Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Validation of the Cossee-Arlman Mechanism for Propylene Oligomerization on Ni/UiO-66

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S1. Propylene Oligomerization Time on Stream, Selectivities, and Kinetics on Ni/UiO-66

Previously, we reported enhancements in rate on Ni/UiO-66 on-stream during ethylene oligomerization. This observation was attributed to the increase in the density of nickel sites upon exposing the catalyst to higher ethylene pressures.[1] We sought to determine if this phenomena occurred during propylene oligomerization to correctly normalize reaction rates. In Figure S1, the propylene pressure was increased from 5 kPa to 500 kPa and the pressure was returned to 5 kPa. No enhancement in rate was determined at 5 kPa after exposing the catalyst to higher propylene pressures (0 – 250 minutes and 750 – 1500 minutes) to suggest that nickel site densities do not increase after exposing the catalyst to high propylene pressures.

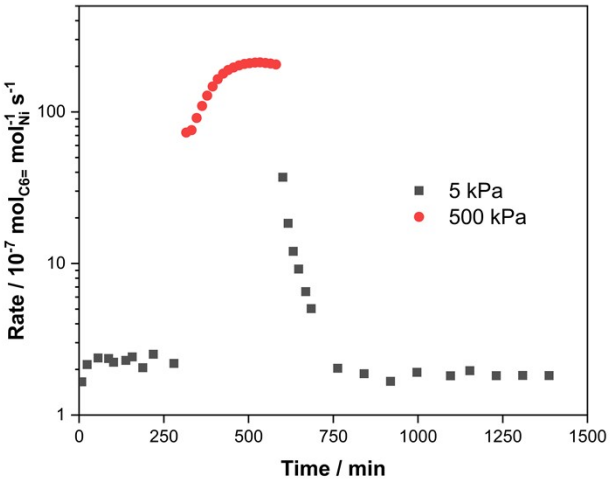


Figure S1: Time on stream after increasing propylene partial pressure from 5 kPa to 500 kPa and then decreasing the pressure back 5 kPa on Ni/UiO-66 at 473 K

Hexadiene formation is observed during the induction period and decreases with time on stream as hexene formation increases with time on stream before both reach steady state, as shown in Figure S2. This observation is consistent with in-situ generation of relevant nickel-hydride or nickel-alkyl intermediates required for the Cossee-Arlman mechanism.[1–4]

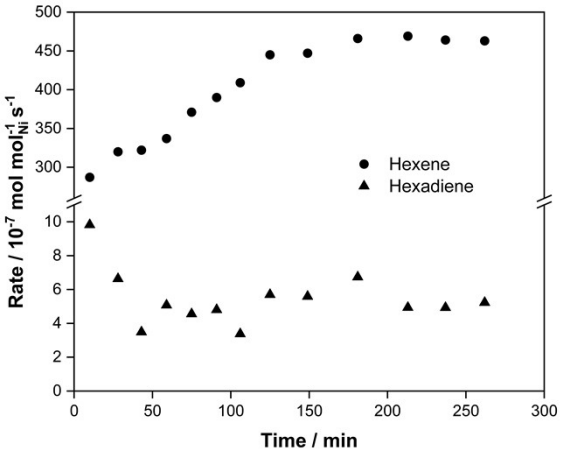


Figure S2: Time on stream showing hexene (●) and hexadiene (▲) formation on 80.6 mg of Ni/UiO-66 at 500 kPa of 0.83 cm^3 s^{-1} of propylene at 473 K.

The stability of Ni/UiO-66 was examined further by changing propylene partial pressures with time on stream on the same catalyst at 473 K. In Figure S3, the reaction rate decreases by ~10% with time on stream at 420 kPa initially (~0-6 ks). However, after changing the propylene partial pressure to 249 kPa, 331 kPa, and returning to 420 kPa (~6-24 ks), the reference pressure, the catalyst is stable at 420 kPa, with the reaction rate at 420 kPa ~30% lower than the initial rate at 420 kPa (~0-6 ks). The partial pressure of propylene was decreased to 331 kPa (~24-30 ks) which yielded reaction rates within 10% of the previous condition at 331 kPa. After increasing partial pressure of propylene back to 420 kPa (~30-36 ks), the rate was within 10% of the reaction rate at 420 kPa at ~21-24 ks. Subsequently, after changing partial pressures of propylene to 497 kPa and 177 kPa, the rates of reaction at the reference partial pressure of 420 kPa were within 10%. In this case, we consider that rates from ~15-42 ks to be steady state rates. We note that although the catalyst appears to be stable initially (Fig. 1 in the main text), changes in process conditions and returning to the same reference process conditions shows a decrease in the rate of reaction initially, and thus, is not the steady state rate for propylene oligomerization.

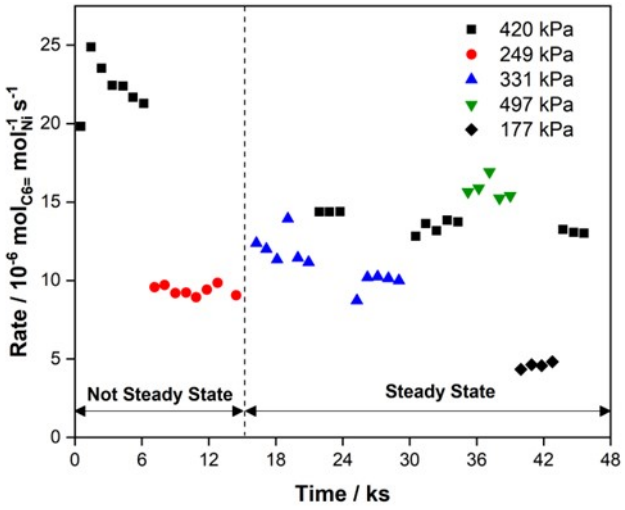


Figure S3: Propylene oligomerization rates as a function of time on stream on 18.2 mg of Ni/UiO-66 at 420 kPa (■), 249 kPa (●) 331 kPa (▲), 497 kPa (▼), and 177 kPa (◆) of 0.83 $cm^3\ s^{-1}$ of propylene at 473 K.

In Figure S4, no effect on oligomerization rates at 259 kPa and 473 K are observed with changes in propylene flowrate (0.17 – 0.83 $cm^3\ s^{-1}$) to suggest kinetics were not measured in the presence of external mass transfer limitations or product inhibition. We note that the rate decreases by ~10% over 700 minutes. The individual hexene product selectivities are tabulated in Table S1.

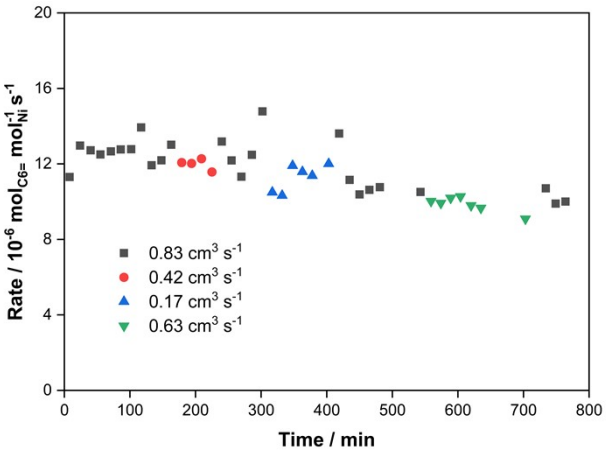


Figure S4: Time on stream after changing propylene flow rate (0.17 – 0.83 cm^3 s^{-1}) at 259 kPa and 473 K on 13.5 mg of Ni/UiO-66

Table S1: Individual hexene product selectivities at 259 kPa and 473 K at 0.002% conversion on Ni/UiO-66

Product	Selectivity / %
4-methyl-1-pentene	12.3
4-methyl-2-pentene	2.7
2,3-dimethyl-1-butene	6.1
2,3-dimethyl-2-butene	9.6
1-hexene	7.6
2-hexene	22.0
3-hexene	16.9
2-methyl-1-pentene	15.6
2-methyl-2-pentene	7.4

Rates of propylene oligomerization recorded at varying times-on-stream while changing temperature (453 - 493 K) at 259 kPa and 0.42 cm^3 s^{-1} propylene are shown in Figure S5. The rates decrease by <10% when returning the temperature back to the reference temperature (483 K). These data were used to extract the Arrhenius plot in Figure 3b in the main text.

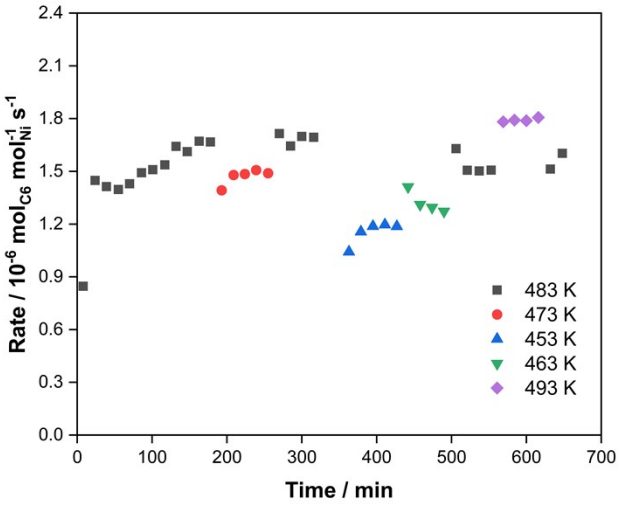


Figure S5: Time on stream with changes in temperature (453 – 493 K) on 259 kPa of 0.42 cm^3 s^{-1} of propylene on 18.8 mg of Ni/UiO-66

S2. Supplemental in-situ NO Titrations

In Figure S6 below, we present a supplemental in-situ NO titration at 500 kPa and 473 K on Ni/UiO-66 during propylene oligomerization This titration gives ~15 $\mu mol_{Ni}\ g_{cat}^{-1}$, which is in good agreement with the NO titration shown in Fig. 2 in the main text.

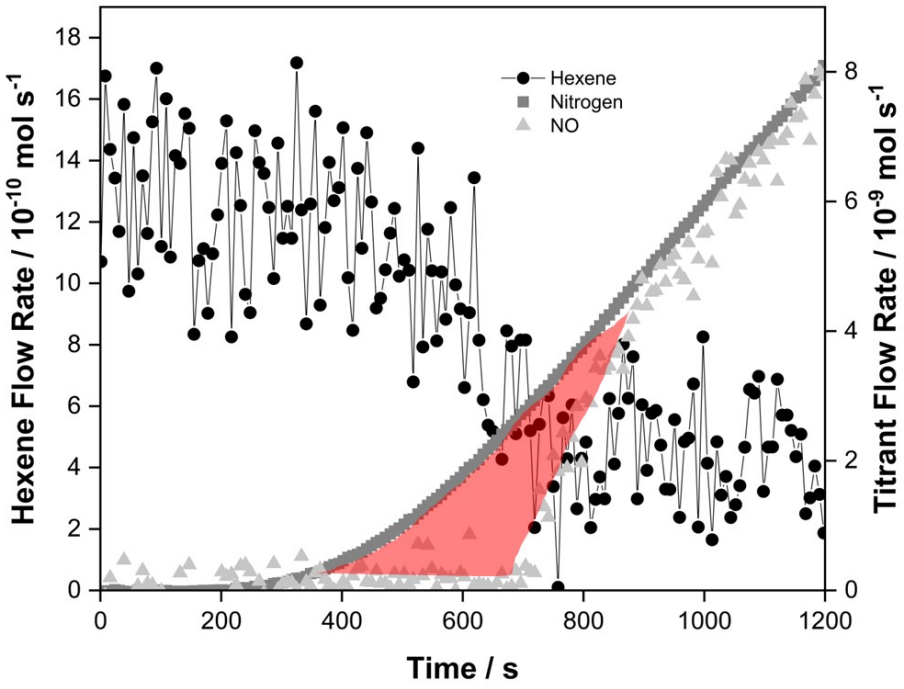


Figure S6: In situ NO titration showing a decrease in the rate of hexene formation (●) upon introduction of 0.083 $cm^3\ s^{-1}$ of 1% NO (▲, light grey) and 99% N_2 (■, dark gray) in 0.83 $cm^3\ s^{-1}$ at a total pressure of 500 kPa at 473 K on 80.6 mg of Ni/UiO-66. The amount of nickel titrated is calculated by integration of the red shaded area.

S3. Supplemental XAS Data

All XAS spectra were collected at beamline 9-3 at Stanford Synchrotron Radiation Light source (SSRL). All experiments were carried out in fluorescence mode with a passivated implanted planar silicon (PIPS) detector and with a water cooled double-crystal monochromator with Si (220) crystals. Six inch long, nitrogen-filled, ion chambers were used to measure the relative intensity of the X-ray beam before and after the sample, and before and after the reference foil. A foil located downbeam of the sample was used as an internal reference to calibrate the photon energy of each spectrum. For the *in-situ* measurements the as synthesized Ni/UiO-66 (~3 mg) was loaded in an *in-situ* XAS cell[5] forming an approximately 1 cm long catalyst bed located in between two quartz wool plugs inside the 1 mm OD, 0.96 mm ID, quartz capillary. Continuous extended X-ray absorption fine structure (EXAFS) spectra at the Ni-K edge (8333 eV) were collected for the as-synthesized sample in helium (0.33 $cm^3\ s^{-1}$) at ambient temperature. Continuous EXAFS spectra were collected while the temperature was ramped at 0.083 K s^{-1} until 573 K and held for 4 hours where continuous EXAFS spectra for the Ni-K edge were obtained. After 4 hours, the reactor was allowed to cool to reaction temperature (473 K) before propylene (0.17 $cm^3\ s^{-1}$) was introduced. Continuous EXAFS spectra were collected for 3 hours, where the catalyst was assumed to be at steady state (Figure 1 in the main text). Each continuous EXAFS spectrum took approximately 2 minutes to collect, and nine EXAFS spectra were merged to improve signal to noise.

The X-ray adsorption near edge structure (XANES) and EXAFS spectra are presented in Figures S7a and S7b, respectively, for Ni/UiO-66 as-synthesized, thermally treated, and during propylene oligomerization. The pre-edge feature at 8333 eV in the XANES spectrum that persists in Ni/UiO-66 in the thermally treated sample and reaction is consistent with the pre-edge feature from α-Ni-OH_2 to suggest that nickel remains in the 2+ oxidation state.[6]

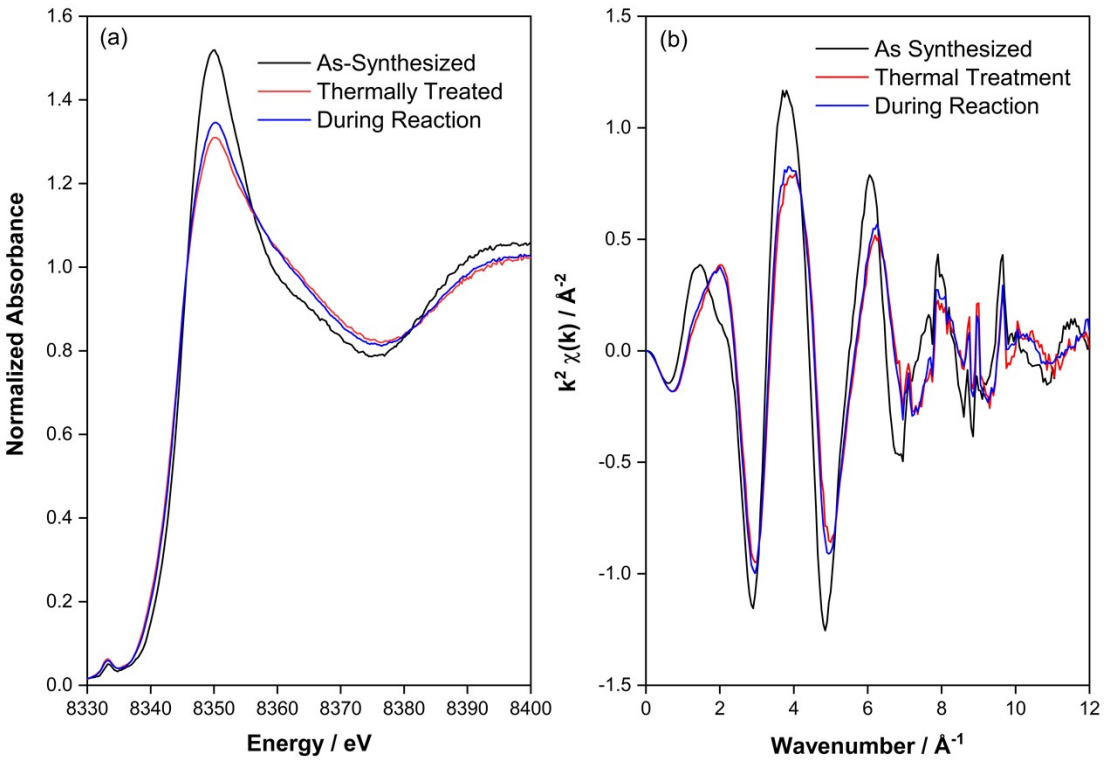
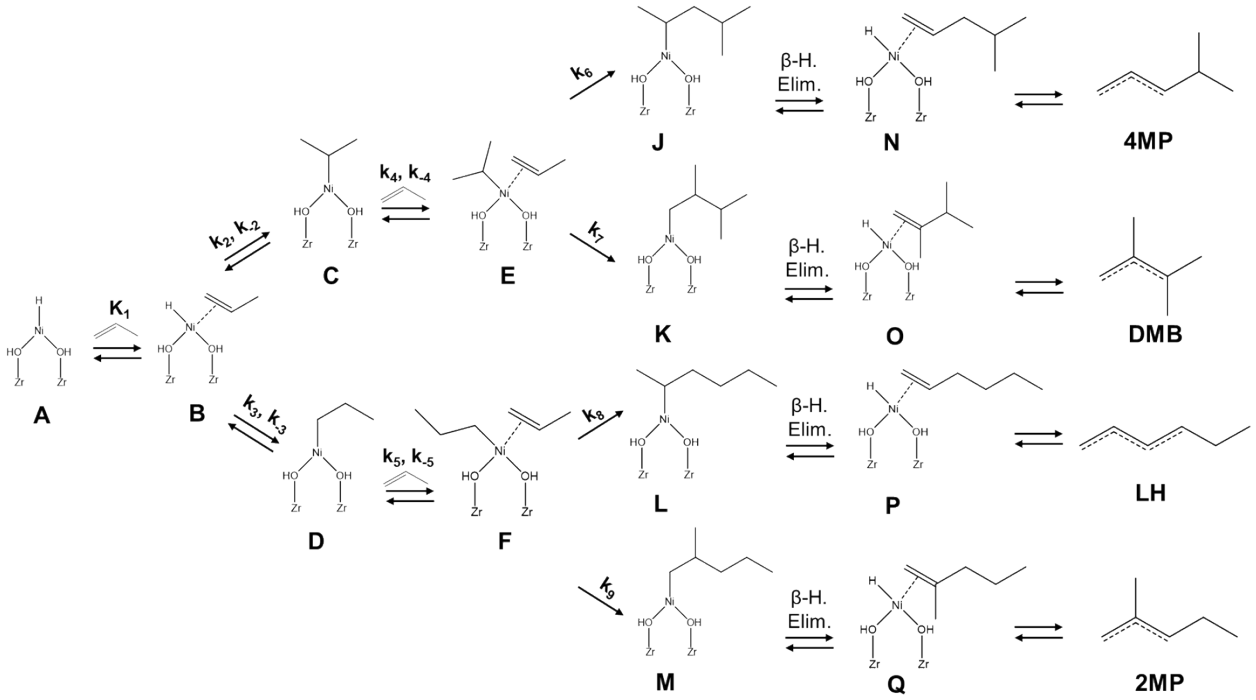


