0.071255	0.578024	-1.220962
O	-0.088867	-2.473565	-1.282756
C	0.658971	-2.515656	-0.226313
H	1.741739	-2.734715	-0.336290
H	0.017674	0.756821	0.953156
C	0.066399	-2.650051	1.163674
H	-0.838417	-3.277102	1.185463
H	0.812380	-2.982769	1.903776
H	-0.288466	-1.618102	1.566172

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Complex 24'

C	-5.550804	-0.073800	2.688934
C	-5.058233	-0.819171	3.775641
C	-3.743890	-1.309929	3.747119
C	-2.923698	-1.062790	2.632451
C	-3.408894	-0.324789	1.532696
C	-4.733335	0.176313	1.576940
P	-2.317865	-0.016539	0.054840
C	-3.213971	-0.920689	-1.297786
C	-2.697020	-0.818142	-2.615107
C	-3.277253	-1.541991	-3.667451
C	-4.369671	-2.393013	-3.421323
C	-4.880460	-2.513101	-2.119471
C	-4.310071	-1.780939	-1.062994
Ru	-0.028116	-0.468532	0.134096
C	0.510816	-2.405073	0.761705
C	-0.141936	-2.892267	-0.549693
P	2.222742	0.049349	0.016418
C	3.094335	0.327932	1.638911
C	3.745040	1.545699	1.942726

C	4.353437	1.738135	3.194963
C	4.326280	0.717129	4.157813
C	3.680827	-0.497158	3.867761
C	3.061528	-0.692997	2.622842
C	-2.735833	1.761287	-0.296778
C	-2.110691	2.764120	0.481960
C	-2.417891	4.117624	0.279234
C	-3.347122	4.492050	-0.707479
C	-3.970694	3.505637	-1.487030
C	-3.672189	2.146574	-1.281604
C	2.681758	1.597818	-0.911423
C	1.732088	2.616821	-1.135570
C	2.101137	3.801251	-1.796494
C	3.419508	3.979418	-2.245049
C	4.373593	2.969474	-2.029126
C	4.009886	1.787656	-1.365378
C	3.318159	-1.188847	-0.839226
C	2.941116	-1.593968	-2.143174
C	3.695078	-2.550353	-2.838648
C	4.832649	-3.121812	-2.240572
C	5.212673	-2.728940	-0.947852
C	4.462295	-1.766567	-0.248955
O	1.364000	-3.063809	1.369477
H	-1.832566	-0.171481	-2.801462
H	-2.871956	-1.445592	-4.679744
H	-4.816667	-2.962724	-4.241866
H	-5.728207	-3.176580	-1.920827
H	-4.721738	-1.870567	-0.053844
H	-1.891708	-1.427966	2.613997
H	-3.349507	-1.880413	4.593968
H	-5.696534	-1.007977	4.644514
H	-6.572052	0.319667	2.711519
H	-5.113348	0.773623	0.742286
H	-4.157141	1.383639	-1.897302
H	-1.375650	2.473485	1.240143
H	-1.927680	4.881512	0.891290
H	-3.581606	5.549075	-0.867673
H	-4.694024	3.789513	-2.258224
H	4.753177	1.001240	-1.202801
H	5.402064	3.099878	-2.380660
H	3.703469	4.899673	-2.765415
H	1.350880	4.580328	-1.965312
H	0.701258	2.464143	-0.804059
H	2.053677	-1.148805	-2.607666
H	4.754850	-1.471854	0.762483
H	6.095185	-3.172770	-0.476066
H	3.394928	-2.850489	-3.847820
H	5.417415	-3.872825	-2.780915
H	2.544880	-1.636180	2.408471
H	3.778660	2.342541	1.195392
H	4.850418	2.688896	3.413517
H	4.803108	0.867511	5.131715
H	3.652368	-1.298024	4.613934
H	0.054934	0.797457	1.072849
H	-0.188443	-1.661643	1.492904
H	-0.045086	0.514265	-1.144023
H	0.609883	-3.469730	-1.107307
H	-1.039117	-3.499974	-0.345985
H	-0.497484	-2.058709	-1.226014

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Complex 25'

