

Supporting Information

Selective Methane Oxidation to Methanol on Dinuclear Copper-oxo Stabilized by Zirconia Nodes of NU-1000 Metal–Organic Framework

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Catalyst synthesis

Cu-NU-1000 samples were synthesized via an ion-exchange route in aqueous solution under ambient condition. Copper acetate was chosen as the Cu precursor. In a typical experiment, 0.5 g NU-1000 (0.23 mmol) was mixed with 300 ml of 0.001 to 0.01 M copper acetate solutions under stirring. A typical exchange time was 24 h. The measured pH values of the solution were 5.0–6.0 during exchange. After exchange, the product collected by centrifugation and was washed with deionized water at least 3 times and separated by centrifugation. After the last water washing, the sample was suspended in 50 ml acetone for 12 hours to allow solvent exchange. This step was repeated for 3 times and separated by centrifugation. The solvent exchanged sample was then collected and dried in vacuum oven overnight at 120 °C. The concentration of Cu in Cu-NU-1000 samples was determined from inductively coupled plasma–atomic emission spectroscopy (ICP-AES) measurements.

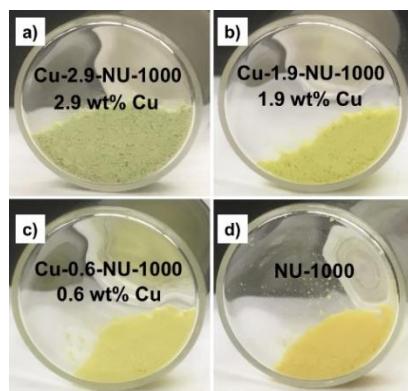


Figure S1. Color comparison of as prepared Cu-2.9-NU-1000, Cu-1.9-NU-1000, Cu-0.6-NU-1000, and pristine NU-1000. The color change of the MOF samples evidences the deposition of Cu. We also note that the sample with higher Cu loading (Cu-2.9-NU-1000, Figure S1a) shows more obvious blue-like color than the lower Cu loaded Cu-0.6-NU-1000 (Figure S1c).

Catalytic testing setup

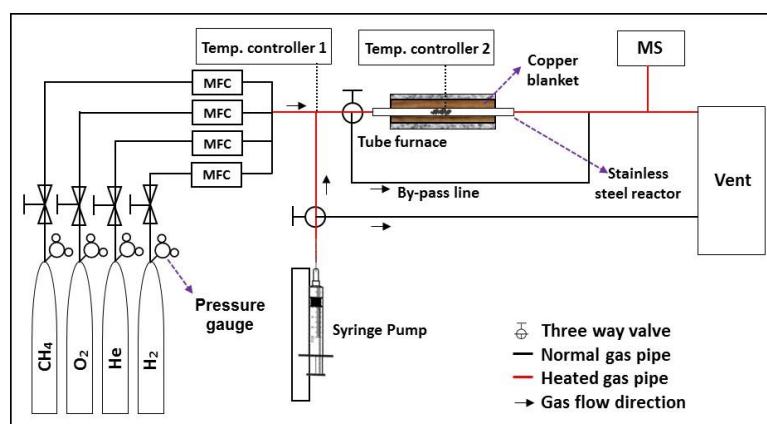


Figure S2. Schematic setup for testing direct methane oxidation over Cu-exchanged NU-1000

Effect of solvent exchange on the crystallinity and porosity of water treated NU-1000

Figure S3 and S4 show the comparison of XRD and N₂-sorption data of water treated NU-1000 with and without solvent exchange. For **acetone exchanged**, we firstly soaked NU-1000 in water to allow the pores to be filled with water. Then we replaced water with acetone and soaked NU-1000 in acetone overnight and following dried in an 80 °C oven for 4 hours. For the **non-acetone exchanged**, we directly dried it after water treatment without solvent exchange. The fresh synthesized parent NU-1000 is used as a reference. XRD and nitrogen sorption results confirm that direct drying water adsorbed NU-1000 leads to the crystallinity and porosity loss. An additional solvent exchange with acetone is necessary to retain the structure of NU-1000.