Figure S7: (a) XANES and (b) EXAFS data for Ni/UiO-66 as synthesized (black), after thermal treatment (red, 573 K, 0.33 $cm^3\ s^{-1}$ of helium) and during propylene oligomerization (blue, 473 K, 0.17 $cm^3\ s^{-1}$ of propylene)

S4. Cossee-Arlman and Metallacycle Mechanisms and Rate Expressions

The Cossee-Arlman has been proposed for olefin oligomerization and is shown in Scheme S1. The nomenclature is the same as the main text up until the Ni-hexyl species, and additional designation is made for Ni-hexyl species (**J**, **K**, **L**, and **M**) and the Ni-hydride species with the absorbed hexene product (**N**, **O**, **P**, and **Q**) for products **4MP**, **DMB**, **LH**, and **2MP**, respectively, in the Cossee-Arlman mechanism. This designation is made for identification of intermediates in Section S5.



Scheme S1: Cossee-Arlman mechanism for propylene oligomerization on Ni/UiO-66. Entire node omitted for clarity.

For the Cossee-Arlman mechanism, the rate limiting step is the olefin insertion step (k_6, k_7, k_8, and k_9).[2,6–10] Thus, the rate expressions are for **4MP**, **DMB**, **LH**, and **2MP** are shown below in Equations S1-S4

$$r_{4MP} = k_6[E] \qquad (Eq.\,S1)$$

$$r_{DMB} = k_7[E] \qquad (Eq.\,S2)$$

$$r_{LH} = k_8[F] \qquad (Eq.\,S3)$$

$$r_{2MP} = k_9[F] \qquad (Eq.\,S4)$$

The rate expressions for the products can be written in terms of propylene pressure by assuming that the first adsorption step is quasi-equilibrated and all other intermediates are at pseudo-steady state. Assuming species **E** and **F** are at steady state, the rate expression for **E** and **F** is shown in Equation S5 and S6, respectively, with the concentration of **E** and **F** solved for in terms of concentrations of species **C** and **D**, respectively, and propylene pressure, as shown in Equations S7 and S8.

$$r_E = 0 = k_4[C]\,P_{C_3H_6} - k_{-4}[E] - k_6[E] - k_7[E] \qquad (Eq.\,S5)$$

$$r_F = 0 = k_5[D]\,P_{C_3H_6} - k_{-5}[F] - k_8[F] - k_9[F] \qquad (Eq.\,S6)$$

$$[E] = \frac{k_4[C]P_{C_3H_6}}{k_{-4} + k_6 + k_7} \qquad (Eq.\,S7)$$

$$[F] = \frac{k_5[D]P_{C_3H_6}}{k_{-5} + k_8 + k_9} \qquad (Eq.\,S8)$$

The concentration of **C** and **D** can be solved for by assuming steady state on these species by solving the rate expressions shown in Equations S9 and S10, respectively. The concentrations of **C** and **D**, shown in Equations S11 and S12 respectively, are solved for by substituting Equations S7 and S8 into Equations S9 and S10, respectively.

$$r_C = \ 0 = k_2[B] - k_{-2}[C] + k_{-4}[E] - k_4[C]P_{C_3H_6} \qquad (Eq.\,S9)$$

$$r_D = \ 0 = k_3[B] - k_{-3}[D] + k_{-5}[F] - k_5[D]P_{C_3H_6} \qquad (Eq.\,S10)$$

$$[C] = \frac{k_2[B]}{k_{-2} - \dfrac{k_{-4}k_4P_{C_3H_6}}{k_{-4} + k_6 + k_7} + k_4P_{C_3H_6}} \qquad (Eq.\,S11)$$

$$[D] = \frac{k_3[B]}{k_{-3} - \dfrac{k_{-5}k_5P_{C_3H_6}}{k_{-5} + k_8 + k_9} + k_5P_{C_3H_6}} \qquad (Eq.\,S12)$$

The concentration of species **B** can be solved by assuming the first adsorption of the propylene molecule from **A** to **B** to be quasi-equilibrated, as shown in Equation S13.

$$[B] = K_1[A]P_{C_3H_6} \qquad (Eq.\,S13)$$

By substituting Equations S13, S11, and S7 into Equations S1 and S2 and by substituting Equations S13, S12, and S8 into Equations S3 and S4, the rate expressions for the hexene products for the Cossee-Arlman mechanism can be written in terms of propylene pressure and **A**, unoccupied nickel sites, as shown in Equations S14, S15, S16, and S17, for **4MP**, **DMB**, **LH**, and **2MP**.

$$r_{4MP} = \frac{k_6k_4k_2K_1[A]P_{C_3H_6}^{\ 2}}{(k_{-4} + k_6 + k_7)\left(k_{-2} - \dfrac{k_{-4}k_4P_{C_3H_6}}{k_{-4} + k_6 + k_7} + k_4P_{C_3H_6}\right)} \qquad (Eq.\,S14)$$

$$r_{DMB} = \frac{k_7 k_4 k_2 K_1 [A] P_{C_3H_6}^{\ 2}}{(k_{-4} + k_6 + k_7)\left(k_{-2} - \frac{k_{-4} k_4 P_{C_3H_6}}{k_{-4} + k_6 + k_7} + k_4 P_{C_3H_6}\right)} \qquad (Eq.\ S15)$$

$$r_{LH} = \frac{k_8 k_5 k_3 K_1 [A] P_{C_3H_6}^{\ 2}}{(k_{-5} + k_8 + k_9)\left(k_{-3} - \frac{k_{-5} k_5 P_{C_3H_6}}{k_{-5} + k_8 + k_9} + k_5 P_{C_3H_6}\right)} \qquad (Eq.\ S16)$$

$$r_{2MP} = \frac{k_9 k_5 k_3 K_1 [A] P_{C_3H_6}^{\ 2}}{(k_{-5} + k_8 + k_9)\left(k_{-3} - \frac{k_{-5} k_5 P_{C_3H_6}}{k_{-5} + k_8 + k_9} + k_5 P_{C_3H_6}\right)} \qquad (Eq.\ S17)$$

The ratio of selectivities for **4MP** to **DMB** and **LH** to **2MP**, shown in Equations S18 and S19, respectively, can be solved for by either dividing Equation S14 by S15 or dividing S1 by S2 and by either dividing Equation S16 by S17 or dividing S3 by S4, respectively.

$$S_{\frac{4MP}{DMB}} = \frac{k_6}{k_7} \qquad (Eq.\ S18)$$

$$S_{\frac{LH}{2MP}} = \frac{k_8}{k_9} \qquad (Eq.\ S19)$$

The ratio of selectivities for LH + 2MP to 4MP + DMB shown in Equation S22 can be solved for by adding Equations S16 and S17 and by adding S14 and S15, respectively, as shown in Equations S20 and S21, and dividing Equation S20 by S21. Equation S22 shows that if propylene oligomerization occurs via the Cossee-Arlman mechanism, the ratio of LH + 2MP to 4MP + DMB is pressure dependent.

$$r_{LH} + r_{2MP} = \frac{(k_8 + k_9) k_5 k_3 K_1 [A] P_{C_3H_6}^{\ 2}}{(k_{-5} + k_8 + k_9)\left(k_{-3} - \frac{k_{-5} k_5 P_{C_3H_6}}{k_{-5} + k_8 + k_9} + k_5 P_{C_3H_6}\right)} \qquad (Eq.\ S20)$$

$$r_{4MP} + r_{DMB} = \frac{(k_6 + k_7) k_4 k_2 K_1 [A] P_{C_3H_6}^{\ 2}}{(k_{-4} + k_6 + k_7)\left(k_{-2} - \frac{k_{-4} k_4 P_{C_3H_6}}{k_{-4} + k_6 + k_7} + k_4 P_{C_3H_6}\right)} \qquad (Eq.\ S21)$$

$$S_{\frac{(LH+2MP)}{(4MP+DMB)}} = \frac{\left(k_{-2} - \frac{k_{-4}k_4 P_{C_3H_6}}{k_{-4}+k_6+k_7} + k_4 P_{C_3H_6}\right)}{\left(k_{-3} - \frac{k_{-5}k_5 P_{C_3H_6}}{k_{-5}+k_8+k_9} + k_5 P_{C_3H_6}\right)} * \frac{(k_8+k_9)k_5k_3(k_{-4}+k_6+k_7)}{(k_6+k_7)k_4k_2(k_{-5}+k_8+k_9)} \quad (Eq.\ S22)$$

The individual product selectivity expressions for 4MP, DMB, LH, and 2MP in Equations S23-S26 can be determined from Equations S14-S17

$$s_{4MP} = \frac{\dfrac{k_6k_4k_2K_1[A]P_{C_3H_6}^2}{(k_{-4}+k_6+k_7)\left(k_{-2} - \frac{k_{-4}k_4P_{C_3H_6}}{k_{-4}+k_6+k_7} + k_4P_{C_3H_6}\right)}}{\dfrac{(k_6+k_7)k_4k_2K_1[A]P_{C_3H_6}^2}{(k_{-4}+k_6+k_7)\left(k_{-2} - \frac{k_{-4}k_4P_{C_3H_6}}{k_{-4}+k_6+k_7} + k_4P_{C_3H_6}\right)} + \dfrac{(k_8+k_9)k_5k_3K_1[A}{(k_{-5}+k_8+k_9)\left(k_{-3} - \frac{k_{-5}k}{k_{-5}+}\right.}}$$

$$s_{DMB} = \frac{\dfrac{k_7k_4k_2K_1[A]P_{C_3H_6}^2}{(k_{-4}+k_6+k_7)\left(k_{-2} - \frac{k_{-4}k_4P_{C_3H_6}}{k_{-4}+k_6+k_7} + k_4P_{C_3H_6}\right)}}{\dfrac{(k_6+k_7)k_4k_2K_1[A]P_{C_3H_6}^2}{(k_{-4}+k_6+k_7)\left(k_{-2} - \frac{k_{-4}k_4P_{C_3H_6}}{k_{-4}+k_6+k_7} + k_4P_{C_3H_6}\right)} + \dfrac{(k_8+k_9)k_5k_3K_1[A}{(k_{-5}+k_8+k_9)\left(k_{-3} - \frac{k_{-5}k}{k_{-5}+}\right.}}$$

$$s_{LH} = \frac{\dfrac{k_8k_5k_3K_1[A]P_{C_3H_6}^2}{(k_{-5}+k_8+k_9)\left(k_{-3} - \frac{k_{-5}k_5P_{C_3H_6}}{k_{-5}+k_8+k_9} + k_5P_{C_3H_6}\right)}}{\dfrac{(k_6+k_7)k_4k_2K_1[A]P_{C_3H_6}^2}{(k_{-4}+k_6+k_7)\left(k_{-2} - \frac{k_{-4}k_4P_{C_3H_6}}{k_{-4}+k_6+k_7} + k_4P_{C_3H_6}\right)} + \dfrac{(k_8+k_9)k_5k_3K_1[A}{(k_{-5}+k_8+k_9)\left(k_{-3} - \frac{k_{-5}k}{k_{-5}+}\right.}}$$

$$s_{2MP} = \frac{\dfrac{k_8 k_5 k_3 K_1 [A] P_{C_3H_6}^{\,2}}{(k_{-5} + k_8 + k_9)\left(k_{-3} - \dfrac{k_{-5} k_5 P_{C_3H_6}}{k_{-5} + k_8 + k_9} + k_5 P_{C_3H_6}\right)}}{\dfrac{(k_6 + k_7) k_4 k_2 K_1 [A] P_{C_3H_6}^{\,2}}{(k_{-4} + k_6 + k_7)\left(k_{-2} - \dfrac{k_{-4} k_4 P_{C_3H_6}}{k_{-4} + k_6 + k_7} + k_4 P_{C_3H_6}\right)} + \dfrac{(k_8 + k_9) k_5 k_3 K_1 [A}{(k_{-5} + k_8 + k_9)\left(k_{-3} - \dfrac{k_{-5} k}{k_{-5} +}\right.}}$$

Using the parameters α, β, γ, δ and ε from the main text and defined below in Equations S27-S31, Equations S23-S26 can be simplified, as shown in Equations S32-S35.

$$\alpha = k_{-2} \qquad (Eq.S27)$$

$$\beta = k_{-3} \qquad (Eq.S28)$$

$$\gamma = k_4 - \frac{k_{-4} k_4}{k_{-4} + k_6 + k_7} \qquad (Eq.S29)$$

$$\delta = k_5 - \frac{k_{-5} k_5}{k_{-5} + k_8 + k_9} \qquad (Eq.S30)$$

$$\varepsilon = \frac{(k_8 + k_9) k_5 k_3 (k_{-4} + k_6 + k_7)}{(k_6 + k_7) k_4 k_2 (k_{-5} + k_8 + k_9)} \qquad (Eq.S31)$$

$$s_{4MP} = \frac{\dfrac{k_6}{k_6 + k_7}(\beta + \delta P_{C_3H_6})}{\varepsilon\left(\alpha + \gamma P_{C_3H_6}\right) + (\beta + \delta P_{C_3H_6})} \qquad (Eq.S32)$$

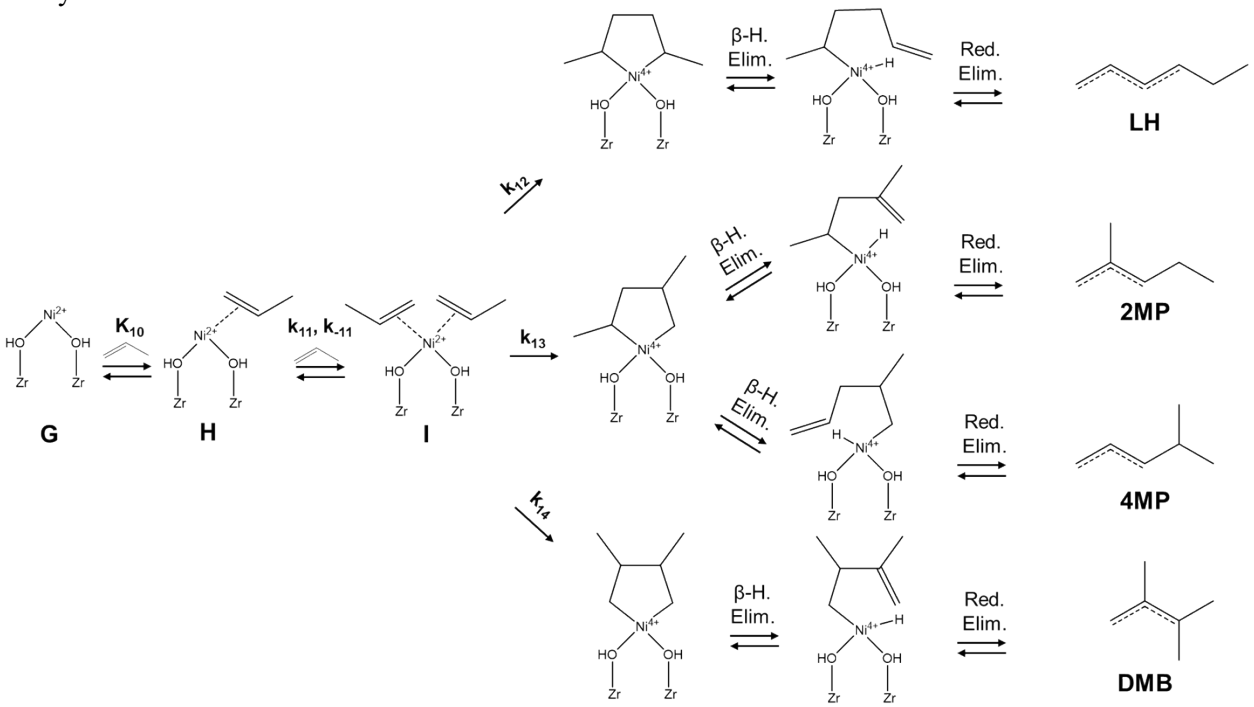
$$s_{DMB} = \frac{\dfrac{k_7}{k_6 + k_7}(\beta + \delta P_{C_3H_6})}{\varepsilon\left(\alpha + \gamma P_{C_3H_6}\right) + (\beta + \delta P_{C_3H_6})} \qquad (Eq.S33)$$

$$s_{LH} = \frac{\dfrac{k_8}{k_8 + k_9}\left(\alpha + \gamma P_{C_3H_6}\right)}{\left(\alpha + \gamma P_{C_3H_6}\right) + \dfrac{1}{\varepsilon}(\beta + \delta P_{C_3H_6})} \qquad (Eq.S34)$$

$$s_{2MP} = \frac{\dfrac{k_9}{k_8 + k_9}\left(\alpha + \gamma P_{C_3H_6}\right)}{\left(\alpha + \gamma P_{C_3H_6}\right) + \dfrac{1}{\varepsilon}(\beta + \delta P_{C_3H_6})} \qquad (Eq.S35)$$

From Equations S32-S35, the individual product selectivities for 4MP, DMB, LH, and 2MP are a function of propylene pressure. This is consistent with Figure 4 in the main text where the individual product selectivities of 4MP, DMB, LH, and 2MP are a function of propylene pressure.