Ru	-0.010111	-0.170668	0.028331
P	-2.323775	0.102701	-0.061169
P	2.306731	0.099765	-0.057407
C	-2.988731	1.837960	-0.079556
C	-4.338926	-1.766508	3.728017
C	-3.485032	-0.653755	3.838812
C	-2.913555	-0.087302	2.690358
C	-3.243489	-0.672474	-1.483367
C	-2.690911	-1.810238	-2.116240
C	-3.376585	-2.443161	-3.167076
C	-4.611056	-1.941671	-3.609714
C	-5.163135	-0.803907	-2.996582
C	-4.487164	-0.174401	-1.939116
C	3.212279	-0.641973	-1.504262
C	-2.266593	2.865291	-0.725779
C	2.558478	-0.741650	-2.751996
C	3.233484	-1.250124	-3.873371
C	4.568354	-1.672763	-3.764687
C	5.227606	-1.585857	-2.527263
C	4.557693	-1.073924	-1.404041
C	3.229288	-0.639593	1.377909
C	3.367934	-2.048427	1.464897
C	3.975464	-2.633909	2.587382
C	4.443705	-1.828017	3.639613
C	4.304151	-0.432598	3.564228
C	-2.786756	4.167534	-0.796238
C	3.702254	0.160808	2.441697
C	2.961391	1.847656	-0.068721
C	4.215683	2.159064	-0.644956
C	4.713952	3.470720	-0.605860
C	3.970721	4.491455	0.010683
C	2.722371	4.195944	0.581171
C	2.217280	2.885221	0.537781
C	-4.031725	4.463677	-0.216375
C	-4.755149	3.452436	0.436743
C	-4.240352	2.147107	0.505183
C	-3.199779	-0.620287	1.408659
C	-4.058442	-1.736907	1.307164
C	-4.621142	-2.306567	2.463630
H	-1.719702	-2.193085	-1.790594
H	-2.935309	-3.324564	-3.643151
H	-5.139001	-2.430864	-4.434526
H	-6.120114	-0.401322	-3.343792
H	-4.916362	0.718551	-1.475151
H	-2.237957	0.771242	2.774163
H	-3.260968	-0.228752	4.822397
H	-4.779274	-2.210840	4.626002
H	-5.283838	-3.172870	2.371227
H	-4.287915	-2.156021	0.323569
H	-4.799227	1.366295	1.029237
H	-1.285477	2.640341	-1.155154
H	-2.213132	4.952276	-1.299602
H	-4.433520	5.480520	-0.267375
H	-5.721622	3.678401	0.898555
H	5.071500	-1.025596	-0.439434
H	6.265209	-1.921712	-2.432258
H	5.090504	-2.075683	-4.638129
H	2.709308	-1.324283	-4.831424
H	1.509952	-0.436870	-2.829153
H	3.009186	-2.682266	0.646732
H	3.605733	1.248823	2.383359
H	4.670989	0.200789	4.378249
H	4.082799	-3.722129	2.637342
H	4.916243	-2.286934	4.513499
H	1.233394	2.649712	0.957312
H	4.793618	1.374543	-1.141022
H	5.683259	3.694838	-1.062639
H	4.360496	5.514015	0.038762
H	2.131603	4.986322	1.055438
H	-0.041214	-0.634831	-1.510721
H	0.018239	1.035598	-1.002063
C	0.062761	-2.129273	0.100762
O	0.144211	-3.212773	-0.446666
H	-0.075264	1.148812	1.088103
C	-0.024375	-1.977487	1.693588
H	-0.936893	-2.503462	2.008670
H	0.889632	-2.434582	2.100258
H	-0.079713	-0.952397	2.130223

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Complex 26'a

C	4.892254	3.009771	1.245142
C	4.664015	3.988502	0.265696
C	3.753962	3.735525	-0.776154
C	3.072279	2.511433	-0.833451
C	3.301662	1.513308	0.145195
C	4.220286	1.775827	1.184820
P	2.330092	-0.067521	0.029816
C	3.124358	-0.871902	-1.453747
C	2.537136	-2.035159	-2.002814

C	3.134882	-2.692426	-3.088923
C	4.325015	-2.195854	-3.648391
C	4.914853	-1.039429	-3.114583
C	4.321975	-0.381469	-2.023000
Ru	-0.002091	0.155461	0.006120
C	0.018210	0.735018	-2.166699
P	-2.334766	-0.074951	0.017679
C	-3.049913	-0.996619	1.469641
C	-4.051377	-1.982145	1.325432
C	-4.568970	-2.643715	2.452810
C	-4.105095	-2.320654	3.737566
C	-3.114294	-1.335500	3.893916
C	-2.585338	-0.683626	2.769757
C	-0.015233	2.078129	0.311684
O	-0.026051	3.227125	0.516508
C	3.097833	-1.067811	1.403470
C	4.369963	-1.667690	1.239681
C	4.962716	-2.383470	2.291548
C	4.297728	-2.510344	3.523066
C	3.035987	-1.919821	3.697102
C	2.438544	-1.205438	2.644721
C	-3.149453	-0.944425	-1.414475
C	-2.442491	-1.920658	-2.150016
C	-3.065535	-2.613437	-3.201155
C	-4.401168	-2.337444	-3.535219
C	-5.113378	-1.363168	-2.815022
C	-4.494240	-0.670057	-1.762721
C	-3.328181	1.498763	0.060064
C	-3.071610	2.472205	-0.936116
C	-3.787015	3.678126	-0.954225
C	-4.762104	3.935330	0.025883
C	-5.020592	2.979661	1.020361
C	-4.312073	1.764808	1.037424
H	1.600313	-2.409572	-1.577405
H	2.666526	-3.591266	-3.502726
H	4.786933	-2.706451	-4.499184
H	5.839538	-0.643835	-3.546837
H	4.782871	0.522941	-1.616715
H	2.352180	2.321758	-1.636262
H	3.567614	4.495523	-1.541531
H	5.188971	4.947602	0.314097
H	5.597619	3.201093	2.060157
H	4.412291	1.013176	1.944279
H	1.448592	-0.759149	2.774324
H	4.887766	-1.582757	0.279942
H	5.944008	-2.846337	2.146083
H	4.759639	-3.071919	4.341242
H	2.508168	-2.019015	4.651034
H	-5.050254	0.092981	-1.210429
H	-6.152904	-1.138448	-3.074011
H	-4.884026	-2.873966	-4.358045
H	-2.501376	-3.363625	-3.764398
H	-1.395191	-2.115283	-1.898388
H	-2.304083	2.278457	-1.692904
H	-4.520202	1.023865	1.813916
H	-5.777322	3.174410	1.787079
H	-3.577441	4.420666	-1.730619
H	-5.315084	4.879774	0.014346
H	-1.796950	0.066132	2.889872
H	-4.423235	-2.230350	0.328043
H	-5.337724	-3.412080	2.322564
H	-4.510299	-2.835554	4.614324
H	-2.747018	-1.077969	4.892549
H	0.014169	-1.277269	-0.778358
H	-0.021512	-1.157093	0.941372
H	-0.010659	0.313449	1.633802
H	0.066825	1.827801	-2.312892
H	0.889847	0.283340	-2.666385
H	-0.891693	0.363899	-2.665313