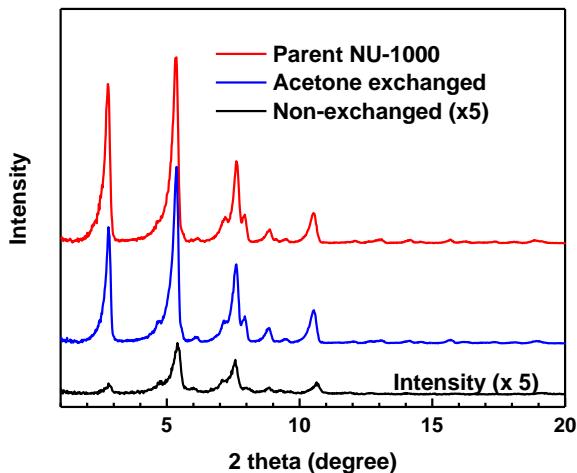


Figure S3. XRD patterns of NU-1000 samples with and without solvent exchange.

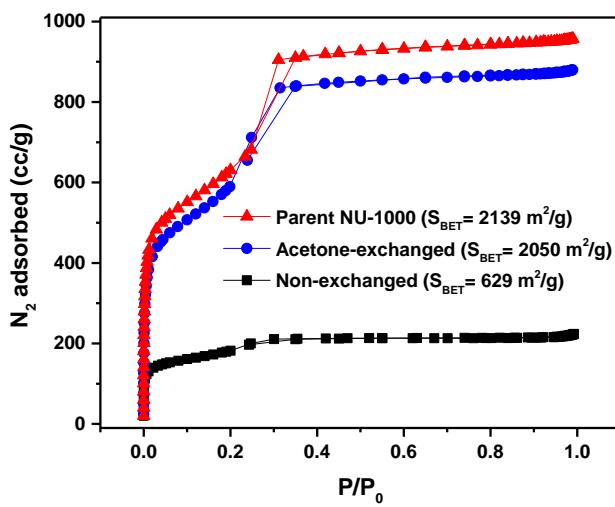


Figure S4. N₂ adsorption and desorption isotherms measured at 77 K of NU-1000 samples with and without solvent exchange.

Additional electron microscopy of Cu-2.9-NU-1000

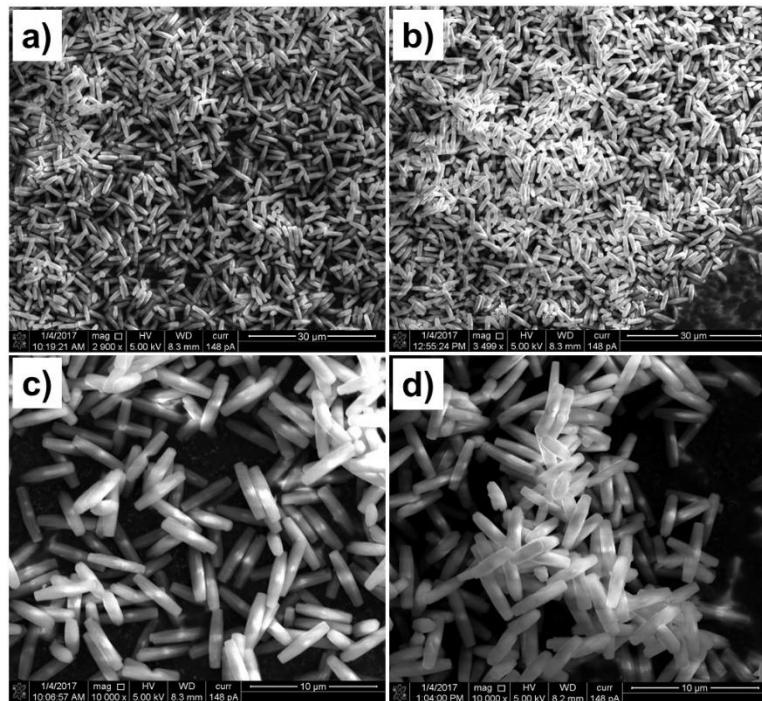


Figure S5. SEM image of (a, c) NU-1000 and (b, d) Cu-2.9-NU-1000. SEM images demonstrate that no change in the morphology or crystal size of NU-1000 MOF after Cu deposition