While the Cossee-Arlman mechanism has been proposed for olefin oligomerization, the metallacycle mechanism, as shown in Scheme S2, has also been proposed for olefin oligomerization on nickel-based catalyst.



Scheme 2: Metallacycle mechanism for propylene oligomerization on Ni/UiO-66. Entire node omitted for clarity.

The kinetically relevant step in the metallacycle mechanism is the oxidative coupling step (k_{12}, k_{13}, and k_{14}).[2,6,7] The rate expressions for products **4MP**, **DMB**, **LH**, and **2MP** for the metallacycle mechanism are shown in Equations S36-S39.

$$r_{4MP} = k_{13}[I] \qquad (Eq.\,S36)$$

$$r_{DMB} = k_{14}[I] \qquad (Eq.\,S37)$$

$$r_{LH} = k_{12}[I] \qquad (Eq.\,S38)$$

$$r_{2MP} = k_{13}[I] \qquad (Eq.\,S39)$$

The rate expressions for the products can be written in terms of propylene pressure by assuming that the first adsorption step is quasi-equilibrated, and all other intermediates are at pseudo-steady state. Assuming that species **I** is at pseudo-steady state (Equation S40), the concentration of **I** can be solved for as shown in Equation S41.

$$r_I = 0 = k_{11}[H]P_{C_3H_6} - k_{-11}[I] - k_{12}[I] - k_{13}[I] - k_{14}[I] \qquad (Eq.\,S40)$$

$$[I] = \frac{k_{11}[H]P_{C_3H_6}}{k_{-11} + k_{12} + k_{13} + k_{14}} \qquad (Eq.S41)$$

The concentration of species **H** can be solved by assuming the first adsorption of the propylene molecule from **G** to **H** to be quasi-equilibrated, as shown in Equation S42.

$$[H] = K_{10}[G]P_{C_3H_6} \qquad (Eq.S42)$$

By substituting Equations S41 and S42 into Equations S36-S39, the rate expressions for the hexene products for the metallacycle mechanism can be written in terms of propylene pressure and **G**, unoccupied nickel sites, as shown in Equations S43, S44, S45, and S46, for **4MP**, **DMB**, **LH**, and **2MP**.

$$r_{4MP} = k_{13}[I] = \frac{k_{13}k_{11}K_{10}[G]P_{C_3H_6}^2}{k_{-11} + k_{12} + k_{13} + k_{14}} \qquad (Eq.S43)$$

$$r_{DMB} = k_{14}[I] = \frac{k_{14}k_{11}K_{10}[G]P_{C_3H_6}^2}{k_{-11} + k_{12} + k_{13} + k_{14}} \qquad (Eq.S44)$$

$$r_{LH} = k_{12}[I] = \frac{k_{12}k_{11}K_{10}[G]P_{C_3H_6}^2}{k_{-11} + k_{12} + k_{13} + k_{14}} \qquad (Eq.S45)$$

$$r_{2MP} = k_{13}[I] = \frac{k_{13}k_{11}K_{10}[G]P_{C_3H_6}^2}{k_{-11} + k_{12} + k_{13} + k_{14}} \qquad (Eq.S46)$$

The ratio of selectivities for the metallacycle mechanism can be found by either dividing any of the rate expressions from Equations S36-S39 by one other or dividing any of the rate expressions from Equations S43-S46 by one another. This yields ratios of selectivities that are solely a function of rate constants. This arises from **4MP**, **DMB**, **LH**, and **2MP** originating from the same intermediates, and the ratio of selectivities comes from the kinetically relevant olefin insertion step, where the metallacycle mechanism branches off. The ratio of **LH** + **2MP** to **4MP** + **DMB** for the metallacycle mechanism is shown in Equation S47.

$$S_{\frac{(LH+2MP)}{(4MP+DMB)}} = \frac{k_{12} + k_{13}}{k_{13} + k_{14}} \qquad (Eq.S47)$$

The selectivity expressions shown in Equations S48-S51 derived from the metallacycle mechanism for **4MP**, **DMB**, **LH**, and **2MP** from the rate expressions shown in Equations S43-S46.

$$s_{4MP} = \frac{k_{13}}{k_{12} + 2k_{13} + k_{14}} \qquad (Eq.S48)$$

$$s_{DMB} = \frac{k_{14}}{k_{12} + 2k_{13} + k_{14}} \qquad (Eq.S49)$$

$$s_{LH} = \frac{k_{12}}{k_{12} + 2k_{13} + k_{14}} \qquad (Eq.S50)$$

$$s_{2MP} = \frac{k_{13}}{k_{12} + 2k_{13} + k_{14}} \qquad (Eq.S51)$$

In contrast to the pressure-dependent ratio of selectivities in Equation S22 and selectivity expressions in Equation S32-S35, the ratio of selectivities shown in Equation S47 and selectivity expressions in Equations S48-S51 are pressure-independent. Observations from Figures 4 and 5 in the main text suggest that propylene oligomerization does not proceed via the metallacycle mechanism on Ni/UiO-66.

The curvature of the ratio of product selectivities described in Equation S22 or Equation 20 in the main text is determined by the parameters α, β, γ, and δ (Equations 13-17 in the main text). By taking the first derivative of Equation 20 as shown in Equation S52, an increase in the ratio of **LH** and **2MP** to **4MP** and **DMB** arises when the product of β and γ is greater than the product of α and δ and a decrease in the ratio of **LH** and **2MP** to **4MP** and **DMB** arises when the product of β and γ is less than the product of α and δ.

$$\frac{d}{dP_{C_3H_6}}\left(\frac{\left(\alpha + \gamma\, P_{C_3H_6}\right)}{\left(\beta + \delta\, P_{C_3H_6}\right)} * \varepsilon\right) = \frac{(\beta * \gamma - \alpha * \delta)}{\left(\beta + \delta\, P_{C_3H_6}\right)^2} * \varepsilon \qquad (Eq.S52)$$

S5. Supplemental DFT Calculations

The enthalpy and free energy diagrams for **4MP**, **DMB**, **LH**, and **2MP** for the Cossee-Arlman mechanism (Scheme S1) are shown in Figures S8-S11, respectively. In all cases, the kinetically relevant step for each hexene product is the olefin insertion step with free energies ranging from 88 kJ mol^{-1} to 143 kJ mol^{-1}. The apparent activation energy for each hexene product is calculated from the difference in enthalpy between the nickel-propyl species and the kinetically relevant olefin insertion step. A comparison of apparent activation energies from experiment and computation are tabulated in Table S2. The differences in the calculated energy barriers and those from experiment are 5-27 kJ mol^{-1} and are within the range of 8-23 kJ mol^{-1}, consistent with differences in experimental and computed enthalpy barriers found in olefin oligomerization on Ni/UiO-66 and Ni/NU-1000 MOF materials using the M06L functional.[1,6,9] Electronic energy, enthalpy, and Gibbs free energy (hartree) for all intermediates and TS structures for species in Scheme S1 are reported in Table S3. The spin state in all species is in the singlet spin state (2S+1 = 0) based on previous calculations on Ni/UiO-66.[1,6]

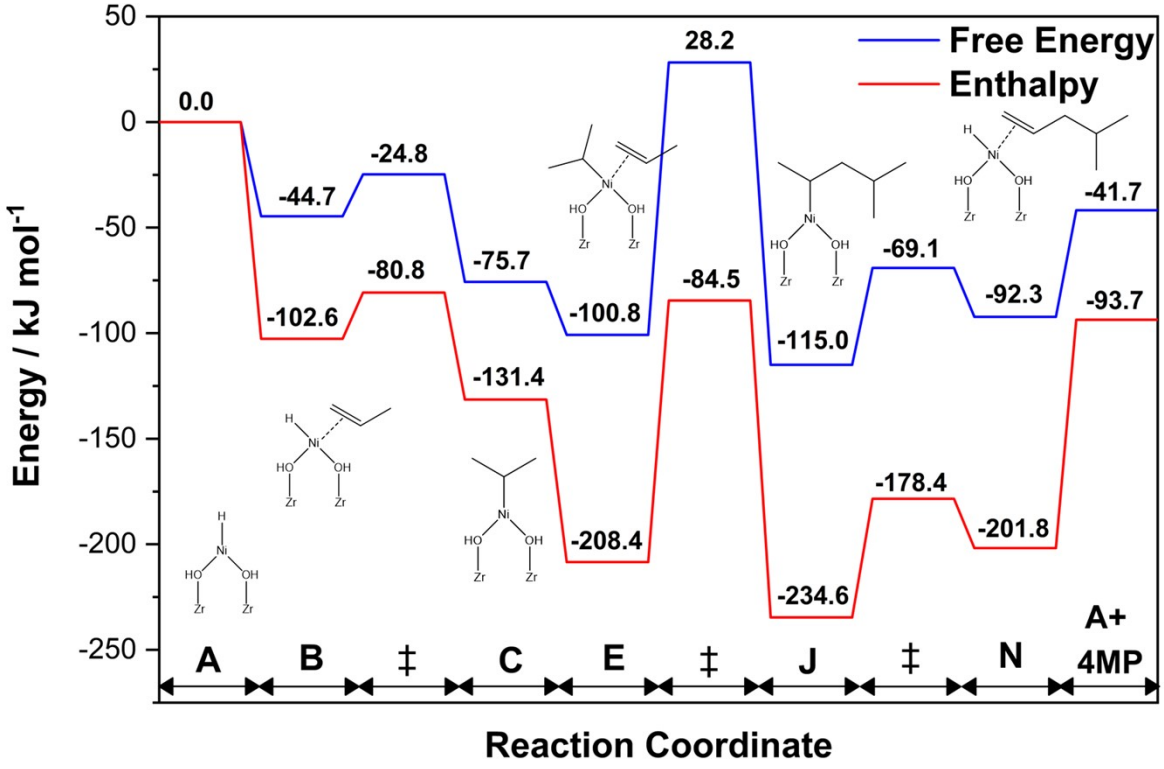


Figure S8: Free energy (blue) and enthalpy (red) diagram for **4MP** following the Cossee-Arlman mechanism on cluster models during propylene oligomerization of Ni/UiO-66 at 101.3 kPa and 298 K.

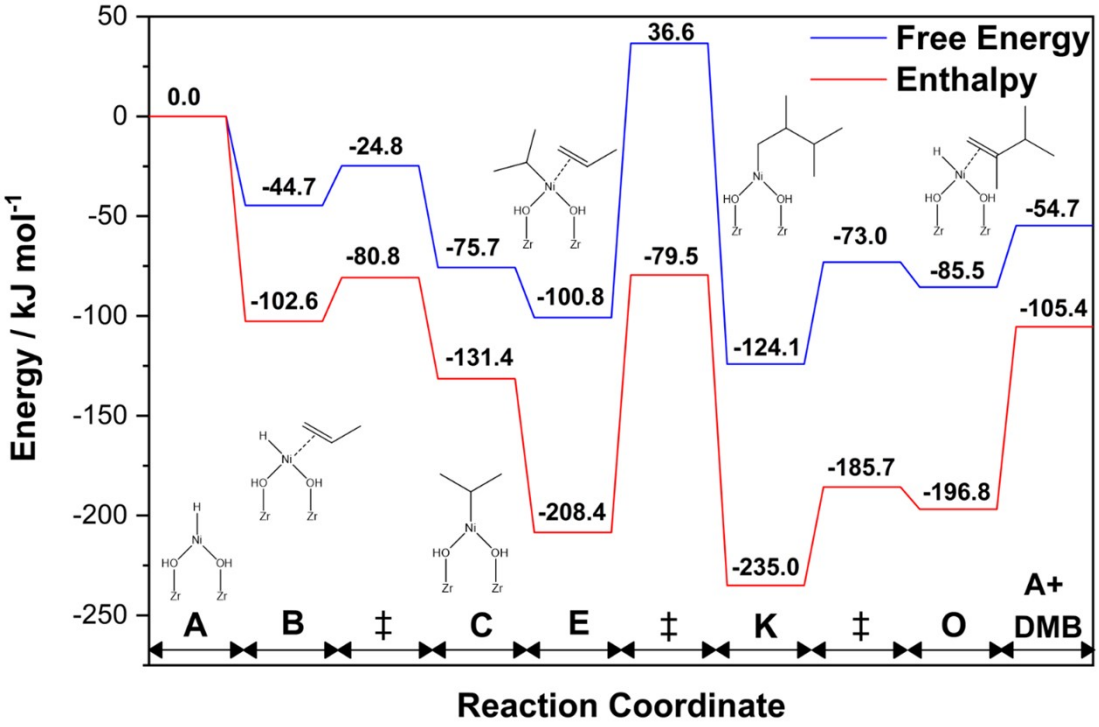


Figure S9: Free energy (blue) and enthalpy (red) diagram for **DMB** following the Cossee-Arlman mechanism on cluster models during propylene oligomerization of Ni/UiO-66 at 101.3 kPa and 298 K.

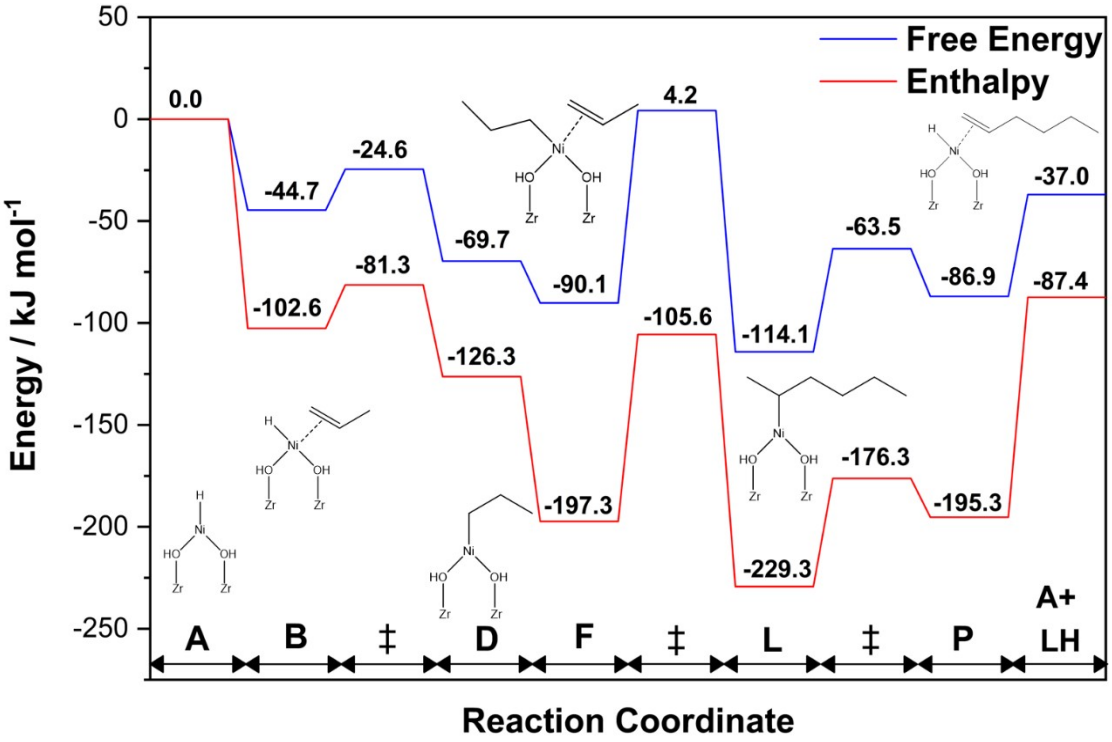


Figure S10: Free energy (blue) and enthalpy (red) diagram for **LH** following the Cossee-Arlman mechanism on cluster models during propylene oligomerization of Ni/UiO-66 at 101.3 kPa and 298 K.