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TS′[13H-23]

Ru	0.014940	-0.489261	-0.142980
P	2.242448	0.033607	-0.021671
P	-2.297404	-0.029693	-0.044395
C	2.670974	1.764952	0.512890
C	4.537883	-0.282700	-4.099886
C	5.206681	0.209018	-2.964474
C	4.532621	0.308785	-1.738404
C	3.296840	-0.989643	1.120287
C	3.157161	-0.815483	2.520676
C	3.832874	-1.660088	3.414425
C	4.647796	-2.698463	2.929531
C	4.789012	-2.882470	1.544771
C	4.121527	-2.034931	0.643524
C	-2.672013	1.782875	-0.241555
C	1.759472	2.807209	0.231261
C	-2.114640	2.464064	-1.350064
C	-2.392885	3.822313	-1.565149
C	-3.225716	4.523162	-0.675027
C	-3.782579	3.857698	0.428115
C	-3.512754	2.494229	0.642860
C	-3.019360	-0.410346	1.625386
C	-2.422915	0.164734	2.776334
C	-2.900532	-0.147935	4.058199
C	-3.966805	-1.051383	4.214447
C	-4.558000	-1.634280	3.082244
C	2.079791	4.137051	0.547829
C	-4.092540	-1.314013	1.795175
C	-3.569322	-0.762343	-1.186075
C	-4.859770	-0.193509	-1.317242
C	-5.813233	-0.782634	-2.160648
C	-5.489516	-1.943283	-2.886996
C	-4.209742	-2.507650	-2.771800
C	-3.249221	-1.922474	-1.927122
C	3.306372	4.444583	1.159569
C	4.212421	3.413935	1.459309
C	3.900463	2.082582	1.137201
C	3.177489	-0.085812	-1.630687
C	2.512045	-0.575150	-2.777858
C	3.193330	-0.673045	-4.004574
H	2.521544	-0.009888	2.903633
H	3.722807	-1.507051	4.492921
H	5.171423	-3.357923	3.628500
H	5.426512	-3.685101	1.160009
H	4.253850	-2.170385	-0.434021
H	5.054621	0.708265	-0.864448
H	6.253607	0.521016	-3.036111
H	5.065322	-0.356296	-5.056308
H	2.665393	-1.054840	-4.884387
H	1.462865	-0.886468	-2.701643
H	4.601329	1.283212	1.395584
H	0.788807	2.560947	-0.209054
H	1.360945	4.931959	0.324942
H	3.551202	5.481387	1.410936
H	5.163920	3.643945	1.949636
H	-3.944829	1.982271	1.507465
H	-4.431896	4.396911	1.125390
H	-3.437871	5.583907	-0.841830
H	-1.955859	4.334340	-2.428452
H	-1.456439	1.921192	-2.037119
H	-1.579989	0.853301	2.654702
H	-4.566184	-1.758397	0.915625
H	-5.388288	-2.338481	3.196642
H	-2.434585	0.310421	4.936367
H	-4.332711	-1.300187	5.215444
H	-2.236747	-2.334348	-1.854649
H	-5.108903	0.718581	-0.765830
H	-6.806984	-0.333237	-2.255779
H	-6.233946	-2.399478	-3.547597
H	-3.948724	-3.402510	-3.346074
H	-0.251673	-1.397848	2.695642
H	0.087427	0.461659	-1.372720
O	-0.163679	-2.103899	-1.676927
C	0.668640	-2.488709	-0.752536
H	0.470681	-1.604866	2.628663
H	-0.031922	0.727303	0.913636

H	1.750096	-2.520012	-1.010805
C	0.232030	-3.490871	0.306925
H	0.105948	-4.483939	-0.168600
H	0.984980	-3.587535	1.105821
H	-0.742596	-3.211723	0.746223

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TS′[23-24]