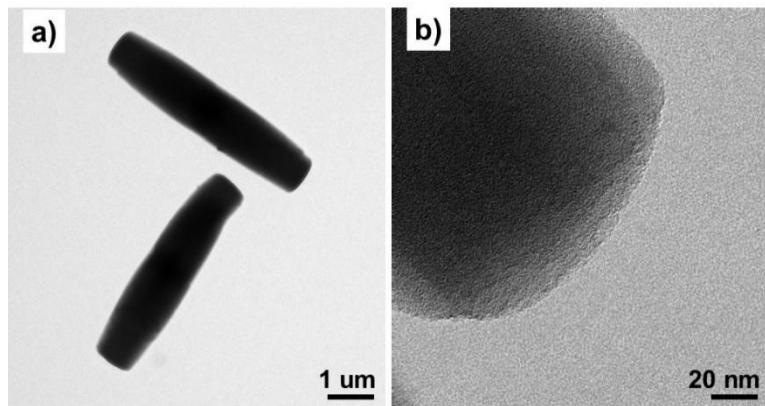


Figure S6. TEM image of Cu-2.9-NU-1000. TEM images confirm the absence of larger Cu nanoparticles (> 2 nm) in Cu-2.9-NU-1000.

XRD of three Cu-exchanged NU-1000 and pristine NU-1000

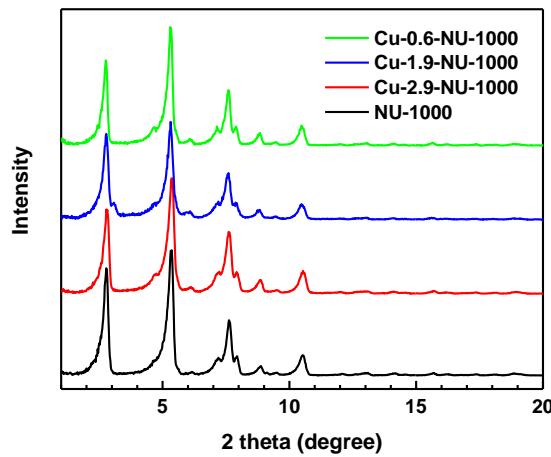


Figure S7. XRD patterns of three Cu-exchanged NU-1000 samples and the pristine NU-1000

N_2 -sorption of three Cu-exchanged NU-1000 and pristine NU-1000

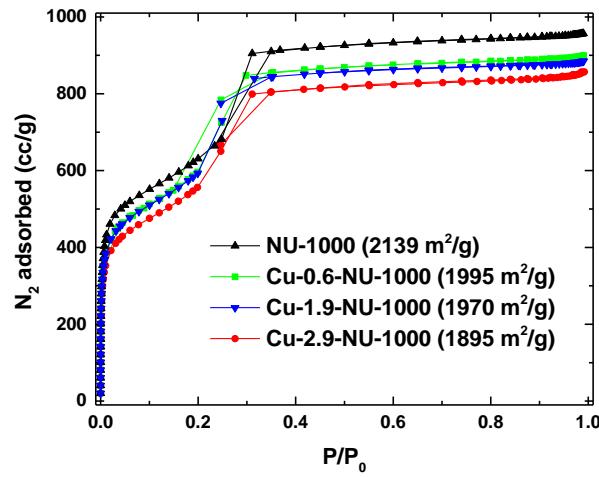


Figure S8. N_2 -sorption isotherms of Cu-exchanged NU-1000 samples and the pristine NU-1000

IR spectra of Cu-exchanged NU-1000 and pristine NU-1000

Figure S9 shows the FTIR spectra of Cu-exchanged NU-1000 and the pristine NU-1000. The sample pellets were firstly evacuated to 1.0×10^{-6} mbar at 150 °C for 2 h to remove the physically adsorbed water. Infrared spectra were then recorded after the system cooled to room temperature. In general, there is no significant change in all IR bands after Cu deposition (**Figure S9a**). However, as shown in **Figure S9b**, the height and the area of the peak at $\sim 3674\text{cm}^{-1}$ (terminal –OH group on the Zr₆ node) clearly decreases as more Cu was deposited. We integrated the area of this peak based on the normalization of the peak at 3074 cm⁻¹, which is assigned to the aromatic C-H stretching vibration from the 1,3,6,8-tetrakis(p-benzoicacid) pyrene (H₄TBAPy) linker. As listed in **Table S1**, the pristine NU-1000 gives a peak area of 1.71. The values for Cu loaded samples decrease to 1.56, 1.42, and 1.39 for Cu-0.6-NU-1000, Cu-1.9-NU-1000, and Cu-2.9-NU-1000, respectively. Since the pristine NU-1000 has 4 terminal –OH groups on each Zr₆ node, there are still 3.65, 3.31, and 3.28 terminal –OH groups retained for Cu-NU-1000 samples with the low, medium, and high Cu loading. Thus, there are 0.35, 0.69, and 0.72 –OH groups on each node consumed by 0.3, 0.9, and 1.3 Cu atoms. The information confirms that Cu species was successfully deposited onto and modified the Zr₆ nodes. Furthermore, it also suggests that Cu mainly presents as isolated Cu cations in Cu-0.6-NU-1000 and clusters in Cu-1.9-NU-1000 and Cu-2.9-NU-1000.