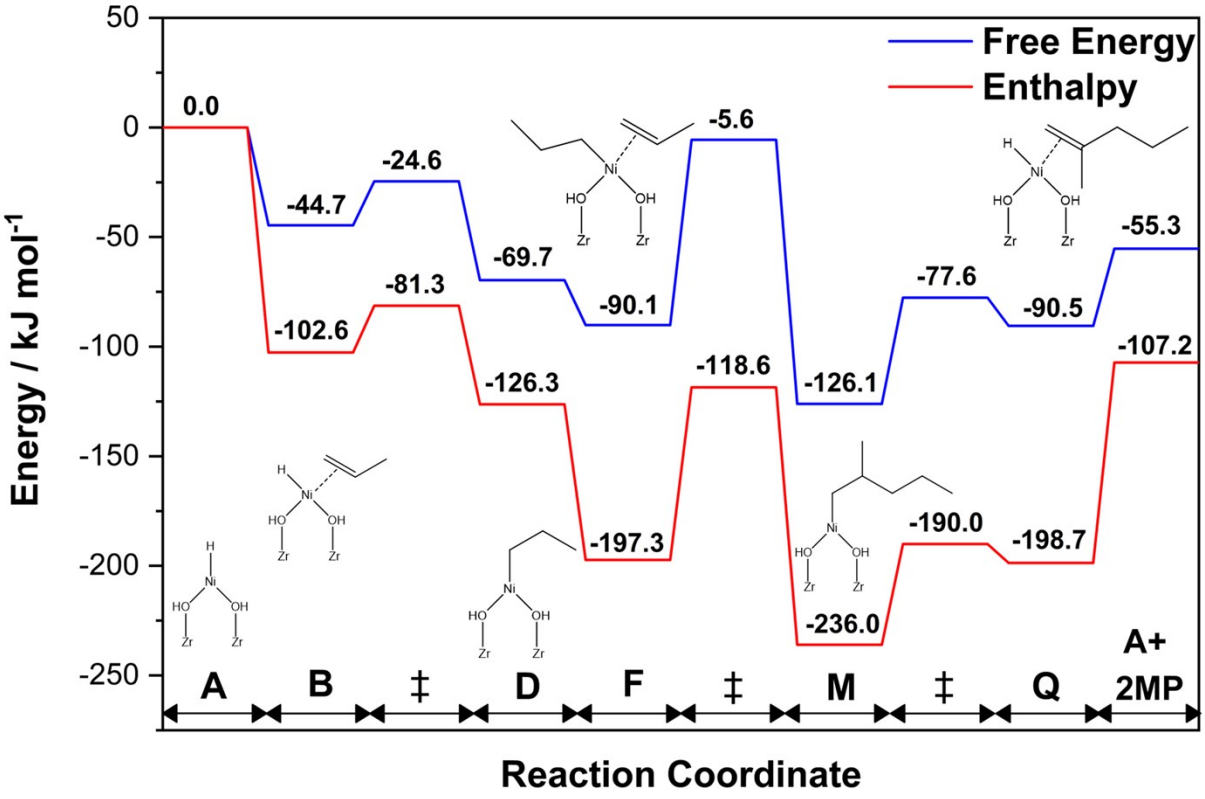


Figure S11: Free energy (blue) and enthalpy (red) diagram for **2MP** following the Cossee-Arlman mechanism on cluster models during propylene oligomerization of Ni/UiO-66 at 101.3 kPa and 298 K.

Table S2: Apparent activation energies from experiment and DFT for 4MP, DMB, LH, and 2MP on Ni/UiO-66 during propylene oligomerization at 259 kPa.

Hexene Product	Experimental Activation Energy / kJ mol^{-1}	Computed Activation Energy / kJ mol^{-1}
4MP	21.0 ± 3.4	46.9
DMB	24.6 ± 3.8	51.9
LH	15.7 ± 2.2	20.7
2MP	17.5 ± 2.8	7.7

Table S3: Electronic energy, enthalpy, and Gibbs free energy (hartree) for all intermediates and transition state TS structures for the Cossee-Arlman mechanism in Scheme S1 at 298 K and 101.3 kPa. The relative enthalpies and free energies (kJ mol^{-1}) with respect to **A** and two propylene molecules are reported.

Structure	E / hartree	H / hartree	G / hartree	△H / kJ mol^{-1}	△G / kJ mol^{-1}
Propylene	-117.71998	-117.714938	-117.744969	-	-
4MP	-235.4743	-235.465555	-235.505839	-	-
DMB	-235.47893	-235.470026	-235.510782	-	-
LH	-235.472	-235.463178	-235.504029	-	-
2MP	-235.47948	-235.470712	-235.51099	-	-
Production of 4-methylpentenes (4MP)					
A	-4627.5525	-4627.494089	-4627.632369	0.0	0.0
B	-4745.3099	-4745.248111	-4745.394354	-102.6	-44.7
B to C TS	-4745.3025	-4745.239784	-4745.386784	-80.8	-24.8
C	-4745.3219	-4745.259092	-4745.406182	-131.4	-75.7
E	-4863.0708	-4863.00334	-4863.160706	-208.4	-100.8
E to J TS	-4863.0229	-4862.956152	-4863.111564	-84.5	28.2
J	-4863.0777	-4863.011623	-4863.166105	-203.7	-115.0
J to N TS	-4863.0587	-4862.991937	-4863.148625	-178.5	-69.1
N	-4863.0677	-4863.000829	-4863.157453	-201.83	-92.3
A + 4MP	-4863.0268	-4862.959644	-4863.138208	-93.7	-41.7
A	-4627.552	-4627.4941	-4627.632	0.0	0
B	-4745.31	-4745.2481	-4745.394	-102.6	-44.7
B to C TS	-4745.302	-4745.2398	-4745.387	-80.8	-24.8
C	-4745.322	-4745.2591	-4745.406	-131.4	-75.7
E	-4863.071	-4863.0033	-4863.161	-208.4	-100.8
E to K TS	-4863.021	-4862.9542	-4863.108	-79.5	36.6
K	-4863.08	-4863.0135	-4863.17	-235.0	-124.1
Kto O TS	-4863.061	-4862.9947	-4863.15	-185.7	-73.0
O	-4863.066	-4862.9989	-4863.155	-196.8	-85.5
A + DMB	-4863.031	-4862.9641	-4863.143	-105.4	-54.7
Production of linear hexenes (LH)					
A	-4627.5525	-4627.494	-4627.632369	0	0.0
B	-4745.3099	-4745.248	-4745.394354	-102.6	-44.7
B to D TS	-4745.3026	-4745.24	-4745.3867	-81.3	-24.6
D	-4745.3198	-4745.257	-4745.403871	-126.3	-69.7
F	-4863.0665	-4862.999	-4863.156638	-197.3	-90.1
F to L TS	-4863.031	-4862.964	-4863.120695	-105.6	4.2
L	-4863.0759	-4863.009	-4863.165782	-223.4	-114.1
L to P TS	-4863.0575	-4862.991	-4863.146506	-176.3	-63.5
P	-4863.0652	-4862.998	-4863.155421	-195.3	-86.9
A + LH	-4863.0245	-4862.957	-4863.136398	-87.4	-37.0
Production of 2-methylpentenes (2MP)					
A	-4627.55	-4627.4941	-4627.63	0	0.0
B	-4745.31	-4745.2481	-4745.39	-102.6	-44.7
B to D TS	-4745.3	-4745.24	-4745.39	-81.3	-24.6
D	-4745.32	-4745.2571	-4745.4	-126.3	-69.7
F	-4863.07	-4862.9991	-4863.16	-197.3	-90.1
F to M TS	-4863.04	-4862.9691	-4863.12	-118.6	-5.6

M	-4863.08	-4863.0139	-4863.17	-236.0	-126.1
M to Q TS	-4863.06	-4862.9963	-4863.15	-190.0	-77.6
Q	-4863.07	-4862.9996	-4863.16	-198.7	-90.5
A + 2MP	-4863.03	-4862.9648	-4863.14	-107.2	-55.3

S6. Atomic Coordinates

A

C	-1.248539	-33.130699	-23.059703
C	3.414473	-27.919858	-17.352661
C	3.091481	-32.678955	-23.546704
C	3.883483	-32.285010	-17.224719
C	-1.743494	-28.525194	-23.194700
C	-1.165504	-28.398058	-16.837658
C	1.489575	-34.960051	-20.155870
C	5.485462	-30.003967	-20.616767
C	2.595477	-28.072968	-23.681697
C	0.524550	-25.989960	-20.416891
C	-0.697582	-32.762857	-16.710698
H	1.545927	-33.156253	-18.161364
H	0.951871	-27.622082	-18.324780
H	3.588250	-30.261189	-22.464098
O	2.997591	-27.742711	-22.537749
O	-0.935123	-29.405332	-23.612411
O	-0.183737	-29.124108	-16.538688
O	2.145713	-31.917767	-23.881217
O	2.975585	-31.545982	-16.762759
O	5.044475	-31.181173	-20.553849
O	-0.527229	-26.648100	-20.220190
O	2.534823	-34.272086	-20.284486
O	-3.015238	-29.276688	-19.788256
O	4.041527	-32.609992	-18.431417
O	-1.571144	-28.105649	-17.987965
O	3.545674	-32.850076	-22.387442
O	-1.886014	-28.152597	-22.012997
O	1.833565	-29.034825	-23.964646
O	2.682571	-28.808213	-16.843533
O	-0.639695	-32.126821	-23.532845
O	0.105516	-31.828774	-16.460343
O	-2.671045	-32.469108	-19.690955
O	1.692621	-26.446852	-20.514276
O	0.320787	-34.529933	-19.991753
O	4.804273	-28.945625	-20.619207
O	-1.022987	-33.202559	-17.839465
O	3.505759	-27.637715	-18.576923
O	-1.320032	-33.452773	-21.856742
O	0.953706	-28.419781	-18.861636
O	2.860715	-30.321892	-21.838456
O	1.382993	-32.409359	-18.744567
O	-1.386471	-30.760785	-21.275778
O	1.045924	-31.956238	-21.215613
O	2.586429	-30.277287	-19.337285
O	-0.346865	-30.583598	-19.023740
O	0.735326	-29.076229	-21.300767

Zr	-0.955854	-28.837915	-20.045433
Zr	-0.564509	-32.475293	-19.938677
Zr	2.584572	-28.519090	-20.457745
Zr	0.765754	-30.572962	-22.714893
Zr	1.274988	-30.370604	-17.713509
Zr	2.965809	-32.058324	-20.353700
H	-1.768739	-33.780795	-23.794711
H	1.614153	-36.063145	-20.183753
H	3.576646	-33.255316	-24.362474
H	-1.161458	-33.260558	-15.831792
H	-1.728629	-27.958462	-15.986191
H	0.412482	-24.888941	-20.507977
H	2.951897	-27.455499	-24.533021
H	4.036481	-27.321574	-16.654086
H	6.587821	-29.887466	-20.682225
H	4.613951	-32.696352	-16.496656
H	-2.385947	-28.044943	-23.962941
H	-3.484784	-28.886585	-19.044377
H	-3.049213	-32.903365	-18.919950
Ni	-3.637623	-30.981802	-20.498400
H	-5.171412	-31.143872	-20.360411
H	-1.813659	-30.829964	-22.138087

B

C	-1.248611	-33.130685	-23.059805
C	3.414480	-27.919953	-17.352701
C	3.091479	-32.678930	-23.546596
C	3.883493	-32.285001	-17.224641
C	-1.743627	-28.525031	-23.194664
C	-1.165541	-28.397672	-16.837791
C	1.489630	-34.960049	-20.155927
C	5.485466	-30.003978	-20.616673
C	2.595492	-28.073039	-23.681651
C	0.524521	-25.989952	-20.417018
C	-0.697400	-32.763289	-16.710600
H	1.530786	-33.152607	-18.160781
H	0.938108	-27.627881	-18.322926
H	3.562296	-30.263819	-22.476948
O	3.004258	-27.739565	-22.538406
O	-0.911429	-29.361119	-23.645150
O	-0.184112	-29.117851	-16.531883
O	2.140867	-31.924044	-23.874529
O	2.973151	-31.548395	-16.761461
O	5.045176	-31.180903	-20.553892
O	-0.526551	-26.647753	-20.215306
O	2.537017	-34.275499	-20.279437
O	-3.136103	-29.052381	-19.838501
O	4.041156	-32.610558	-18.430206
O	-1.573526	-28.106663	-17.988979

O	3.553077	-32.851347	-22.387782
O	-1.862932	-28.158610	-22.007450
O	1.827380	-29.029363	-23.958287
O	2.679482	-28.806084	-16.842206
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O	0.108436	-31.836524	-16.452094
O	-2.745115	-32.687333	-19.717043
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O	0.321490	-34.528927	-19.988013
O	4.805047	-28.945777	-20.619873
O	-1.027770	-33.198636	-17.841324
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O	1.375860	-32.404880	-18.745053
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O	1.061601	-31.972164	-21.205714
O	2.580178	-30.277708	-19.336159
O	-0.397519	-30.586773	-18.973036
O	0.747262	-29.055234	-21.291319
Zr	-0.944360	-28.839001	-20.065954
Zr	-0.553217	-32.470116	-19.959943
Zr	2.588064	-28.516204	-20.465636
Zr	0.720070	-30.576976	-22.715317
Zr	1.276997	-30.370007	-17.717797
Zr	2.969978	-32.060381	-20.361616
H	-1.814958	-33.769452	-23.770166
H	1.610889	-36.063556	-20.190121
H	3.579732	-33.250447	-24.364336
H	-1.167663	-33.261945	-15.833795
H	-1.734798	-27.959950	-15.987457
H	0.409490	-24.889628	-20.515576
H	2.956194	-27.460192	-24.534903
H	4.038847	-27.324480	-16.653466
H	6.588125	-29.887478	-20.680608
H	4.615670	-32.693014	-16.496100
H	-2.430722	-28.066507	-23.937111
H	-3.396914	-28.578309	-19.039095
H	-2.915769	-33.161772	-18.893260
Ni	-3.420302	-30.920913	-19.654770
H	-2.048274	-30.846434	-21.735057
C	-3.596640	-30.829587	-17.482108
H	-3.389289	-29.807154	-17.156155
H	-2.925587	-31.604642	-17.109996
C	-4.790761	-31.142212	-18.087978
H	-5.048469	-32.202210	-18.215764
C	-5.902568	-30.180153	-18.332176
H	-6.732432	-30.374016	-17.633279
H	-5.589207	-29.137457	-18.192339
H	-6.318021	-30.279538	-19.345047

H	-3.621307	-30.992718	-21.140981

B to C TS

C	10.482563	13.517234	23.859346
C	13.495905	16.642081	23.854624
C	16.909376	13.434781	23.954829
C	10.368201	16.571672	26.878761
C	13.610906	16.682548	30.228008
C	16.948977	10.422001	26.990989
C	13.577425	10.302574	30.245528
C	16.707673	16.768007	27.232027
C	10.521521	10.244956	27.157966
C	16.745475	13.719074	30.304600
C	10.415721	13.285819	30.195707
O	13.755097	11.720094	23.345250
Zr	13.691159	13.484258	24.533712
O	10.072134	13.422403	25.044448
O	11.670364	13.556797	23.466405
O	15.733377	13.435403	23.508754
O	13.609691	15.455394	23.454375
Zr	13.728817	10.971845	27.077899
Zr	11.119880	13.413287	27.025657
O	15.045260	14.945148	25.660918
O	12.309555	12.008235	25.611990
O	12.574294	14.495532	26.007119
O	14.739243	12.483705	26.057205
O	13.494824	17.045656	25.044369
O	17.271036	13.540599	25.151101
Zr	13.555033	16.003053	27.050742
Zr	16.156493	13.570541	27.115295
H	11.774194	11.416400	25.068874
H	15.595464	15.527097	25.129312
H	11.572559	15.416407	29.004175
O	12.151465	14.874986	28.460265
O	15.507825	17.130836	27.141985
O	11.545576	17.008421	26.947878
O	13.564013	17.077687	29.035695
Zr	13.590592	13.495836	29.584853
O	14.627693	14.570830	28.124913
H	15.646457	11.589255	29.089276
O	15.083435	12.122054	28.520852
O	11.714806	9.869088	27.191298
O	15.781931	9.962098	27.062289
O	13.677535	9.902226	29.057183
O	12.604983	12.425713	28.097991
O	17.173517	13.678278	29.123784
O	17.150375	15.592203	27.194947
O	17.296385	11.628503	27.059528
O	10.029110	13.327216	29.001468
O	10.097595	11.427212	27.055038