Ru	-0.031008	-0.254919	-0.083593
P	-2.326198	0.047104	-0.046426
P	2.266633	0.070710	-0.047503
C	-2.986786	1.621220	-0.788833
C	-4.177933	0.272000	4.256213
C	-2.815310	-0.014412	4.080763
C	-2.271425	-0.080879	2.786063
C	-3.370849	-1.249524	-0.873763
C	-3.255149	-1.411437	-2.278216
C	-3.923890	-2.455586	-2.934120
C	-4.705499	-3.366869	-2.200957
C	-4.815190	-3.225247	-0.808850
C	-4.155333	-2.173953	-0.147622
C	2.889196	1.604587	-0.901362
C	-2.281457	2.823530	-0.549987
C	1.998625	2.642353	-1.249966
C	2.471872	3.807841	-1.877328
C	3.838524	3.950539	-2.163804
C	4.734675	2.921206	-1.824740
C	4.265673	1.755791	-1.199557
C	3.372116	-1.198308	-0.844491
C	3.110604	-1.531424	-2.195731
C	3.881771	-2.501238	-2.852813
C	4.921418	-3.157322	-2.170052
C	5.187933	-2.833736	-0.830466
C	-2.767698	4.044766	-1.040819
C	4.420926	-1.858744	-0.169080
C	3.000520	0.259354	1.655467
C	3.685898	1.428696	2.057628
C	4.173094	1.556143	3.369384
C	3.988401	0.517634	4.296037
C	3.307868	-0.649211	3.908595
C	2.808130	-0.779206	2.602433
C	-3.960990	4.083585	-1.782986
C	-4.666993	2.895492	-2.029493
C	-4.187437	1.670964	-1.533389
C	-3.085622	0.137176	1.652772
C	-4.455401	0.438429	1.842545
C	-4.996414	0.501207	3.135197
H	-2.638338	-0.711904	-2.852705
H	-3.831093	-2.560875	-4.019747
H	-5.221350	-4.184271	-2.713899
H	-5.419162	-3.931677	-0.230522
H	-4.258444	-2.061621	0.935365
H	-1.202686	-0.282823	2.650544
H	-2.169423	-0.181283	4.948482
H	-4.601985	0.326170	5.263794
H	-6.056946	0.736715	3.269820
H	-5.090158	0.638105	0.973776
H	-4.736482	0.747394	-1.737870
H	-1.348345	2.786224	0.021921
H	-2.212537	4.967766	-0.844749
H	-4.336710	5.036163	-2.169498
H	-5.595222	2.918027	-2.609600
H	4.963085	0.950755	-0.948446
H	5.800614	3.023917	-2.051959
H	4.205562	4.856970	-2.655643
H	1.767298	4.601002	-2.147585
H	0.934084	2.517114	-1.035213
H	2.302038	-1.020313	-2.730722
H	4.625707	-1.618606	0.877871
H	5.995323	-3.341801	-0.293261
H	3.671168	-2.745571	-3.899040
H	5.519159	-3.918325	-2.681426
H	2.261189	-1.683635	2.310425
H	3.843873	2.237547	1.339477
H	4.700509	2.469470	3.663311
H	4.371056	0.618073	5.316793
H	3.159008	-1.463986	4.624939
H	0.004932	1.154661	0.661350
O	1.137580	-2.979054	1.088887
C	0.127981	-2.521893	0.513167
H	-0.758051	-2.179284	1.135942
H	0.034056	0.497667	-1.459653
C	-0.130591	-2.615742	-0.969848
H	0.680891	-3.174319	-1.459586
H	-1.129280	-3.015471	-1.209261
H	-0.127729	-1.572965	-1.495435

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TS′[24-25]

C	-5.575301	-0.550181	2.600914
C	-5.211587	-1.678283	3.357538
C	-3.972205	-2.298830	3.134444
C	-3.098133	-1.795370	2.156185
C	-3.454771	-0.668930	1.385321
C	-4.704554	-0.046371	1.622306
P	-2.300359	-0.041888	0.064833
C	-3.170456	-0.570329	-1.492735
C	-2.534270	-0.312809	-2.733427
C	-3.129162	-0.717697	-3.938244
C	-4.359843	-1.397434	-3.924422
C	-4.993716	-1.667675	-2.701080
C	-4.406285	-1.256401	-1.492018
Ru	-0.011041	-0.551743	0.116382
C	0.518612	-2.467689	0.483962
C	-0.117941	-2.859860	-0.889643
P	2.221618	0.032330	0.024584
C	3.142946	0.068573	1.644669
C	3.928892	1.175144	2.041185
C	4.584924	1.179021	3.283818
C	4.470210	0.077229	4.145926
C	3.691373	-1.028143	3.763355
C	3.025228	-1.035454	2.526980
C	-2.670440	1.778813	0.126968
C	-2.089550	2.554653	1.158276
C	-2.360629	3.927805	1.253444
C	-3.208137	4.548065	0.318022
C	-3.786332	3.787830	-0.710210
C	-3.524363	2.409257	-0.804538
C	2.625236	1.712366	-0.663750
C	1.659456	2.741280	-0.663294
C	1.986028	4.024460	-1.133808
C	3.276687	4.293653	-1.616965
C	4.245025	3.274767	-1.627865
C	3.924604	1.993203	-1.152561
C	3.301368	-1.043834	-1.041630
C	2.917805	-1.222634	-2.393900
C	3.662546	-2.055491	-3.241816
C	4.795820	-2.728646	-2.750867
C	5.180741	-2.562162	-1.411438
C	4.440561	-1.723477	-0.558998
O	1.220761	-3.252939	1.116314
H	-1.568650	0.204904	-2.738846
H	-2.627914	-0.505444	-4.888009
H	-4.819525	-1.719138	-4.864104
H	-5.949824	-2.200478	-2.683316
H	-4.908127	-1.464289	-0.543051
H	-2.120070	-2.260879	1.999362
H	-3.677332	-3.170487	3.727179
H	-5.889837	-2.066170	4.124012
H	-6.536320	-0.056836	2.777892
H	-4.983778	0.841523	1.046603
H	-3.974685	1.822021	-1.609681
H	-1.416755	2.075288	1.877307
H	-1.905452	4.514688	2.057636
H	-3.414332	5.620485	0.391322
H	-4.446029	4.264029	-1.442674
H	4.678786	1.200506	-1.167748
H	5.250954	3.475571	-2.010133
H	3.527036	5.291964	-1.989731
H	1.223800	4.810084	-1.128752
H	0.646650	2.521067	-0.313593
H	2.034098	-0.697675	-2.774684