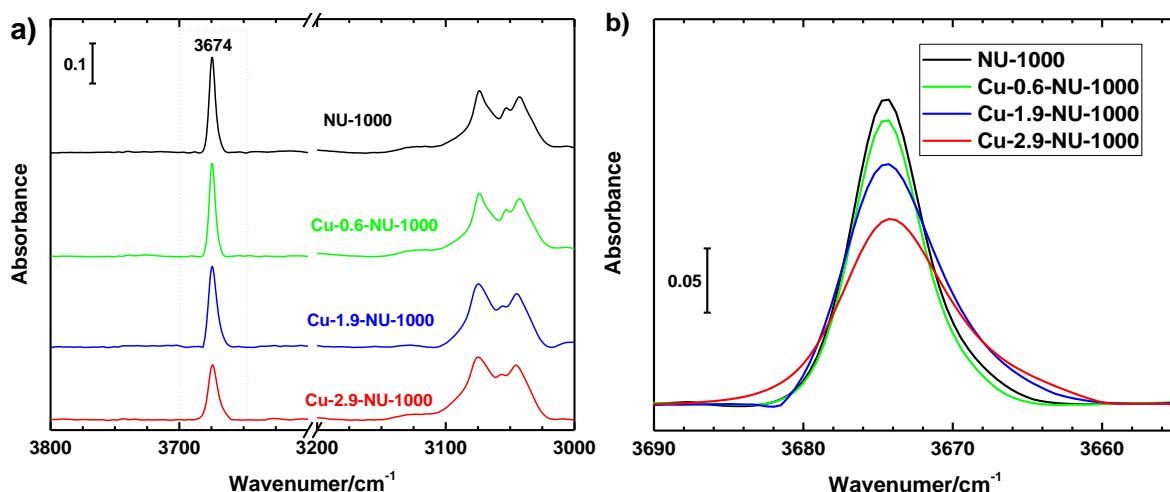


Figure S9. Transmission FTIR spectra of Cu-exchanged NU-1000 samples and the pristine NU-1000.

Table S1. The parameters determined from IR spectra by integrating the 3674 cm⁻¹ peak: ^a calculated based on the peak area at 3674 cm⁻¹ compared to the peak area of pristine NU-1000, ^b pristine NU-1000 has 4 terminal –OH groups on each Zr₆ node; ^c calculated based on the difference of terminal –OH groups between pristine NU-1000 and Cu-exchanged NU-1000.

| Sample | Cu loading | Deposited Cu atoms per Zr ₆ node | 3674 cm ⁻¹ peak height | 3674 cm ⁻¹ peak area | Amount of –OH groups per Zr ₆ node ^a | Number of consumed –OH groups per Zr ₆ node ^c |
|----------------|------------|---|-----------------------------------|---------------------------------|--|---|
| NU-1000 | -- | -- | 0.237 | 1.71 | 4 ^b | 0 |
| Cu-0.6-NU-1000 | 0.6 wt% | 0.3 | 0.221 | 1.56 | 3.65 | 0.35 |
| Cu-1.9-NU-1000 | 1.9 wt% | 0.9 | 0.187 | 1.42 | 3.31 | 0.69 |

| | | | | | | |
|----------------|---------|-----|-------|------|------|------|
| Cu-2.9-NU-1000 | 2.9 wt% | 1.3 | 0.149 | 1.39 | 3.28 | 0.72 |
|----------------|---------|-----|-------|------|------|------|