O	9.998171	15.372748	26.937218
O	13.585818	15.493984	30.636370
O	13.568133	11.493698	30.645205
O	15.551451	13.623835	30.684772
O	11.597539	13.375636	30.616388
O	13.784179	9.765872	25.288319
H	14.031809	8.851215	25.462924
H	9.744094	9.451672	27.217164
H	9.695778	13.565147	23.072734
H	13.395762	17.420584	23.067926
H	13.496707	9.516371	31.026586
H	13.671550	17.471768	31.008094
H	17.461350	17.576482	27.347511
H	17.509203	13.840244	31.102802
H	9.625945	13.164754	30.968075
H	17.722173	13.343443	23.201217
H	9.566494	17.332284	26.761595
H	17.768793	9.680550	26.871847
H	14.586069	11.661656	22.860605
Ni	12.888465	9.949658	23.580602
C	12.198397	9.935206	21.705928
H	12.676172	9.072804	21.217073
C	11.201800	9.624736	22.651896
H	10.512918	10.418449	22.980883
H	10.750199	8.629764	22.696233
C	12.273295	11.215755	20.946208
H	13.303757	11.479368	20.673583
H	11.716034	11.110180	20.000207
H	11.853542	12.061243	21.503672
H	12.260652	8.681698	23.806382

B to D TS

C	10.482563	13.517234	23.859346
C	13.495905	16.642081	23.854624
C	16.909376	13.434781	23.954829
C	10.368201	16.571672	26.878761
C	13.610906	16.682548	30.228008
C	16.948977	10.422001	26.990989
C	13.577425	10.302574	30.245528
C	16.707673	16.768007	27.232027
C	10.521521	10.244956	27.157966
C	16.745475	13.719074	30.304600
C	10.415721	13.285819	30.195707
O	13.734525	11.732604	23.320484
Zr	13.680871	13.485556	24.529053
O	10.073365	13.419961	25.045663
O	11.669649	13.546172	23.464462
O	15.732802	13.423106	23.512445
O	13.606314	15.455671	23.453770
Zr	13.722169	10.963792	27.079033

Zr	11.118653	13.414263	27.027174
O	15.042610	14.945522	25.657624
O	12.301544	12.001915	25.614381
O	12.570109	14.498266	26.005824
O	14.730614	12.487775	26.054094
O	13.494717	17.046033	25.044421
O	17.272567	13.537772	25.151459
Zr	13.553619	16.003412	27.049509
Zr	16.148943	13.571400	27.111551
H	11.720902	11.442958	25.080257
H	15.591834	15.530608	25.128444
H	11.573258	15.418114	29.004951
O	12.151078	14.875946	28.460689
O	15.508124	17.131805	27.141220
O	11.545483	17.008761	26.948992
O	13.563993	17.078076	29.035788
Zr	13.589144	13.495338	29.583318
O	14.626858	14.571970	28.124999
H	15.645964	11.591855	29.088416
O	15.080857	12.116989	28.514939
O	11.715024	9.871452	27.195719
O	15.781073	9.958122	27.036040
O	13.682308	9.898604	29.059199
O	12.603195	12.426387	28.098630
O	17.171908	13.676710	29.123122
O	17.148811	15.591584	27.192649
O	17.293705	11.627022	27.065178
O	10.028095	13.327416	29.002019
O	10.095596	11.426473	27.053661
O	9.997401	15.373314	26.938557
O	13.586557	15.493812	30.636068
O	13.566106	11.494490	30.642945
O	15.551458	13.620073	30.684793
O	11.597510	13.377256	30.616198
O	13.803909	9.782178	25.293455
H	14.391046	9.020796	25.331664
H	9.745791	9.450287	27.217792
H	9.695053	13.574951	23.075097
H	13.399082	17.421363	23.068219
H	13.496651	9.518469	31.028816
H	13.671464	17.471573	31.008350
H	17.462200	17.575502	27.348766
H	17.508868	13.847329	31.101975
H	9.626422	13.165096	30.968683
H	17.721839	13.351430	23.199594
H	9.566842	17.332647	26.761199
H	17.771451	9.680912	26.884871
H	14.638620	11.573478	23.025348
Ni	12.807635	10.011489	23.642943
C	11.863335	8.998305	22.164474
H	11.015270	8.372357	22.464911

C	11.658965	10.384244	22.100990
H	12.251060	11.017680	21.436020
H	10.708010	10.812162	22.435369
C	12.897751	8.283991	21.351250
H	13.321811	7.423107	21.885242
H	12.441718	7.890572	20.428605
H	13.722606	8.945799	21.054817
H	12.136466	8.771443	23.980416

C

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.739531	11.731568	23.299180
Zr	13.687148	13.484383	24.538138
O	10.070749	13.406344	25.044386
O	11.670109	13.581012	23.472732
O	15.733058	13.436409	23.508541
O	13.617343	15.456032	23.455712
Zr	13.719197	10.954485	27.081799
Zr	11.116424	13.410427	27.021204
O	15.043291	14.945642	25.660962
O	12.315601	11.994376	25.596423
O	12.574732	14.494076	26.007647
O	14.738368	12.481063	26.051911
O	13.491018	17.046224	25.044600
O	17.270512	13.534695	25.152106
Zr	13.553674	16.004986	27.050792
Zr	16.148737	13.569797	27.113606
H	11.782792	11.420471	25.029142
H	15.592112	15.526295	25.126505
H	11.572306	15.417415	29.003760
O	12.149951	14.876067	28.458464
O	15.507844	17.131790	27.142208
O	11.545271	17.009103	26.949525
O	13.564044	17.078928	29.035826
Zr	13.585703	13.493888	29.579302
O	14.626474	14.571018	28.124468
H	15.643512	11.594343	29.093417
O	15.078508	12.113719	28.514602
O	11.712492	9.867242	27.190247

O	15.782699	9.956560	27.027530
O	13.679285	9.893942	29.061136
O	12.597366	12.426477	28.092765
O	17.172845	13.674937	29.123295
O	17.148877	15.591716	27.193449
O	17.293923	11.626127	27.072187
O	10.027999	13.327302	29.001849
O	10.097117	11.426580	27.051574
O	9.998601	15.372496	26.932238
O	13.585851	15.493515	30.634757
O	13.563892	11.495740	30.639462
O	15.551058	13.619585	30.683215
O	11.597538	13.377587	30.616020
O	13.783122	9.702533	25.368641
H	14.617134	9.219357	25.345845
H	9.742856	9.453088	27.224436
H	9.696945	13.559748	23.072136
H	13.393655	17.419936	23.067642
H	13.501333	9.521441	31.032331
H	13.672063	17.471119	31.008728
H	17.462018	17.575896	27.347117
H	17.508142	13.849146	31.102331
H	9.626504	13.164911	30.968803
H	17.722319	13.342326	23.201522
H	9.566063	17.332583	26.766140
H	17.772852	9.682190	26.884289
H	14.500887	11.719978	22.707726
Ni	13.011665	9.992666	23.563930
C	12.045884	9.789141	21.963856
H	12.734290	9.697278	21.109464
C	10.921880	10.751673	21.725127
H	11.304313	11.759170	21.511786
H	10.293023	10.452266	20.868091
H	10.251952	10.827616	22.596392
C	11.798000	8.528493	22.699806
H	10.753132	8.357331	22.999342
H	12.211006	7.616249	22.246938
H	12.325223	8.503290	23.749694

D

C	10.482685	13.517077	23.859501
C	13.495993	16.641965	23.854693
C	16.909489	13.434778	23.954791
C	10.368266	16.571600	26.878820
C	13.610909	16.682540	30.228067
C	16.948748	10.422218	26.990830
C	13.577337	10.302725	30.245392
C	16.707759	16.768009	27.232025
C	10.521477	10.244906	27.157980
C	16.745407	13.719135	30.304545

C	10.415671	13.285793	30.195741
O	13.741075	11.747680	23.302062
Zr	13.687029	13.483071	24.528691
O	10.073613	13.412773	25.046150
O	11.668444	13.544856	23.463902
O	15.734936	13.438873	23.507749
O	13.606017	15.455085	23.455215
Zr	13.722203	10.961278	27.085355
Zr	11.120374	13.414391	27.024843
O	15.043356	14.944931	25.658837
O	12.310782	12.002959	25.615636
O	12.570584	14.498399	26.005398
O	14.735538	12.483116	26.053607
O	13.495426	17.046737	25.044334
O	17.270185	13.530988	25.152955
Zr	13.553615	16.003247	27.048689
Zr	16.148992	13.570849	27.112385
H	11.747294	11.434397	25.072140
H	15.593469	15.528150	25.128490
H	11.573083	15.418521	29.004415
O	12.150965	14.876008	28.460516
O	15.508124	17.131528	27.141777
O	11.545423	17.008955	26.949104
O	13.563990	17.077779	29.035838
Zr	13.588195	13.496087	29.583832
O	14.626493	14.570652	28.125001
H	15.645959	11.592967	29.092415
O	15.080732	12.114436	28.515692
O	11.714278	9.871773	27.198571
O	15.779234	9.960222	27.018421
O	13.684631	9.896246	29.060386
O	12.601991	12.425376	28.099944
O	17.171913	13.676510	29.123200
O	17.148982	15.591519	27.192437
O	17.295246	11.625219	27.075012
O	10.029241	13.323994	29.001408
O	10.093639	11.424653	27.043199
O	9.997829	15.372966	26.937124
O	13.586740	15.493737	30.636265
O	13.564537	11.495020	30.641331
O	15.551302	13.619143	30.684474
O	11.597068	13.379221	30.617016
O	13.781140	9.727947	25.333658
H	14.538982	9.135533	25.282868
H	9.745621	9.449449	27.221396
H	9.693379	13.584147	23.077695
H	13.398769	17.420582	23.067712
H	13.495817	9.519830	31.029832
H	13.671415	17.471586	31.008365
H	17.462246	17.575559	27.348465
H	17.508489	13.848478	31.101995

H	9.625805	13.166273	30.968302
H	17.723723	13.343934	23.202415
H	9.566642	17.332470	26.762441
H	17.770304	9.679376	26.889596
H	14.588404	11.671114	22.849506
Ni	12.871710	10.011039	23.694338
C	9.886684	10.075878	22.785575
H	9.838089	10.555230	23.775734
H	9.695105	10.850270	22.031111
H	9.062096	9.351987	22.738804
C	11.726638	8.531409	23.669907
H	11.102367	8.436735	24.567848
H	12.227395	7.591005	23.405220
C	11.213287	9.372113	22.568630
H	11.261344	8.882377	21.580789
H	11.996469	10.231249	22.323676

E

C	10.482568	13.517215	23.859364
C	13.495868	16.642084	23.854622
C	16.909384	13.434807	23.954813
C	10.368212	16.571668	26.878765
C	13.610918	16.682546	30.228008
C	16.948976	10.421983	26.991016
C	13.577380	10.302576	30.245531
C	16.707682	16.768011	27.232019
C	10.521539	10.244966	27.157942
C	16.745484	13.719071	30.304603
C	10.415731	13.285819	30.195703
O	13.757073	11.729638	23.355223
Zr	13.684237	13.480988	24.536428
O	10.075034	13.422542	25.045960
O	11.669211	13.552111	23.463077
O	15.735009	13.440652	23.506733
O	13.606872	15.455744	23.454093
Zr	13.722770	10.967581	27.074646
Zr	11.114775	13.409687	27.023580
O	15.042417	14.945599	25.661468
O	12.309742	11.987865	25.603501
O	12.568672	14.491766	26.009939
O	14.739077	12.485617	26.058500
O	13.493297	17.045107	25.045168
O	17.269979	13.533604	25.152414
Zr	13.552263	16.001732	27.049912
Zr	16.151534	13.572509	27.115236
H	11.794773	11.406092	25.030526
H	15.589642	15.529764	25.129253
H	11.573089	15.417700	29.005719
O	12.149344	14.874499	28.460792
O	15.507834	17.130733	27.143128

O	11.545630	17.008258	26.948415
O	13.562906	17.077785	29.035708
Zr	13.587906	13.495233	29.582352
O	14.627217	14.571808	28.126435
H	15.642060	11.590169	29.092082
O	15.080604	12.116947	28.516563
O	11.716957	9.882450	27.222748
O	15.779954	9.958857	27.029207
O	13.688712	9.898230	29.059929
O	12.604018	12.428367	28.091713
O	17.173434	13.677029	29.123697
O	17.150266	15.591983	27.193026
O	17.295072	11.625613	27.071438
O	10.028670	13.322101	29.001334
O	10.089574	11.423078	27.045225
O	9.997222	15.373124	26.938437
O	13.586289	15.493761	30.636117
O	13.561752	11.495109	30.641792
O	15.551268	13.620472	30.683847
O	11.597341	13.377538	30.615999
O	13.781098	9.734106	25.306548
H	14.407071	9.007985	25.408739
H	9.751136	9.443591	27.202970
H	9.693293	13.566949	23.076249
H	13.399598	17.422227	23.068983
H	13.495161	9.519184	31.029362
H	13.672652	17.471650	31.008151
H	17.461737	17.576286	27.346697
H	17.508258	13.846749	31.102682
H	9.625809	13.169523	30.968663
H	17.723904	13.340369	23.202965
H	9.566918	17.332766	26.761821
H	17.770500	9.679827	26.885049
H	14.621009	11.693706	22.928485
Ni	13.044393	9.823082	23.505778
C	12.745758	9.776651	21.481907
H	12.807025	8.713970	21.215792
C	11.619715	10.206241	22.186688
H	11.404089	11.279381	22.237883
H	10.786041	9.527990	22.391190
C	13.623796	10.667148	20.666713
H	14.692934	10.442282	20.801725
H	13.416749	10.497766	19.597664
H	13.457161	11.729263	20.878549
C	12.498360	7.945218	23.632238
H	11.950478	7.730375	22.699381
C	11.583673	7.699458	24.804284
H	10.685876	8.335625	24.769626
H	11.225774	6.653657	24.804786
H	12.072751	7.881700	25.769631
C	13.765868	7.121566	23.649342

H	14.447884	7.364510	22.819411
H	14.332998	7.223076	24.588159
H	13.538199	6.043912	23.559536

F

C	10.482561	13.517237	23.859347
C	13.495913	16.642078	23.854626
C	16.909374	13.434773	23.954836
C	10.368199	16.571673	26.878761
C	13.610903	16.682548	30.228008
C	16.948976	10.422007	26.990982
C	13.577433	10.302576	30.245524
C	16.707671	16.768006	27.232027
C	10.521521	10.244956	27.157967
C	16.745473	13.719075	30.304599
C	10.415719	13.285819	30.195707
O	13.739646	11.728690	23.332072
Zr	13.683891	13.480699	24.530525
O	10.074027	13.419006	25.045098
O	11.669946	13.559016	23.465109
O	15.733838	13.429466	23.509558
O	13.608960	15.455985	23.453678
Zr	13.724119	10.968462	27.077614
Zr	11.118283	13.413714	27.025766
O	15.043171	14.944814	25.659251
O	12.304418	11.997065	25.607489
O	12.570587	14.494842	26.007710
O	14.734729	12.486993	26.056371
O	13.493663	17.045407	25.044899
O	17.271164	13.536633	25.151745
Zr	13.553537	16.002246	27.049121
Zr	16.151240	13.572276	27.113479
H	11.751511	11.430712	25.054409
H	15.591218	15.529900	25.128835
H	11.573410	15.418183	29.004994
O	12.150687	14.875240	28.460899
O	15.507992	17.131060	27.141727
O	11.545408	17.008465	26.949300
O	13.563782	17.077704	29.035751
Zr	13.589097	13.495725	29.583897
O	14.627115	14.571553	28.125770
H	15.644618	11.590667	29.089486
O	15.080953	12.118202	28.516799
O	11.715905	9.872272	27.195973
O	15.781050	9.958566	27.041691
O	13.681676	9.899791	29.058624
O	12.603707	12.426841	28.095401
O	17.172668	13.676975	29.123435
O	17.149713	15.591821	27.193274
O	17.294211	11.626957	27.065475