H	4.740500	-1.601551	0.485365
H	6.060238	-3.085930	-1.023505
H	3.358512	-2.179950	-4.286157
H	5.373861	-3.382638	-3.411250
H	2.410818	-1.898085	2.243927
H	4.026738	2.036468	1.375754
H	5.185189	2.047120	3.575023
H	4.982063	0.080857	5.113638
H	3.593277	-1.890655	4.430624
H	0.091082	0.556788	1.231122
H	-0.216392	-1.599251	1.428362
H	-0.070018	0.603866	-1.061283
H	0.668452	-3.339362	-1.491605
H	-0.959777	-3.550683	-0.722369
H	-0.528705	-2.004645	-1.487843

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TS'[25-26a]

Ru	-0.000905	-0.214108	-0.018118
P	-2.319785	0.053888	-0.055107
P	2.317568	0.081720	-0.054999
C	-2.952033	1.796278	-0.220229
C	-4.319532	-1.411875	3.917488
C	-3.353393	-0.389512	3.926467
C	-2.779699	0.048351	2.724260
C	-3.307033	-0.794021	-1.388325
C	-2.735640	-1.856912	-2.121488
C	-3.480748	-2.524022	-3.109636
C	-4.800139	-2.132194	-3.383538
C	-5.376608	-1.068574	-2.666895
C	-4.637623	-0.403231	-1.676721
C	3.263690	-0.699636	-1.455188
C	-2.340145	2.670301	-1.147583
C	2.635911	-0.858269	-2.710281
C	3.339165	-1.398860	-3.798754
C	4.678021	-1.795001	-3.649451
C	5.312356	-1.649309	-2.404388
C	4.613763	-1.105438	-1.314091
C	3.225549	-0.584161	1.423577
C	3.414821	-1.982443	1.559231
C	4.007820	-2.509448	2.717662
C	4.410990	-1.654659	3.757860
C	4.221784	-0.268541	3.633898
C	-2.834206	3.970294	-1.335445
C	3.634044	0.266213	2.475257
C	2.936838	1.839199	-0.119989
C	4.203239	2.151239	-0.668189
C	4.673440	3.473795	-0.675494
C	3.889229	4.505363	-0.132379
C	2.628946	4.209291	0.410923
C	2.151846	2.887458	0.412648
C	-3.942832	4.419895	-0.597699
C	-4.556649	3.561622	0.327799
C	-4.069090	2.256407	0.515054
C	-3.177324	-0.521326	1.489146
C	-4.146876	-1.548129	1.490354
C	-4.710805	-1.990995	2.700491
H	-1.704777	-2.157569	-1.918559
H	-3.021947	-3.347469	-3.666035
H	-5.377643	-2.648475	-4.156970
H	-6.402138	-0.752261	-2.882753
H	-5.085399	0.435101	-1.134549
H	-2.012732	0.830845	2.729682
H	-3.040859	0.063241	4.872819
H	-4.760148	-1.757866	4.857659
H	-5.459054	-2.789883	2.687070
H	-4.464267	-1.995087	0.544187
H	-4.545845	1.597361	1.245942
H	-1.466460	2.329805	-1.711861
H	-2.347310	4.634457	-2.056641
H	-4.323329	5.435948	-0.741920
H	-5.417776	3.905435	0.909815
H	5.108352	-1.012513	-0.342756
H	6.353166	-1.964043	-2.277570
H	5.222911	-2.223038	-4.496653
H	2.834192	-1.518503	-4.762534
H	1.584760	-0.572629	-2.817556
H	3.108658	-2.654065	0.750290
H	3.498835	1.347546	2.379278
H	4.538334	0.403133	4.438260
H	4.153442	-3.590713	2.806075
H	4.871337	-2.068234	4.660404
H	1.159162	2.655159	0.810727
H	4.813188	1.357626	-1.108570
H	5.652511	3.697341	-1.111172
H	4.256367	5.536580	-0.140371
H	2.006046	5.007588	0.827062
H	-0.030849	-0.327206	-1.620728
H	0.020223	1.200166	-0.768551
C	0.104591	-2.124141	-0.143511
O	0.216113	-3.250008	-0.536262
H	-0.077761	1.002242	1.130658
C	-0.023065	-1.905278	1.684453
H	-0.934636	-2.492827	1.852188
H	0.888177	-2.454823	1.953488
H	-0.068164	-1.004048	2.315261