In situ FTIR of pyridine adsorption

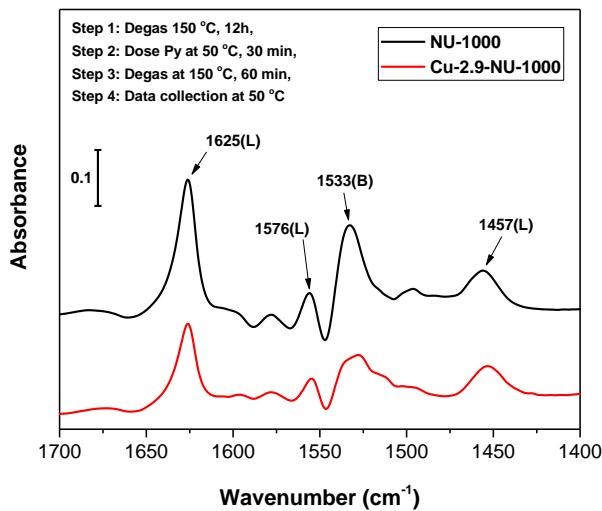


Figure S10. IR spectra of pyridine (Py) adsorption in parent NU-1000 and Cu-2.9-NU-1000. The samples were pressed into self-supported pellets and placed under dynamic vacuum ($<10^3$ mbar) at 150 °C overnight to remove surface-adsorbed water. After cooled to 50 °C, 1 mbar of pyridine was dosed to the IR cell and allowed the adsorption proceed for 30 min. After adsorption, the system was heated to 150 °C and kept this temperature for 60 min under vacuum, to remove any physisorbed pyridine. After cooled the IR cell to 50 °C, the data were collected in a transmission way. The adsorption of pyridine causes the appearance of several IR bands attributed to pyridinium ions coordinated with Lewis and Brönsted acid sites in the MOF. These observations agree with the fact that NU-1000 is an excellent Lewis acid catalyst owing to the high concentration of the Lewis acidic oxo-zirconium clusters in its structure.¹⁻² Deposition of Cu ions onto the node of NU-1000 decrease the intensity of the bands by 10-20%. This is consistent with that the loading of Cu is about 1 Cu atom per Zr₆ node (2.9 wt%). Due to the limited amount of Cu, the majority of the oxo-zirconium sites retain the same property as that of parent NU-1000.

EPR spectra of Cu-0.6-NU-1000 and Cu-2.9-NU-1000

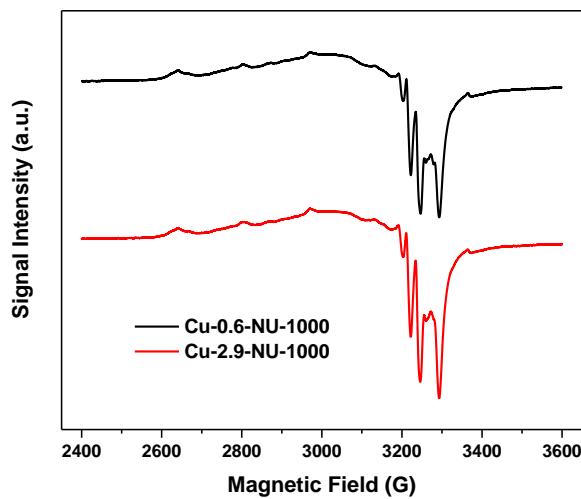


Figure S11. Electron paramagnetic resonance (EPR) spectra of fresh Cu-0.6-NU-1000 and Cu-2.9-NU-1000. EPR was used to quantify isolated Cu²⁺ ions in the samples, since other Cu sites are EPR silent. Experiments were conducted on a Bruker E580 X-band spectrometer equipped with a SHQE resonator and a continuous flow cryostat. ~10 mg of powder samples were contained in 4 mm OD quartz tubes and sealed with a rubber septa. In order to avoid signal loss, the data were collected at 125 K to freeze mobility of Cu ions. Quantification of isolated Cu²⁺ ions was done by using standard solutions of Cu(II)-imidazole. The two lines show more or less the same intensity of the spectra, although Cu-2.9-NU-1000 has near 5 time higher Cu loading than that of Cu-0.6-NU-1000. It suggests that the percentage of EPR active sites, namely, isolated Cu²⁺ are much higher in Cu-0.6-NU-1000. According to the quantification of the paramagnetic signals, isolated Cu²⁺ species accounts for 70–80% and 20–30 % of total in the Cu-0.6-NU-1000 and Cu-2.9-NU-1000.