O	10.028549	13.326505	29.001721
O	10.094692	11.425579	27.054975
O	9.997603	15.372934	26.937369
O	13.586222	15.493735	30.636275
O	13.565508	11.494548	30.643160
O	15.551320	13.621225	30.684488
O	11.597638	13.376279	30.615987
O	13.807685	9.777301	25.290076
H	14.349781	8.986723	25.385859
H	9.746653	9.448500	27.214229
H	9.694715	13.563566	23.074599
H	13.397793	17.421829	23.068829
H	13.497684	9.518038	31.028387
H	13.671970	17.471577	31.008268
H	17.461836	17.575986	27.347686
H	17.508671	13.846115	31.102338
H	9.626130	13.166925	30.968594
H	17.722899	13.347392	23.201187
H	9.566652	17.332507	26.761971
H	17.770609	9.680817	26.880192
H	14.634055	11.625913	22.987124
Ni	12.891585	9.892421	23.580399
C	12.583251	9.698602	21.580296
H	12.478089	8.621981	21.411202
C	11.534982	10.368191	22.211436
H	11.496845	11.461631	22.167142
H	10.603535	9.852436	22.461504
C	13.620742	10.362695	20.737040
H	14.632869	9.982379	20.942387
H	13.425410	10.134831	19.676678
H	13.622081	11.451837	20.855114
C	12.026728	8.219630	24.046453
H	11.299057	8.614039	24.780838
H	12.790137	7.685311	24.636167
C	11.364068	7.269496	23.076416
H	10.657183	7.793602	22.410158
H	12.117088	6.818046	22.407436
C	10.619070	6.154823	23.796128
H	9.821052	6.555535	24.438503
H	10.153732	5.451313	23.091135
H	11.291944	5.575363	24.445145

E to J TS

C	10.482595	13.517215	23.859340
C	13.495822	16.642122	23.854605
C	16.909395	13.434876	23.954722
C	10.368238	16.571654	26.878775
C	13.610928	16.682528	30.228006
C	16.948960	10.421935	26.991080
C	13.577332	10.302576	30.245571

C	16.707694	16.768000	27.232026
C	10.521552	10.244949	27.157961
C	16.745478	13.719077	30.304602
C	10.415747	13.285814	30.195698
O	13.808970	11.750954	23.299605
Zr	13.689406	13.486479	24.540386
O	10.073418	13.415104	25.046617
O	11.669852	13.563805	23.469298
O	15.738724	13.483399	23.501195
O	13.609384	15.455276	23.456976
Zr	13.719243	10.954344	27.072285
Zr	11.116578	13.410065	27.017773
O	15.042033	14.948673	25.664803
O	12.324556	11.984866	25.585258
O	12.572385	14.493745	26.008369
O	14.742303	12.481888	26.050822
O	13.492879	17.047254	25.044449
O	17.267839	13.520255	25.154986
Zr	13.553480	16.005399	27.051538
Zr	16.149822	13.570195	27.114423
H	11.815935	11.408773	25.002649
H	15.590327	15.525068	25.125252
H	11.572347	15.416450	29.004545
O	12.149354	14.875281	28.458400
O	15.507972	17.132282	27.145611
O	11.545524	17.008986	26.947754
O	13.562564	17.079716	29.036029
Zr	13.585624	13.492310	29.576770
O	14.626511	14.571376	28.124666
H	15.642204	11.594596	29.093657
O	15.079108	12.113549	28.512699
O	11.711956	9.870706	27.231345
O	15.780405	9.957796	27.007555
O	13.690060	9.893459	29.062434
O	12.599454	12.427591	28.085203
O	17.173939	13.676563	29.123760
O	17.149266	15.591783	27.192374
O	17.295466	11.623682	27.083077
O	10.028980	13.319948	29.000806
O	10.097197	11.423737	27.032921
O	9.997855	15.373010	26.936584
O	13.586767	15.493298	30.633980
O	13.558709	11.496459	30.638272
O	15.550898	13.617882	30.682340
O	11.597255	13.379384	30.615786
O	13.734284	9.689419	25.360240
H	14.565842	9.199819	25.373198
H	9.743195	9.450548	27.203653
H	9.695238	13.565348	23.075063
H	13.397543	17.420061	23.067136
H	13.496725	9.522418	31.033021

H	13.672569	17.470788	31.009058
H	17.462545	17.575812	27.345185
H	17.507346	13.849390	31.103138
H	9.625796	13.169761	30.968734
H	17.724502	13.316705	23.206937
H	9.566494	17.332678	26.764057
H	17.771949	9.679861	26.892206
H	14.469260	11.872477	22.608079
Ni	13.288014	9.924884	23.373099
C	13.568996	8.256671	22.182304
H	13.205466	7.390484	21.613880
C	13.414007	9.560745	21.524598
H	14.311058	10.026371	21.094587
H	12.524370	9.694646	20.894144
C	14.947234	7.915367	22.722911
H	14.901401	7.206609	23.560923
H	15.551054	7.435988	21.936115
H	15.503205	8.801430	23.065102
C	12.073596	8.058266	23.284474
H	11.494481	7.709815	22.420180
C	11.127577	9.071000	23.947383
H	10.933971	9.970776	23.338262
H	10.148000	8.574290	24.062628
H	11.455637	9.352113	24.954205
C	12.374355	6.906703	24.210186
H	12.907820	6.086851	23.708827
H	12.966763	7.235908	25.076058
H	11.438305	6.487450	24.609674

E to K TS

C	10.482568	13.517215	23.859364
C	13.495868	16.642084	23.854622
C	16.909384	13.434807	23.954813
C	10.368212	16.571668	26.878765
C	13.610918	16.682546	30.228008
C	16.948976	10.421983	26.991016
C	13.577380	10.302576	30.245531
C	16.707682	16.768011	27.232019
C	10.521539	10.244966	27.157942
C	16.745484	13.719071	30.304603
C	10.415731	13.285819	30.195703
O	13.696639	11.713565	23.306936
Zr	13.686589	13.474603	24.536047
O	10.068582	13.391698	25.043007
O	11.669237	13.614634	23.479900
O	15.732672	13.430206	23.508983
O	13.625327	15.457071	23.455991
Zr	13.718518	10.961904	27.082819
Zr	11.113778	13.408518	27.017257
O	15.043367	14.944884	25.661602

O	12.321260	11.985228	25.589189
O	12.577078	14.486679	26.009451
O	14.742626	12.481892	26.052897
O	13.486443	17.045756	25.045193
O	17.271567	13.538167	25.151564
Zr	13.553007	16.002296	27.048629
Zr	16.149277	13.572182	27.113290
H	11.833535	11.392363	25.001924
H	15.590056	15.526134	25.125695
H	11.572186	15.419003	29.002686
O	12.148559	14.876534	28.457172
O	15.507885	17.131155	27.141577
O	11.545156	17.008691	26.949851
O	13.564427	17.078478	29.035842
Zr	13.584675	13.495625	29.578962
O	14.626655	14.571904	28.125469
H	15.640412	11.594366	29.094180
O	15.077206	12.116964	28.516647
O	11.711634	9.863038	27.181280
O	15.786562	9.950629	27.054660
O	13.674631	9.893746	29.060955
O	12.593547	12.428352	28.091870
O	17.173519	13.674218	29.123558
O	17.150077	15.592125	27.194636
O	17.291877	11.626564	27.066424
O	10.027133	13.329692	29.002261
O	10.098264	11.426951	27.057743
O	9.998510	15.372033	26.926491
O	13.584335	15.493604	30.635450
O	13.564476	11.495788	30.639477
O	15.551023	13.621957	30.683412
O	11.597680	13.377310	30.615997
O	13.820193	9.706760	25.382546
H	14.630073	9.191005	25.467152
H	9.741132	9.454427	27.225422
H	9.698953	13.546777	23.069758
H	13.390709	17.420217	23.068159
H	13.504243	9.521686	31.033046
H	13.673103	17.471214	31.008640
H	17.461607	17.576472	27.346792
H	17.508301	13.847830	31.102573
H	9.627000	13.163232	30.969086
H	17.722302	13.345763	23.200799
H	9.565771	17.332940	26.770844
H	17.773814	9.685393	26.866464
H	14.366500	11.767447	22.615580
Ni	13.145842	9.861279	23.491190
C	11.879926	9.722038	22.065691
H	12.292998	9.418729	21.089201
C	11.692633	8.621475	23.007222
H	11.163247	8.896905	23.941501

H	11.283589	7.658177	22.686331
C	10.895651	10.846992	21.988294
H	11.355824	11.780391	21.637516
H	10.062621	10.610828	21.302925
H	10.440642	11.050020	22.970680
C	13.377930	7.742205	23.156302
H	13.128853	7.212522	22.226964
C	13.226638	6.809571	24.333526
H	12.239586	6.327612	24.349448
H	13.981212	6.008920	24.290567
H	13.346818	7.334681	25.290333
C	14.825272	8.186075	22.898509
H	14.918865	8.865044	22.038288
H	15.347910	8.644851	23.747629
H	15.400632	7.279684	22.637109

F to L TS

C	10.482553	13.517254	23.859342
C	13.495921	16.642086	23.854632
C	16.909360	13.434764	23.954844
C	10.368195	16.571677	26.878757
C	13.610901	16.682552	30.228001
C	16.948983	10.421995	26.990989
C	13.577443	10.302570	30.245526
C	16.707663	16.768006	27.232027
C	10.521529	10.244945	27.157968
C	16.745474	13.719078	30.304595
C	10.415721	13.285821	30.195702
O	13.706254	11.722043	23.299394
Zr	13.687861	13.476248	24.537612
O	10.069292	13.391436	25.042988
O	11.668931	13.612540	23.478473
O	15.733162	13.437342	23.508050
O	13.624149	15.456879	23.455993
Zr	13.721034	10.958198	27.080095
Zr	11.114629	13.407595	27.018125
O	15.043295	14.945785	25.662211
O	12.323357	11.981465	25.585291
O	12.576165	14.486692	26.009116
O	14.741309	12.483149	26.053110
O	13.486629	17.045741	25.045098
O	17.271054	13.537019	25.151833
Zr	13.553164	16.002266	27.049302
Zr	16.149989	13.571651	27.113439
H	11.824197	11.393528	25.005105
H	15.590232	15.526261	25.125724
H	11.572441	15.418437	29.002961
O	12.148614	14.875966	28.457262
O	15.507831	17.131279	27.142037
O	11.545137	17.008752	26.949934

O	13.564013	17.078695	29.035809
Zr	13.585118	13.494629	29.578030
O	14.626810	14.572084	28.125324
H	15.641108	11.593997	29.092856
O	15.077575	12.117080	28.516057
O	11.711841	9.865743	27.189911
O	15.786716	9.950845	27.056870
O	13.677187	9.893924	29.061177
O	12.595592	12.428279	28.088926
O	17.173741	13.674595	29.123626
O	17.150070	15.592157	27.194620
O	17.291702	11.627057	27.065137
O	10.027333	13.328064	29.001983
O	10.097645	11.426807	27.052794
O	9.998640	15.371957	26.926967
O	13.584560	15.493551	30.635089
O	13.563521	11.495918	30.639329
O	15.550962	13.621611	30.683132
O	11.597680	13.376967	30.615645
O	13.820445	9.715237	25.372047
H	14.588199	9.140771	25.472852
H	9.741654	9.453824	27.223269
H	9.698277	13.547080	23.070032
H	13.391609	17.420220	23.068040
H	13.503153	9.521691	31.032950
H	13.673182	17.471173	31.008671
H	17.461634	17.576490	27.346427
H	17.508107	13.847807	31.102739
H	9.626757	13.164945	30.969090
H	17.722418	13.340809	23.201609
H	9.565727	17.332855	26.770255
H	17.773804	9.685608	26.866552
H	14.365345	11.799151	22.599435
Ni	13.216899	9.844677	23.441475
C	12.034111	9.725486	21.935610
H	12.507264	9.420513	20.989395
C	11.776975	8.647605	22.872191
H	11.100849	8.877854	23.713216
H	11.563310	7.635662	22.515760
C	11.097546	10.885967	21.810079
H	11.605665	11.806188	21.493950
H	10.301701	10.676582	21.074479
H	10.594449	11.099308	22.765099
C	13.552975	7.860441	23.298684
H	13.281422	7.300750	24.205289
H	14.523389	8.371237	23.499120
C	13.770539	6.975739	22.089456
H	12.904765	6.310624	21.934292
H	13.832917	7.594983	21.178782
C	15.030357	6.138622	22.218970
H	15.002464	5.504191	23.116957

H	15.163660	5.475334	21.353690
H	15.931128	6.765374	22.291899

F to M TS

C	10.482561	13.517237	23.859347
C	13.495913	16.642078	23.854626
C	16.909374	13.434773	23.954836
C	10.368199	16.571673	26.878761
C	13.610903	16.682548	30.228008
C	16.948976	10.422007	26.990982
C	13.577433	10.302576	30.245524
C	16.707671	16.768006	27.232027
C	10.521521	10.244956	27.157967
C	16.745473	13.719075	30.304599
C	10.415719	13.285819	30.195707
O	13.786736	11.716931	23.361547
Zr	13.687896	13.488055	24.542080
O	10.070926	13.417385	25.045522
O	11.670316	13.561681	23.468625
O	15.735056	13.451856	23.505681
O	13.612259	15.455609	23.456094
Zr	13.717479	10.953242	27.067287
Zr	11.118087	13.413706	27.022147
O	15.044266	14.948328	25.662945
O	12.308587	12.007986	25.603054
O	12.572787	14.500694	26.008672
O	14.738129	12.486919	26.057661
O	13.493840	17.047560	25.044169
O	17.269670	13.528552	25.153157
Zr	13.554391	16.006510	27.052347
Zr	16.149830	13.569739	27.115591
H	11.777784	11.432249	25.035645
H	15.592243	15.528745	25.127447
H	11.573384	15.415088	29.006532
O	12.150752	14.875029	28.459702
O	15.508198	17.132705	27.143916
O	11.545294	17.009296	26.949868
O	13.563233	17.080166	29.036106
Zr	13.586437	13.490342	29.577317
O	14.626952	14.571295	28.125791
H	15.641340	11.591933	29.094331
O	15.078662	12.110361	28.512437
O	11.710634	9.855813	27.153485
O	15.779316	9.961678	27.003579
O	13.668897	9.895997	29.058987
O	12.597431	12.421717	28.092217
O	17.173824	13.674866	29.123722
O	17.149017	15.591803	27.193976
O	17.297389	11.624164	27.078131
O	10.027374	13.328385	29.002198

O	10.101332	11.427674	27.055443
O	9.997457	15.373388	26.936672
O	13.586239	15.493364	30.633908
O	13.568764	11.495053	30.641855
O	15.551164	13.617879	30.682570
O	11.597988	13.374895	30.615436
O	13.762044	9.739120	25.319992
H	14.640621	9.354869	25.217688
H	9.738156	9.462397	27.262697
H	9.696117	13.562993	23.073282
H	13.394692	17.419817	23.067222
H	13.505665	9.520065	31.031526
H	13.672452	17.470793	31.009125
H	17.462569	17.575794	27.345308
H	17.507507	13.850955	31.102711
H	9.626746	13.166512	30.969330
H	17.723592	13.335338	23.203370
H	9.566788	17.332805	26.762040
H	17.770773	9.677710	26.900042
H	14.524865	11.722875	22.742626
Ni	12.898310	10.014653	23.487625
C	12.120329	8.784232	21.975944
H	11.128477	8.357270	21.781796
C	12.226095	10.195096	21.728006
H	13.043319	10.569780	21.101629
H	11.310577	10.796495	21.669632
C	13.227776	7.876644	21.512432
H	13.218514	6.906726	22.027316
H	13.117423	7.675633	20.435664
H	14.220786	8.324492	21.659703
C	11.637896	8.403248	23.864936
H	12.225182	8.457484	24.796065
H	11.663110	7.341974	23.581936
C	10.217787	8.880591	24.082840
H	10.214041	9.881122	24.555436
H	9.699866	9.032154	23.118904
C	9.421241	7.904421	24.931741
H	9.939899	7.676351	25.874496
H	8.423776	8.293032	25.179914
H	9.281476	6.948012	24.406475

J

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019

C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.731890	11.728756	23.302533
Zr	13.686636	13.484329	24.537471
O	10.069649	13.402815	25.043919
O	11.670352	13.589479	23.475175
O	15.732789	13.434274	23.508991
O	13.619628	15.456403	23.455462
Zr	13.719408	10.954590	27.082493
Zr	11.116614	13.410521	27.021048
O	15.043317	14.945393	25.661053
O	12.314529	11.995319	25.596901
O	12.575192	14.494132	26.008029
O	14.737511	12.481055	26.052339
O	13.490005	17.046036	25.044630
O	17.270595	13.535375	25.152058
Zr	13.553720	16.004822	27.050770
Zr	16.148490	13.569722	27.113403
H	11.776815	11.424715	25.030872
H	15.592167	15.526092	25.126680
H	11.572311	15.417622	29.003867
O	12.149716	14.876213	28.458388
O	15.507898	17.131931	27.141866
O	11.545190	17.009147	26.949923
O	13.564124	17.079004	29.035894
Zr	13.585674	13.494053	29.579474
O	14.626411	14.571079	28.124723
H	15.643208	11.594177	29.093625
O	15.078452	12.113845	28.514830
O	11.712665	9.867194	27.188576
O	15.782936	9.956377	27.029834
O	13.678939	9.893888	29.061100
O	12.597055	12.426386	28.093328
O	17.172760	13.674832	29.123280
O	17.148732	15.591683	27.193828
O	17.293836	11.626251	27.071146
O	10.027887	13.327398	29.001890
O	10.096894	11.426378	27.051863
O	9.998565	15.372415	26.931166
O	13.585689	15.493516	30.634746
O	13.564085	11.495696	30.639513
O	15.551064	13.619635	30.683339
O	11.597501	13.377921	30.616031
O	13.788448	9.700968	25.370994
H	14.626376	9.224937	25.344822
H	9.743064	9.452941	27.225683
H	9.697901	13.554843	23.070623
H	13.392845	17.419978	23.067781
H	13.501460	9.521399	31.032311
H	13.672109	17.471054	31.008801