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TS'[26a-27]

Ru	-0.009848	0.199507	0.019063
P	-2.332406	-0.043816	-0.045007
P	2.314138	-0.052668	-0.027483
C	-3.073830	-1.186606	-1.315212
C	-4.619062	3.998330	-0.676133
C	-3.776851	3.806569	0.433294
C	-3.117444	2.582082	0.612498
C	-3.127170	-0.734255	1.494545
C	-2.575048	-1.907252	2.061927
C	-3.148393	-2.485526	3.204054
C	-4.279163	-1.900364	3.800782
C	-4.834634	-0.736538	3.247333
C	-4.265481	-0.156672	2.099600
C	3.084200	-0.871479	1.458633
C	-4.447522	-1.528628	-1.249810
C	2.459471	-2.011586	2.017757
C	3.017288	-2.657113	3.132209
C	4.203659	-2.172121	3.709590
C	4.832716	-1.042301	3.163440
C	4.280251	-0.396642	2.043858
C	3.347002	1.492445	-0.151155
C	3.018760	2.595797	0.672387
C	3.773821	3.777179	0.621149
C	4.862604	3.879412	-0.261930
C	5.194902	2.794222	-1.088189
C	-5.014779	-2.381345	-2.208181
C	4.446110	1.605845	-1.032190
C	3.033848	-1.068611	-1.413641
C	4.160307	-1.901346	-1.219431
C	4.705670	-2.624221	-2.294122
C	4.141925	-2.518372	-3.576138
C	3.026641	-1.688396	-3.780929
C	2.473478	-0.972374	-2.707614
C	-4.219902	-2.910916	-3.240723
C	-2.856412	-2.586513	-3.307513
C	-2.285217	-1.729217	-2.350626
C	-3.303716	1.520124	-0.307638
C	-4.151006	1.725060	-1.418510
C	-4.800367	2.958936	-1.601392
H	-1.690672	-2.359528	1.600883
H	-2.709837	-3.393391	3.630478
H	-4.722645	-2.350047	4.694598
H	-5.714383	-0.274623	3.706818
H	-4.697535	0.754254	1.676337
H	-2.443261	2.446091	1.464825
H	-3.624100	4.615015	1.155227
H	-5.125401	4.957720	-0.820781
H	-5.448565	3.104057	-2.471530
H	-4.303991	0.917071	-2.138960
H	-1.220901	-1.479725	-2.386161
H	-5.064337	-1.133640	-0.436750
H	-6.076874	-2.638732	-2.145133
H	-4.663171	-3.580476	-3.984680

H	-2.229283	-3.003887	-4.101851
H	4.775148	0.483419	1.624963
H	5.756398	-0.658073	3.607792
H	4.633192	-2.672231	4.583245
H	2.520933	-3.537432	3.552933
H	1.530502	-2.383112	1.573461
H	2.162215	2.525553	1.350333
H	4.711560	0.763492	-1.676457
H	6.039066	2.868919	-1.781117
H	3.504529	4.620745	1.264488
H	5.445995	4.804298	-0.308677
H	1.590080	-0.342872	-2.856697
H	4.604614	-1.987013	-0.223889
H	5.572609	-3.271227	-2.126124
H	4.567891	-3.082885	-4.411658
H	2.581102	-1.601600	-4.777237
H	-0.012971	-0.636859	1.393914
C	-0.010550	2.061697	-0.533065
O	-0.006472	3.158998	-0.936181
H	0.008392	-1.422481	-0.209143
H	-0.015627	-0.001878	-1.607227
C	-0.043983	0.900583	2.225742
H	-0.095891	1.998154	2.163193
H	-0.922335	0.545081	2.786328
H	0.863947	0.625503	2.784323

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TS′[13-28]