XANES and EXAFS spectra of three as synthesized Cu-NU-1000 samples

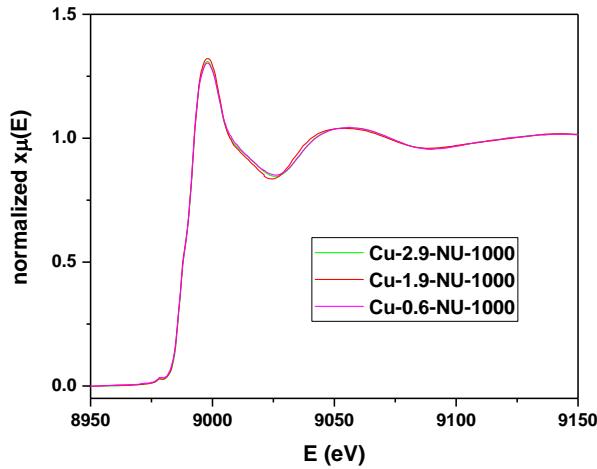


Figure S12. Normalized Cu k-edge XANES spectra of three Cu-exchanged NU-1000 samples. All three samples show nearly identical XANES spectra.

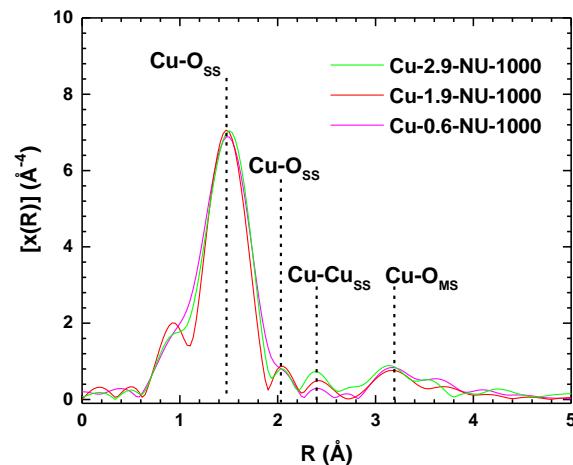


Figure S13. K³-weighted Cu k-edge Mag[$\chi(R)$] spectra of three Cu-exchanged NU-1000. Here the K³-weighted spectra are shown to highlight the high-Z Cu-Cu interaction. It is clear that the higher Cu-loaded sample Cu-2.9-NU-1000 (green curve) shows a more intensive Cu-Cu feature (~2.4 Å) than those of other two samples, although all the samples give weak Cu-Cu scattering feature.

XANES spectra of as-synthesized and O₂-activated Cu-2.9-NU-1000

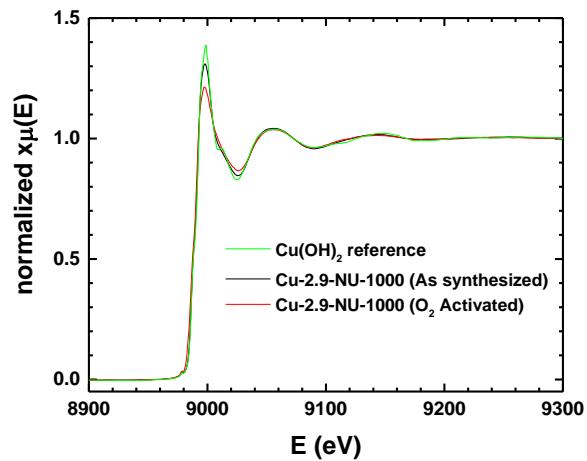


Figure S14. Normalized Cu k-edge XANES spectra of as-synthesized and O₂-activated Cu-2.9-NU-1000. Cu(OH)₂ is used as a reference. XANES spectra show that the structure of both as-synthesized and O₂-activated Cu-NU-1000 still most resemble the structure of Cu(OH)₂, although there is an intensity loss of the white line for the MOF samples.

Fitted result of the as synthesized Cu-2.9-NU-1000

Fitting the as-synthesized Cu-2.9-NU-1000 shows that there are 4 O atoms in the first shell with average Cu-O distance of 1.95 Å. We also note 1 additional O atom assigned to the J-T H₂O molecule with Cu-O distance of 2.37 Å. The coordination number of Cu-Cu is 0.9 and bond length is 2.85 Å.