H	17.462088	17.575819	27.347144
H	17.508188	13.849249	31.102271
H	9.626570	13.164588	30.968844
H	17.722192	13.343785	23.201259
H	9.565995	17.332651	26.766819
H	17.772833	9.682319	26.883181
H	14.483751	11.715637	22.699240
Ni	12.999901	9.991407	23.576697
C	11.990914	9.794149	22.003093
H	12.650317	9.710889	21.125390
C	10.847864	10.753944	21.822060
H	11.252580	11.746074	21.556608
H	10.327623	10.893380	22.789391
C	11.764170	8.528394	22.737590
H	10.727129	8.355745	23.064652
H	12.164082	7.617362	22.270620
H	12.316761	8.500210	23.773933
C	9.797833	10.343257	20.776170
H	9.381460	9.365668	21.089907
C	8.659494	11.350262	20.752381
H	8.194372	11.466977	21.742377
H	9.019085	12.343691	20.439596
H	7.868151	11.055073	20.048566
C	10.406160	10.169639	19.393717
H	11.173588	9.382818	19.368985
H	9.642197	9.901202	18.650120
H	10.881183	11.102845	19.050914

K

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.748774	11.742031	23.277307
Zr	13.687636	13.483904	24.538038
O	10.068600	13.411575	25.043936
O	11.670861	13.574715	23.474570
O	15.733959	13.440089	23.506923
O	13.614946	15.455707	23.455546
Zr	13.718162	10.955192	27.080124
Zr	11.115892	13.410400	27.020363
O	15.043039	14.945670	25.660514
O	12.315180	11.996347	25.594543

O	12.574005	14.494856	26.007069
O	14.739639	12.481638	26.050215
O	13.492020	17.046387	25.044418
O	17.269955	13.533572	25.152233
Zr	13.553259	16.004387	27.050650
Zr	16.148711	13.569670	27.113887
H	11.790854	11.417648	25.023681
H	15.591716	15.527116	25.126783
H	11.572196	15.417784	29.003436
O	12.149637	14.876098	28.458265
O	15.507943	17.131876	27.142124
O	11.545358	17.009072	26.948833
O	13.563781	17.079093	29.035919
Zr	13.585496	13.493769	29.579218
O	14.626424	14.571057	28.124350
H	15.642974	11.594012	29.092734
O	15.078501	12.114014	28.513976
O	11.712370	9.867558	27.192424
O	15.781992	9.957621	27.022330
O	13.680087	9.893947	29.061271
O	12.597408	12.427439	28.091488
O	17.172982	13.675315	29.123364
O	17.148887	15.591652	27.193038
O	17.294620	11.625870	27.073831
O	10.027877	13.326865	29.001891
O	10.097238	11.426633	27.050443
O	9.998059	15.372828	26.933476
O	13.585929	15.493421	30.634575
O	13.563421	11.495943	30.639276
O	15.551022	13.619418	30.683081
O	11.597590	13.377851	30.615870
O	13.771764	9.718412	25.360430
H	14.604974	9.234192	25.328850
H	9.742735	9.453174	27.223816
H	9.697815	13.560564	23.070906
H	13.394720	17.420040	23.067590
H	13.501163	9.521656	31.032534
H	13.672177	17.470992	31.008868
H	17.462111	17.575765	27.347593
H	17.508063	13.848927	31.102458
H	9.626612	13.165066	30.968956
H	17.722964	13.340141	23.202378
H	9.566287	17.332811	26.765661
H	17.772601	9.681477	26.887302
H	14.535617	11.728428	22.719927
Ni	13.015243	9.997644	23.532934
C	12.142077	9.682520	21.875875
C	11.769800	8.533107	22.745383
H	10.717294	8.510583	23.062550
H	12.066057	7.539349	22.375566
H	12.331355	8.521701	23.773495

C	11.010435	10.633577	21.492408
H	10.541024	10.974560	22.436980
C	9.927309	9.917276	20.683459
H	9.106569	10.603763	20.429968
H	10.328640	9.532693	19.732935
H	9.486160	9.067454	21.223709
C	11.506132	11.858571	20.740254
H	10.697528	12.590607	20.604116
H	12.319176	12.362048	21.276736
H	11.862347	11.589673	19.733737
C	13.148157	9.399726	20.787961
H	12.671690	9.026255	19.862290
H	13.702517	10.306421	20.504222
H	13.886071	8.643304	21.092169

L

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.733084	11.728986	23.301738
Zr	13.686897	13.484385	24.537601
O	10.069602	13.404134	25.043888
O	11.670469	13.588697	23.475224
O	15.732771	13.434229	23.509000
O	13.619620	15.456373	23.455520
Zr	13.719365	10.954363	27.082445
Zr	11.116735	13.410791	27.021127
O	15.043415	14.945396	25.661065
O	12.314391	11.995712	25.596964
O	12.575227	14.494401	26.008041
O	14.737509	12.481034	26.052343
O	13.490264	17.046137	25.044626
O	17.270605	13.535293	25.152033
Zr	13.553760	16.004967	27.050881
Zr	16.148498	13.569715	27.113406
H	11.776472	11.425132	25.030950
H	15.592138	15.526180	25.126660
H	11.572297	15.417474	29.004054
O	12.149747	14.876249	28.458440
O	15.507918	17.131978	27.141866
O	11.545202	17.009152	26.949800
O	13.564118	17.079060	29.035903

Zr	13.585702	13.493922	29.579455
O	14.626410	14.571097	28.124724
H	15.643364	11.594221	29.093569
O	15.078474	12.113791	28.514818
O	11.712612	9.866993	27.188173
O	15.782935	9.956410	27.029752
O	13.678718	9.893964	29.061114
O	12.597033	12.426325	28.093353
O	17.172741	13.674799	29.123278
O	17.148703	15.591650	27.193854
O	17.293819	11.626254	27.071160
O	10.027840	13.327532	29.001924
O	10.096983	11.426446	27.051934
O	9.998522	15.372481	26.931346
O	13.585703	15.493507	30.634737
O	13.564112	11.495686	30.639572
O	15.551080	13.619618	30.683354
O	11.597514	13.377938	30.616040
O	13.787639	9.701246	25.371031
H	14.625328	9.224884	25.343425
H	9.742985	9.453025	27.225831
H	9.698233	13.553961	23.070147
H	13.392564	17.419897	23.067728
H	13.501635	9.521388	31.032312
H	13.672014	17.471042	31.008830
H	17.462139	17.575799	27.347066
H	17.508191	13.849364	31.102256
H	9.626604	13.164436	30.968856
H	17.722169	13.343663	23.201237
H	9.566027	17.332650	26.766614
H	17.772855	9.682309	26.883493
H	14.487423	11.714189	22.701572
Ni	12.995596	9.994788	23.577565
C	11.983653	9.801626	22.007181
H	12.630493	9.702040	21.120451
C	10.851459	10.771324	21.808968
H	11.269128	11.770954	21.603825
H	10.279447	10.876909	22.751574
C	11.743781	8.541738	22.748054
H	10.705328	8.383220	23.077789
H	12.131993	7.624214	22.284122
H	12.299003	8.511211	23.782783
C	9.888151	10.381551	20.691472
H	9.469714	9.378235	20.894302
H	10.452935	10.271478	19.748023
C	8.754628	11.374208	20.495590
H	8.197934	11.479752	21.443728
H	9.180977	12.374029	20.300525
C	7.803045	10.992887	19.380892
H	7.333167	10.015569	19.567459
H	6.993295	11.725230	19.260518

H	8.322785	10.919604	18.413883

M

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.727002	11.739546	23.285715
Zr	13.686639	13.484098	24.536471
O	10.068883	13.405318	25.043309
O	11.670224	13.592849	23.475666
O	15.733197	13.431968	23.508393
O	13.620590	15.456856	23.454692
Zr	13.719218	10.954562	27.080793
Zr	11.116481	13.409911	27.020772
O	15.043388	14.945193	25.660474
O	12.314376	11.995353	25.595409
O	12.574772	14.493927	26.008110
O	14.738847	12.480654	26.050369
O	13.489699	17.045690	25.044781
O	17.270599	13.536250	25.151786
Zr	13.553291	16.004192	27.050569
Zr	16.148104	13.569586	27.113284
H	11.786350	11.418092	25.026426
H	15.592114	15.527037	25.127242
H	11.572360	15.417704	29.003941
O	12.149555	14.876079	28.458464
O	15.507931	17.131886	27.141591
O	11.545133	17.009268	26.950070
O	13.564069	17.079017	29.035907
Zr	13.585537	13.493751	29.579235
O	14.626475	14.571040	28.124588
H	15.643084	11.593867	29.092564
O	15.078409	12.114013	28.514140
O	11.712525	9.867828	27.191578
O	15.783098	9.956152	27.029492
O	13.679793	9.893927	29.061291
O	12.597229	12.426845	28.092519
O	17.172828	13.674848	29.123308
O	17.148853	15.591683	27.193626
O	17.293860	11.626339	27.070817
O	10.027827	13.327114	29.001931
O	10.096587	11.426424	27.051148

O	9.998438	15.372509	26.931331
O	13.585655	15.493499	30.634792
O	13.563809	11.495825	30.639497
O	15.551069	13.619552	30.683301
O	11.597511	13.377784	30.616064
O	13.784556	9.704328	25.369779
H	14.613588	9.212739	25.350279
H	9.743112	9.452767	27.223911
H	9.698417	13.548858	23.069451
H	13.392188	17.420428	23.068239
H	13.500952	9.521528	31.032414
H	13.672145	17.471080	31.008809
H	17.462039	17.575851	27.347592
H	17.508171	13.849259	31.102320
H	9.626557	13.164961	30.968917
H	17.722590	13.344599	23.201422
H	9.566048	17.332687	26.766431
H	17.773063	9.682410	26.883959
H	14.518952	11.712968	22.735825
Ni	13.007600	9.984862	23.562712
C	12.061065	9.783088	21.935142
C	10.925563	10.772025	21.791925
H	11.357734	11.783856	21.732279
H	10.310427	10.758833	22.711854
C	11.802526	8.528309	22.687923
H	10.758081	8.370227	22.993761
H	12.201365	7.609076	22.232978
H	12.336634	8.496886	23.736160
C	12.977812	9.698964	20.743494
H	12.475914	9.268881	19.857164
H	13.327862	10.700130	20.449565
H	13.862448	9.073775	20.936294
C	10.014180	10.549032	20.582138
H	9.244715	11.338369	20.579039
H	10.592059	10.712367	19.656494
C	9.351809	9.187455	20.538411
H	10.086744	8.371810	20.450854
H	8.760092	8.993730	21.446867
H	8.669016	9.092419	19.682997

J to N TS

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976

C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.732804	11.718102	23.328948
Zr	13.683850	13.475661	24.532552
O	10.074463	13.410011	25.045031
O	11.667171	13.559381	23.460639
O	15.732628	13.424735	23.509746
O	13.609132	15.455219	23.455175
Zr	13.723852	10.962624	27.082919
Zr	11.116953	13.408915	27.023320
O	15.041752	14.944140	25.658779
O	12.313678	11.983764	25.597156
O	12.570856	14.489083	26.005348
O	14.734751	12.487179	26.058792
O	13.492204	17.045784	25.044821
O	17.271043	13.540438	25.150995
Zr	13.552871	16.000921	27.048069
Zr	16.150136	13.572001	27.113436
H	11.771693	11.408368	25.042620
H	15.589277	15.528749	25.127320
H	11.572368	15.417876	29.002247
O	12.149950	14.874972	28.458428
O	15.507696	17.130612	27.141086
O	11.545716	17.008019	26.947901
O	13.563805	17.077369	29.035543
Zr	13.587506	13.496029	29.582270
O	14.626508	14.571996	28.125532
H	15.643082	11.592145	29.092453
O	15.079375	12.117808	28.518063
O	11.714579	9.870921	27.193735
O	15.784566	9.954389	27.055220
O	13.680349	9.896919	29.060017
O	12.600468	12.426998	28.093701
O	17.172680	13.675997	29.123398
O	17.149828	15.591969	27.193315
O	17.292133	11.627905	27.062189
O	10.027992	13.326995	29.001900
O	10.095974	11.426608	27.052221
O	9.997744	15.372694	26.934220
O	13.585201	15.493723	30.636247
O	13.564262	11.495161	30.641331
O	15.551162	13.621940	30.684226
O	11.597593	13.377163	30.615866
O	13.841432	9.750253	25.331205
H	14.491428	9.044573	25.414322
H	9.745109	9.451205	27.220539
H	9.690932	13.577962	23.078036
H	13.399681	17.421207	23.068064
H	13.499860	9.519709	31.030347
H	13.672699	17.471670	31.008119
H	17.461400	17.576298	27.348259

H	17.508665	13.846273	31.102340
H	9.626475	13.165553	30.968851
H	17.722118	13.347512	23.200606
H	9.566542	17.333076	26.765943
H	17.772377	9.683999	26.870800
H	14.569381	11.682029	22.849744
Ni	13.057020	9.859170	23.565859
C	11.986192	10.065207	21.914863
H	12.541012	10.828808	21.360859
C	10.548008	10.360072	22.208585
H	10.480481	11.247711	22.863086
H	10.110786	9.526214	22.783835
C	12.510655	8.765632	21.996465
H	11.839734	7.907472	22.108267
H	13.461118	8.516332	21.510924
H	12.617454	8.492808	23.762133
C	9.679501	10.631961	20.968935
H	9.734420	9.732249	20.326483
C	8.230842	10.828490	21.385187
H	7.841240	9.963385	21.940515
H	8.121084	11.708755	22.038334
H	7.577801	10.985457	20.515176
C	10.190039	11.819137	20.166650
H	11.190948	11.646461	19.747907
H	9.522728	12.046072	19.323288
H	10.254191	12.724701	20.790634

K to O TS

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.745242	11.734669	23.315747
Zr	13.687872	13.483990	24.535356
O	10.067787	13.417685	25.042320
O	11.671887	13.572840	23.473482
O	15.733682	13.429821	23.508414
O	13.613926	15.456333	23.453485
Zr	13.724218	10.966922	27.076903
Zr	11.118248	13.412491	27.024946
O	15.044520	14.947052	25.659751
O	12.308662	12.005277	25.608284
O	12.572295	14.497029	26.008363

O	14.737592	12.490094	26.057070
O	13.492503	17.045578	25.044623
O	17.270793	13.538551	25.151304
Zr	13.553746	16.003359	27.050602
Zr	16.152487	13.572203	27.115038
H	11.779299	11.413263	25.058332
H	15.592261	15.532093	25.129026
H	11.572908	15.417930	29.005419
O	12.150207	14.875712	28.460635
O	15.508057	17.131458	27.141950
O	11.544988	17.009292	26.950094
O	13.563553	17.078458	29.035957
Zr	13.588702	13.495222	29.582997
O	14.627616	14.572641	28.126199
H	15.644939	11.591692	29.091029
O	15.081772	12.118614	28.517319
O	11.714701	9.871621	27.195191
O	15.780774	9.959807	27.037138
O	13.681498	9.899503	29.058873
O	12.602942	12.427702	28.095904
O	17.173475	13.677301	29.123739
O	17.150108	15.592126	27.193680
O	17.295185	11.627112	27.066570
O	10.028604	13.326594	29.001660
O	10.095899	11.426731	27.052139
O	9.998163	15.372623	26.934981
O	13.585886	15.493822	30.635978
O	13.565682	11.494648	30.643220
O	15.551338	13.621523	30.684181
O	11.597375	13.376836	30.616390
O	13.786238	9.795293	25.290948
H	14.323792	8.999096	25.360250
H	9.745179	9.450918	27.219368
H	9.699779	13.550041	23.067303
H	13.394907	17.421145	23.068531
H	13.497701	9.518297	31.028689
H	13.672267	17.471423	31.008460
H	17.461781	17.576154	27.347325
H	17.508476	13.845616	31.102667
H	9.625949	13.166158	30.968417
H	17.722680	13.344625	23.201456
H	9.566065	17.332222	26.763306
H	17.770665	9.680538	26.882662
H	14.618592	11.662057	22.913977
Ni	12.904369	9.957274	23.554094
C	12.207538	9.893739	21.658408
C	11.279594	9.392428	22.603480
H	10.486358	10.060343	22.970965
H	10.967986	8.342559	22.580871
H	12.317910	8.669524	23.829021
C	11.955919	11.245766	21.005535

H	11.740284	11.969893	21.805083
C	10.718824	11.154959	20.109505
H	10.513698	12.122921	19.629432
H	10.851534	10.416620	19.302736
H	9.819824	10.867827	20.673643
C	13.138328	11.775524	20.209658
H	12.942707	12.801989	19.869632
H	14.062589	11.805975	20.800039
H	13.332980	11.171373	19.309625
C	13.050737	8.917401	20.888580
H	12.660272	8.780851	19.864796
H	14.086820	9.269981	20.771778
H	13.083497	7.928091	21.363868