Ru	-0.025191	-0.458277	-0.069113
P	-2.234554	-0.003326	-0.020429
P	2.245179	-0.048689	-0.024931
C	-2.711218	1.772161	0.368460
C	-4.689274	-2.326528	3.264173
C	-3.471602	-1.687768	3.561875
C	-2.779525	-0.984517	2.564629
C	-3.302432	-0.207669	-1.564378
C	-2.785150	-0.984937	-2.622938
C	-3.533733	-1.192672	-3.794680
C	-4.809517	-0.620966	-3.928651
C	-5.329527	0.171356	-2.889369
C	-4.581300	0.380781	-1.718793
C	3.446962	-0.960507	-1.150711
C	-1.925465	2.811744	-0.179266
C	2.918685	-1.613699	-2.285429
C	3.763533	-2.293536	-3.178499
C	5.148329	-2.342470	-2.944577
C	5.684877	-1.709414	-1.809943
C	4.841378	-1.022833	-0.919640
C	3.221261	-0.120456	1.578412
C	2.934687	-1.162400	2.493203
C	3.639866	-1.258230	3.704100
C	4.636251	-0.319915	4.025747
C	4.925082	0.721055	3.128447
C	-2.256409	4.156275	0.049516
C	4.222321	0.822149	1.914325
C	2.645827	1.721896	-0.505901
C	3.628085	2.083887	-1.453995
C	3.855007	3.436222	-1.774014
C	3.115015	4.446940	-1.141336
C	2.137568	4.099299	-0.190527
C	1.898993	2.751797	0.118407
C	-3.370905	4.487408	0.841607
C	-4.151635	3.464100	1.402232
C	-3.827604	2.115528	1.164447
C	-3.301607	-0.889579	1.248288
C	-4.521971	-1.542445	0.960793
C	-5.207660	-2.255955	1.961268
H	-1.770198	-1.389512	-2.506503
H	-3.112456	-1.795237	-4.607237
H	-5.392274	-0.778907	-4.842991
H	-6.316237	0.636520	-2.995152
H	-4.977203	1.025398	-0.927380
H	-1.813759	-0.510530	2.778256
H	-3.051596	-1.747504	4.572003
H	-5.223490	-2.884335	4.041007
H	-6.150820	-2.758053	1.717476
H	-4.934401	-1.488108	-0.050893
H	-4.430025	1.319415	1.612853
H	-1.036724	2.543670	-0.760993
H	-1.633738	4.947075	-0.383174
H	-3.622312	5.537377	1.027859
H	-5.014141	3.712541	2.031119
H	5.260122	-0.544719	-0.028405
H	6.761968	-1.755247	-1.612664
H	5.805867	-2.881343	-3.635987
H	3.335529	-2.798384	-4.051957
H	1.829221	-1.594428	-2.422589
H	2.151996	-1.884600	2.226457
H	4.440966	1.646053	1.228208
H	5.694838	1.461934	3.373206
H	3.404556	-2.070440	4.401195
H	5.181320	-0.396154	4.973440
H	1.115343	2.467371	0.830021
H	4.215380	1.301412	-1.942953
H	4.614838	3.695211	-2.520091
H	3.293405	5.499029	-1.389818
H	1.550581	4.879290	0.307026
H	0.033346	-1.240214	-1.546984
H	-0.016138	0.572506	-1.262370
C	-0.130132	-2.727823	0.351088
O	1.028116	-2.900591	0.846251
H	-0.911964	-2.242638	1.017163
H	-0.008953	0.460445	1.381975
C	-0.671183	-3.704005	-0.689338
H	-1.636874	-3.372776	-1.102320
H	0.059798	-3.806570	-1.508570
H	-0.806957	-4.702045	-0.223067

2-propanol

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TS″[24-25]

Ru	0.018871	-0.543247	-0.212488
P	-2.291963	0.003202	-0.029846
P	2.220601	0.048182	-0.018784
C	-2.714409	1.793379	-0.307503
C	-4.100500	-0.723882	4.237414
C	-4.917777	-0.884125	3.105697
C	-4.392801	-0.680314	1.818901
C	-3.525507	-0.838263	-1.139588
C	-4.252327	-0.148588	-2.134919
C	-5.113119	-0.847596	-2.999590
C	-5.262582	-2.238070	-2.879629
C	-4.542949	-2.935419	-1.892797
C	-3.676947	-2.243294	-1.034478
C	2.578528	1.875169	0.074928
C	-2.026631	2.524259	-1.304201
C	1.543808	2.819744	0.240607
C	1.836658	4.193621	0.314145
C	3.163924	4.639621	0.224636
C	4.203237	3.707189	0.055883
C	3.914052	2.337039	-0.021308
C	3.384854	-0.431109	-1.386698
C	2.922100	-0.290881	-2.715203
C	3.762843	-0.588014	-3.797980
C	5.076231	-1.033449	-3.570537
C	5.544457	-1.179285	-2.255213
C	-2.363019	3.862133	-1.568517
C	4.706533	-0.879465	-1.167363
C	3.073391	-0.580076	1.507957
C	3.304118	0.268484	2.615638
C	3.843341	-0.244076	3.807281
C	4.164739	-1.607051	3.910589
C	3.939629	-2.460205	2.816679
C	3.393648	-1.957547	1.624476
C	-3.381376	4.492188	-0.834342
C	-4.066665	3.778124	0.162960
C	-3.740268	2.436837	0.422041
C	-3.036844	-0.310731	1.646913
C	-2.224458	-0.151804	2.795018