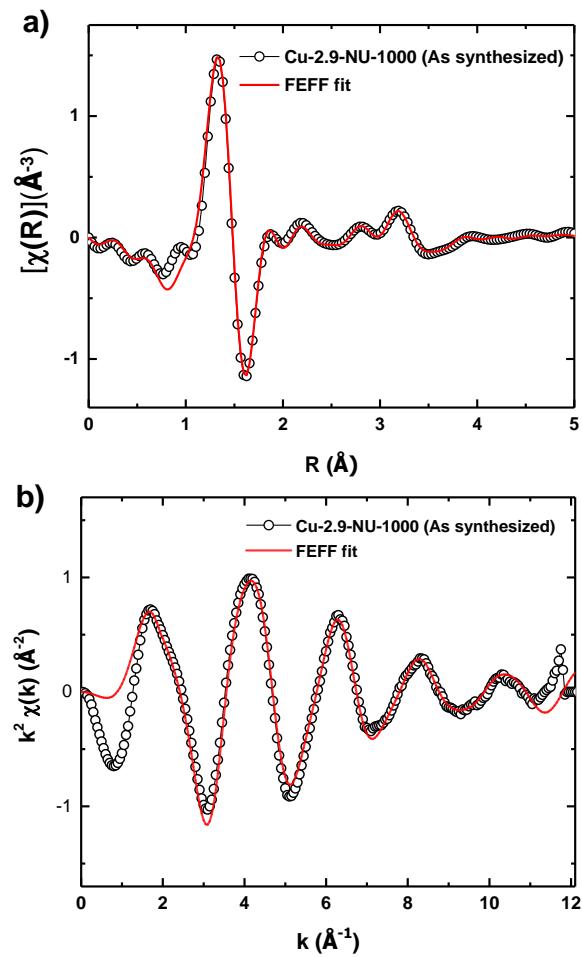


Figure S15. k^2 -weighted Cu K-edge (a) $\text{Img}[\chi(\mathbf{R})]$ and (b) $\chi(\mathbf{k})$ spectra of as-synthesized Cu-2.9-NU-1000 and the obtained FEFF fit. The color-coding is reported in the legend.

Table S2. The parameters determined from freshly prepared Cu-2.9-NU-1000 by fitting the experimental spectrum with a $\text{Cu}(\text{OH})_2$ model derived using FEFF9. Other parameters: amplitude reduction factor (amp) = 0.83, R-factor = 0.001, and $E_0 = -7.6 \pm 0.8$.

| Shell | CN | Distance (\AA) | DWF |
|----------------------|---------------|---------------------------|---------------------|
| Cu-O ₁ SS | 4.2 ± 0.3 | 1.954 ± 0.005 | 0.0040 ± 0.0007 |
| Cu-O ₂ SS | 0.8 ± 0.4 | 2.365 ± 0.011 | 0.0167 ± 0.0046 |
| Cu-Cu SS | 0.9 ± 0.3 | 2.846 ± 0.015 | 0.0081 ± 0.0047 |
| Cu-O MS | -- | 3.870 ± 0.020 | 0.0160 ± 0.0028 |

MS signal of CO₂ recorded during Cu-2.9-NU-1000 activation in O₂

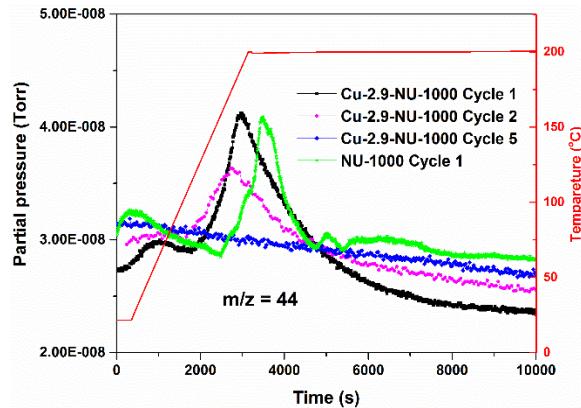


Figure S16. MS signal of CO₂ ($m/z = 44$) recorded during Cu-2.9-NU-1000 activation in O₂ in the first, second, and fifth cycle. The first cycle of pristine NU-1000 is used as a reference. We note that CO₂ was formed in the first cycle. The amount was becoming less in the second cycle and almost completely disappeared in the fifth cycle. CO₂ is also observed from the pristine NU-1000 activation under the same condition, but the peak shifted to a higher temperature.