L to P TS

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.703501	11.714898	23.334089
Zr	13.682632	13.474439	24.531790
O	10.072588	13.404201	25.044784
O	11.667045	13.546116	23.461066
O	15.731254	13.411514	23.513312
O	13.606265	15.454666	23.455662
Zr	13.726298	10.960618	27.085339
Zr	11.119059	13.409336	27.025503
O	15.042004	14.943447	25.657878
O	12.312659	11.988567	25.610260
O	12.569703	14.491354	26.003927
O	14.734899	12.485704	26.058651
O	13.493602	17.046426	25.044583
O	17.272684	13.543951	25.150291
Zr	13.553260	16.001073	27.047593
Zr	16.149876	13.572050	27.112564
H	11.757469	11.422089	25.059237
H	15.589986	15.528820	25.127729
H	11.572790	15.419035	29.002107
O	12.150305	14.875604	28.458762
O	15.507727	17.130646	27.140499
O	11.545595	17.008340	26.948190
O	13.564148	17.077244	29.035503
Zr	13.587788	13.496198	29.583107

O	14.626333	14.571724	28.125107
H	15.644678	11.592690	29.092845
O	15.080174	12.117345	28.518311
O	11.714839	9.871221	27.193001
O	15.785685	9.953016	27.059201
O	13.680844	9.896305	29.060343
O	12.600530	12.426310	28.098484
O	17.172377	13.675752	29.123281
O	17.149690	15.591971	27.193552
O	17.291464	11.628220	27.059774
O	10.028198	13.326204	29.001793
O	10.094227	11.425641	27.049335
O	9.997967	15.372578	26.933890
O	13.585299	15.493856	30.636546
O	13.565186	11.494964	30.641587
O	15.551313	13.621802	30.684616
O	11.597202	13.378302	30.616481
O	13.852373	9.744811	25.336567
H	14.523185	9.057606	25.401701
H	9.745853	9.450276	27.222232
H	9.691873	13.600215	23.079126
H	13.400815	17.420983	23.067699
H	13.498546	9.519742	31.030296
H	13.672395	17.471830	31.008008
H	17.461358	17.576283	27.348571
H	17.508883	13.846634	31.102085
H	9.626208	13.165188	30.968552
H	17.720853	13.355564	23.198435
H	9.566424	17.332967	26.765839
H	17.772905	9.684741	26.869393
H	14.563589	11.619882	22.907812
Ni	12.956576	9.889371	23.627031
C	11.668874	10.143933	22.164408
H	12.120595	10.934818	21.555608
C	10.283751	10.403803	22.683125
H	10.319816	11.041083	23.589626
H	9.834086	9.458561	23.034197
C	12.203940	8.840761	22.123964
H	11.545293	7.974530	22.253744
H	13.079713	8.623206	21.501147
H	12.517202	8.508972	23.762813
C	9.367328	11.079240	21.671770
H	9.310700	10.462090	20.757535
H	9.831032	12.028465	21.346673
C	7.970020	11.338240	22.210095
H	7.495605	10.374464	22.463958
H	8.044093	11.877027	23.171669
C	7.090747	12.112030	21.250541
H	6.976260	11.586205	20.290850
H	6.083232	12.275228	21.655826
H	7.515423	13.102077	21.024666

M to Q TS

C	10.482472	13.517337	23.859336
C	13.496088	16.642020	23.854618
C	16.909266	13.434581	23.954900
C	10.368155	16.571681	26.878756
C	13.610859	16.682526	30.228037
C	16.949072	10.422173	26.990900
C	13.577455	10.302597	30.245503
C	16.707647	16.768005	27.232019
C	10.521585	10.244977	27.157976
C	16.745460	13.719069	30.304601
C	10.415685	13.285780	30.195738
O	13.700027	11.716548	23.334042
Zr	13.685314	13.474534	24.534202
O	10.071631	13.411172	25.044085
O	11.668608	13.570832	23.466423
O	15.731577	13.413598	23.512230
O	13.612765	15.455561	23.455070
Zr	13.725308	10.962426	27.083517
Zr	11.118469	13.410400	27.024778
O	15.043623	14.944579	25.659054
O	12.309512	11.990846	25.605124
O	12.572245	14.491097	26.006968
O	14.735097	12.488483	26.060796
O	13.492067	17.046041	25.044750
O	17.272171	13.543107	25.150447
Zr	13.553565	16.001388	27.048400
Zr	16.150862	13.572514	27.113770
H	11.765568	11.414702	25.052249
H	15.590781	15.530094	25.128276
H	11.572864	15.418724	29.003575
O	12.149984	14.875730	28.459386
O	15.507832	17.130825	27.140828
O	11.545432	17.008443	26.948549
O	13.563933	17.077616	29.035660
Zr	13.587758	13.496015	29.582639
O	14.627065	14.572469	28.126340
H	15.643548	11.592240	29.093410
O	15.079990	12.117667	28.518673
O	11.715045	9.870984	27.189037
O	15.785103	9.953887	27.057478
O	13.679552	9.896823	29.060012
O	12.600235	12.426891	28.096681
O	17.172933	13.675727	29.123517
O	17.150117	15.592154	27.194384
O	17.292020	11.628070	27.060904
O	10.028107	13.326834	29.001853
O	10.094361	11.425825	27.051774
O	9.997936	15.372603	26.933892
O	13.585100	15.493872	30.636486

O	13.565238	11.494968	30.641826
O	15.551315	13.621983	30.684447
O	11.597286	13.377634	30.616397
O	13.853616	9.765879	25.325384
H	14.515775	9.070105	25.390694
H	9.745944	9.450335	27.223861
H	9.694135	13.564229	23.073536
H	13.396691	17.420937	23.068107
H	13.499552	9.519553	31.030214
H	13.672681	17.471711	31.008139
H	17.461383	17.576451	27.347704
H	17.508715	13.846480	31.102305
H	9.626228	13.165164	30.968592
H	17.721258	13.354631	23.198956
H	9.566318	17.332841	26.765596
H	17.772533	9.684269	26.869968
H	14.540889	11.645611	22.866748
Ni	12.968977	9.875454	23.601331
C	11.672974	10.067760	22.077117
C	10.311872	10.263031	22.706618
H	10.338334	11.140948	23.376322
H	10.081700	9.402527	23.358000
C	12.250068	8.779309	22.113360
H	11.630262	7.900734	22.321665
H	13.113311	8.557672	21.472589
H	12.524581	8.524229	23.847338
C	12.094187	11.081937	21.057745
H	11.474110	10.979340	20.150398
H	11.976628	12.108463	21.429928
H	13.138729	10.949244	20.748491
C	9.173657	10.459007	21.704172
H	8.245330	10.645480	22.267259
H	9.349821	11.380541	21.123718
C	8.987373	9.281505	20.769764
H	9.880940	9.098504	20.153230
H	8.786920	8.353446	21.326667
H	8.146064	9.435912	20.080890

N

C	10.482544	13.517259	23.859349
C	13.495917	16.642094	23.854636
C	16.909358	13.434763	23.954851
C	10.368193	16.571681	26.878756
C	13.610903	16.682558	30.227995
C	16.948991	10.421979	26.991002
C	13.577434	10.302560	30.245525
C	16.707661	16.768011	27.232022
C	10.521536	10.244937	27.157959
C	16.745480	13.719082	30.304592
C	10.415725	13.285823	30.195699

O	13.730644	11.730783	23.312985
Zr	13.686442	13.482050	24.525487
O	10.071356	13.407862	25.043359
O	11.669832	13.574250	23.468186
O	15.732906	13.426309	23.510716
O	13.613084	15.456288	23.453692
Zr	13.728394	10.970691	27.083763
Zr	11.121235	13.413702	27.025211
O	15.043453	14.941322	25.659018
O	12.307602	12.000161	25.605730
O	12.573655	14.493282	26.006464
O	14.734471	12.476807	26.050805
O	13.492668	17.044573	25.045062
O	17.271181	13.542303	25.151024
Zr	13.554973	16.001958	27.048750
Zr	16.154122	13.569386	27.112160
H	11.735042	11.428324	25.078873
H	15.594730	15.523287	25.128380
H	11.573547	15.417407	29.003948
O	12.151592	14.874757	28.460324
O	15.507776	17.130615	27.140172
O	11.545325	17.008300	26.949987
O	13.565292	17.076835	29.035458
Zr	13.590648	13.497140	29.585996
O	14.626690	14.568966	28.123331
H	15.647481	11.589005	29.085037
O	15.082011	12.122558	28.519651
O	11.716050	9.871715	27.195447
O	15.783613	9.961218	27.074975
O	13.678640	9.901785	29.057564
O	12.604564	12.424707	28.098013
O	17.172102	13.677321	29.123155
O	17.149302	15.591631	27.193912
O	17.294654	11.629679	27.053632
O	10.029834	13.325299	29.001066
O	10.096470	11.425877	27.045783
O	9.998811	15.372012	26.933115
O	13.586107	15.493840	30.636646
O	13.567282	11.493951	30.644233
O	15.551270	13.624343	30.685219
O	11.597495	13.376722	30.616484
O	13.806593	9.738911	25.303882
H	13.998633	8.813203	25.489883
H	9.746069	9.450331	27.221967
H	9.695757	13.563626	23.072756
H	13.395402	17.421366	23.068851
H	13.498594	9.516707	31.026964
H	13.670633	17.471875	31.007967
H	17.461530	17.576012	27.348416
H	17.509413	13.843211	31.101997
H	9.625565	13.167476	30.968001

H	17.721884	13.345465	23.200799
H	9.566019	17.332219	26.765166
H	17.768667	9.681903	26.863722
H	14.607346	11.633013	22.922970
Ni	12.894922	9.932112	23.639988
C	11.400612	10.405181	22.382964
H	11.507181	11.495250	22.302168
H	12.282955	8.642533	23.896777
C	12.376318	9.635892	21.749287
H	12.203235	8.577081	21.532115
H	13.161723	10.124548	21.163942
C	10.058791	9.913915	22.827175
H	9.833232	10.309852	23.835266
H	10.068072	8.815007	22.931092
C	8.920643	10.330125	21.880953
H	8.969668	11.430077	21.767394
C	9.088287	9.711003	20.502712
H	9.068336	8.610603	20.559209
H	8.279113	10.016777	19.824586
H	10.038298	9.997801	20.029521
C	7.573747	9.980431	22.491600
H	6.743222	10.291423	21.842354
H	7.478793	8.893855	22.644518
H	7.430583	10.463683	23.468844

O

C	10.482544	13.517259	23.859349
C	13.495917	16.642094	23.854636
C	16.909358	13.434763	23.954851
C	10.368193	16.571681	26.878756
C	13.610903	16.682558	30.227995
C	16.948991	10.421979	26.991002
C	13.577434	10.302560	30.245525
C	16.707661	16.768011	27.232022
C	10.521536	10.244937	27.157959
C	16.745480	13.719082	30.304592
C	10.415725	13.285823	30.195699
O	13.703896	11.724424	23.308753
Zr	13.686887	13.476059	24.532095
O	10.070168	13.396556	25.042911
O	11.668915	13.611211	23.476557
O	15.732675	13.427497	23.509400
O	13.623253	15.457329	23.454652
Zr	13.725538	10.973499	27.084434
Zr	11.115183	13.409193	27.018913
O	15.043570	14.943878	25.661526
O	12.322070	11.983929	25.589307
O	12.574895	14.485631	26.010317
O	14.740781	12.482786	26.055444
O	13.486777	17.044201	25.045724

O	17.270997	13.542716	25.150940
Zr	13.553583	16.000575	27.048595
Zr	16.154439	13.572221	27.113506
H	11.820751	11.390045	25.018436
H	15.590413	15.526842	25.127560
H	11.572541	15.417453	29.003271
O	12.149345	14.874381	28.458763
O	15.507628	17.130119	27.141444
O	11.545145	17.008079	26.950676
O	13.564544	17.077055	29.035605
Zr	13.588108	13.497829	29.583466
O	14.627074	14.570585	28.125486
H	15.641961	11.589495	29.089472
O	15.079341	12.121647	28.519992
O	11.715355	9.871139	27.190832
O	15.784309	9.957311	27.071269
O	13.677827	9.899734	29.058570
O	12.600661	12.427387	28.091521
O	17.173269	13.676160	29.123661
O	17.150653	15.592207	27.195029
O	17.293706	11.628355	27.058982
O	10.028806	13.326484	29.001393
O	10.096144	11.426141	27.052367
O	9.998625	15.371650	26.928365
O	13.584771	15.493739	30.636517
O	13.564639	11.494803	30.642367
O	15.550985	13.624221	30.684237
O	11.597709	13.376206	30.615995
O	13.841802	9.739209	25.326786
H	14.331971	8.928712	25.506734
H	9.745384	9.450760	27.222006
H	9.698021	13.539597	23.070026
H	13.392250	17.421313	23.069125
H	13.501607	9.518329	31.029049
H	13.672462	17.471639	31.008115
H	17.461167	17.576764	27.346530
H	17.508691	13.844219	31.102630
H	9.626070	13.166948	30.968521
H	17.722076	13.344079	23.201120
H	9.565779	17.332518	26.768598
H	17.769783	9.683082	26.861227
H	14.485600	11.761095	22.743219
Ni	13.296880	9.735409	23.500363
C	11.791824	9.428298	22.128987
H	13.235651	8.304887	23.646186
C	13.059974	9.553070	21.541269
H	13.583605	8.674124	21.156069
H	13.364528	10.516116	21.120892
C	11.072128	8.088678	22.264222
H	10.806766	7.979130	23.333425
C	9.758640	8.100874	21.477760

H	9.933479	8.318927	20.412530
H	9.274580	7.116427	21.533221
H	9.037634	8.836292	21.856627
C	10.927952	10.643796	22.286782
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H	11.522641	11.563182	22.306009
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C	13.610903	16.682558	30.227995
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C	13.577434	10.302560	30.245525
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C	10.415725	13.285823	30.195699
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O	11.669728	13.575516	23.468209
O	15.732879	13.426077	23.510752
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Zr	13.728371	10.970831	27.083733
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O	12.307462	12.000375	25.605749
O	12.573802	14.493264	26.006598
O	14.734457	12.476828	26.050838
O	13.492567	17.044557	25.045077
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Zr	13.554996	16.001980	27.048776
Zr	16.154146	13.569389	27.112153
H	11.735090	11.427919	25.079348
H	15.594782	15.523294	25.128387
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O	15.507782	17.130625	27.140171
O	11.545320	17.008296	26.949986
O	13.565266	17.076853	29.035468
Zr	13.590670	13.497154	29.585992
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H	15.647463	11.589000	29.085061

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Ni	13.325372	9.748139	23.482539
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H	13.665896	8.619521	21.197559
H	13.550997	10.470298	21.073183

S7. References

1 B. Yeh, S. P. Vicchio, S. Chheda, J. Zheng, J. Schmid, L. Löbbert, R. Bermejo-Deval, O. Y. Gutiérrez, J. A. Lercher, C. C. Lu, M. Neurock, R. B. Getman, L. Gagliardi and A. Bhan, *J. Am. Chem. Soc.*, 2021, **143**, 20274–20280.

2 R. Y. Brogaard and U. Olsbye, *ACS Catal.*, 2016, **6**, 1205–1214.

3 B. Yeh, S. Chheda, S. D. Prinslow, A. S. Hoffman, J. Hong, J. E. Perez-Aguilar, S. R. Bare, C. C. Lu, L. Gagliardi and A. Bhan, *J. Am. Chem. Soc.*, 2023, **145**, 3408–3418.

4 R. Y. Brogaard, M. Kømurcu, M. M. Dyballa, A. Botan, V. Van Speybroeck, U. Olsbye and K. De Wispelaere, *ACS Catal.*, 2019, **9**, 5645–5650.

5 A. S. Hoffman, J. A. Singh, S. F. Bent and S. R. Bare, *J. Synchrotron Radiat.*, 2018, **25**, 1673–1682.

6 J. Zheng, L. Löbbert, S. Chheda, N. Khetrapal, J. Schmid, C. Alberto Gaggioli, B. Yeh, R. Bermejo-Deval, R. Kishan Motkuri, M. Balasubramanian, J. L. Fulton, O. Y. Gutiérrez, J. Ilja Siepmann, M. Neurock, L. Gagliardi and J. A. Lercher, *J. Catal.*, 2022, **413**, 176–183.

7 V. Bernales, A. B. League, Z. Li, N. M. Schweitzer, A. W. Peters, R. K. Carlson, J. T. Hupp, C. J. Cramer, O. K. Farha and L. Gagliardi, *J. Phys. Chem. C*, 2016, **120**, 23576–23583.

8 J. Ye, L. Gagliardi, C. J. Cramer and D. G. Truhlar, *J. Catal.*, 2017, **354**, 278–286.

9 J. Ye, L. Gagliardi, C. J. Cramer and D. G. Truhlar, *J. Catal.*, 2018, **360**, 160–167.

10 E. D. Metzger, R. J. Comito, C. H. Hendon and M. Dincă, *J. Am. Chem. Soc.*, 2017, **139**, 757–762.