C	-2.753649	-0.357539	4.079514
H	-4.146705	0.935755	-2.227837
H	-5.671047	-0.299430	-3.765469
H	-5.934170	-2.779112	-3.553299
H	-4.652786	-4.020136	-1.795134
H	-3.116748	-2.789361	-0.267746
H	-5.030500	-0.818884	0.941369
H	-5.967893	-1.170407	3.222576
H	-4.511868	-0.886873	5.238476
H	-2.109491	-0.232633	4.955680
H	-1.175092	0.135368	2.666555
H	-4.276438	1.885166	1.199682
H	-1.215190	2.040607	-1.857741
H	-1.820147	4.412315	-2.343562
H	-3.637252	5.537148	-1.035789
H	-4.858271	4.264096	0.742102
H	4.724575	1.618326	-0.173739
H	5.240660	4.047808	-0.021837
H	3.390373	5.709196	0.280369
H	1.019649	4.911457	0.438924
H	0.510271	2.468480	0.308684
H	1.893260	0.041758	-2.889143
H	5.072816	-1.011920	-0.145254
H	6.564687	-1.531320	-2.071246
H	3.388851	-0.478754	-4.820962
H	5.729196	-1.271571	-4.415987
H	3.200245	-2.629788	0.782195
H	3.069060	1.333801	2.539339
H	4.018471	0.428076	4.653633
H	4.589772	-2.002879	4.838365
H	4.189224	-3.523971	2.888074
H	0.055523	0.536273	1.015899
O	1.646930	-3.103745	-0.839105
C	0.693642	-2.430175	-0.457532
H	0.140842	0.599300	-1.294061
C	-0.363547	-1.961892	-2.065166
H	0.489273	-2.017005	-2.752642
H	-0.855024	-2.947511	-1.999958
H	-1.126465	-1.258750	-2.433577
C	-0.121185	-2.812981	0.822627
H	0.577959	-3.281162	1.530497
H	-0.604660	-1.954718	1.359055
H	-0.929334	-3.508416	0.547248

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TS"[28-29aperp]

Ru	0.025806	-0.295168	0.018142
P	2.274026	0.044904	0.015867
P	-2.253819	0.062531	0.015848
C	2.870874	1.800935	-0.328378
C	4.501972	-2.390131	-3.330992
C	3.590914	-1.366729	-3.650271
C	2.977251	-0.621678	-2.632611
C	3.326755	-0.238168	1.557160
C	2.697467	-0.695681	2.733268
C	3.437642	-0.900339	3.911330
C	4.818985	-0.651071	3.930812
C	5.457198	-0.184694	2.767050
C	4.717528	0.025823	1.592493
C	-3.277123	-0.481599	1.488790
C	2.157439	2.887540	0.226701
C	-2.658464	-0.522205	2.756910
C	-3.395318	-0.862318	3.902503
C	-4.762529	-1.171188	3.801281
C	-5.387443	-1.144347	2.543384
C	-4.651894	-0.801496	1.395668
C	-3.312969	-0.597994	-1.382484
C	-3.491854	-2.001131	-1.501346
C	-4.217614	-2.534225	-2.579178
C	-4.769981	-1.687026	-3.556022
C	-4.588814	-0.297947	-3.452285
C	2.599508	4.207095	0.043258
C	-3.867364	0.243912	-2.374142
C	-2.781140	1.870324	-0.056163
C	-3.984442	2.338215	0.521399
C	-4.354638	3.690434	0.420159
C	-3.534053	4.598953	-0.268888
C	-2.336206	4.147804	-0.848227
C	-1.959146	2.798526	-0.737569
C	3.757815	4.470306	-0.708794
C	4.469911	3.401558	-1.275485
C	4.034411	2.078276	-1.083382
C	3.278028	-0.872970	-1.268231
C	4.188221	-1.910199	-0.959901
C	4.792451	-2.661215	-1.984605
H	1.615681	-0.878104	2.696010
H	2.929444	-1.255307	4.814908
H	5.396872	-0.811596	4.847667
H	6.532951	0.023809	2.777158
H	5.215759	0.414397	0.699216
H	2.248080	0.159179	-2.877401
H	3.347964	-1.154616	-4.697225
H	4.972946	-2.976985	-4.126696
H	5.493925	-3.461879	-1.724846
H	4.429360	-2.122092	0.085975
H	4.585682	1.253020	-1.543643
H	1.234687	2.678688	0.778787
H	2.028894	5.032961	0.482423
H	4.097621	5.501034	-0.857812
H	5.368381	3.594464	-1.872683
H	-5.136848	-0.802059	0.414925
H	-6.449845	-1.397117	2.451551
H	-5.335421	-1.441408	4.695262
H	-2.894980	-0.897566	4.876741
H	-1.583237	-0.316608	2.813563
H	-3.018407	-2.644631	-0.747974
H	-3.735519	1.326805	-2.296642
H	-5.013247	0.371014	-4.209579
H	-4.344747	-3.619859	-2.657412
H	-5.334243	-2.107094	-4.396241
H	-1.014097	2.437013	-1.158081
H	-4.625933	1.638182	1.064465
H	-5.286804	4.032728	0.883597
H	-3.823099	5.652977	-0.347506
H	-1.683162	4.847699	-1.381291
H	0.003720	-0.614050	1.633482
H	0.001355	1.121971	0.788737
C	-0.271966	-2.387179	0.333527
O	-1.416981	-2.877902	0.560881
H	0.080373	0.689230	-1.366639
C	0.914206	-3.217377	0.890417
H	1.893788	-2.883108	0.511754
H	0.911434	-3.125295	1.989460
H	0.771176	-4.289366	0.645812
C	-0.005334	-2.147922	-1.487984
H	0.478036	-3.138465	-1.508874
H	-0.998996	-2.213330	-1.948383
H	0.656039	-1.502792	-2.088612