MS signals recorded during products desorption after Cu-2.9-NU-1000 loaded with $^{13}\text{CH}_4$

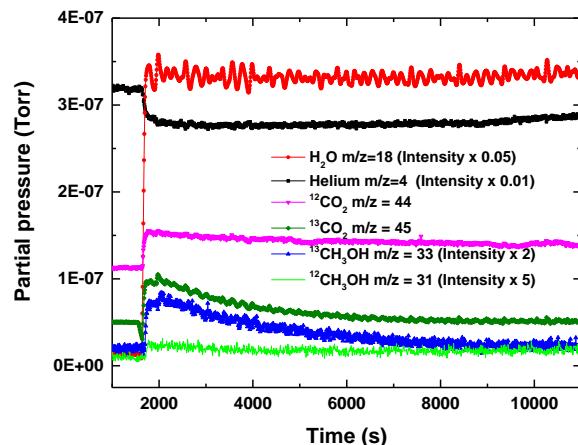


Figure S17. MS signals of H_2O ($m/z = 18$), helium ($m/z = 4$), $^{12}\text{CO}_2$ ($m/z = 44$), $^{13}\text{CO}_2$ ($m/z = 45$), $^{12}\text{CH}_3\text{OH}$ ($m/z = 31$), and $^{13}\text{CH}_3\text{OH}$ ($m/z = 33$) during products desorption at 135°C from Cu-2.9-NU-1000 after $^{13}\text{CH}_4$ loading. The intensity increase of signals for $^{13}\text{CO}_2$ ($\sim 4 \text{ mmol}_{\text{CO}_2}/\text{mol}_{\text{Cu}}$) and $^{13}\text{CH}_3\text{OH}$ ($\sim 9 \text{ mmol}_{\text{CO}_2}/\text{mol}_{\text{Cu}}$) upon steam injecting indicates the products desorption. The observation of $^{12}\text{CO}_2$ ($m/z = 44$) signal is contributed by the $^{12}\text{CO}_2$ from water. Except a very weak feature in the first 30 minutes, this signal is generally constant during the experiment, which suggests that there is only minor amount of $^{12}\text{CO}_2$ from Cu-2.9-NU-1000. This observation further confirms the methanol selectivity and the stability of Cu-2.9-NU-1000.

Additional high pressure experiments

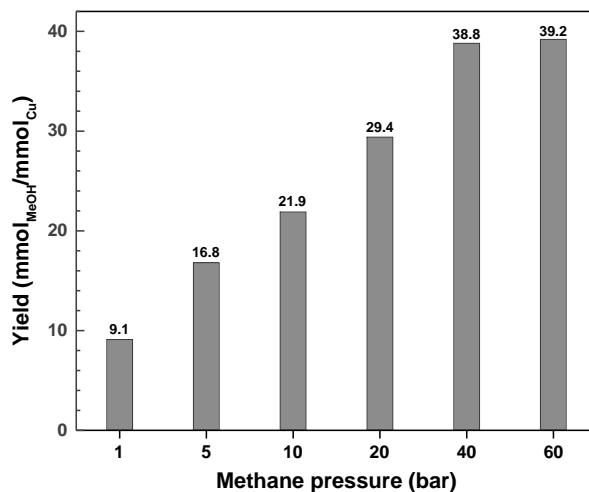


Figure S18. Effect of methane pressure on methanol productivity with Cu-2.9-NU-1000 as the catalyst. The sample was activated in 1 bar oxygen at 200°C for 2 h, then methane (1, 10, 20, 30, 40, and 60 bar) loaded at 200°C for 3 h, and steam-assisted product extracted in the flow of 10% H_2O and 90% He for 3 h at 135°C . The products were analyzed online by a MS spectrometer. We also observed a small amount of DME produced at the higher pressure. Thus, each DME molecule was considered as two methanol molecules for the calculation of total yield of partially oxidized products. It shows that the yield of methanol increased from 9.1 to 38.8 $\text{mmol}_{\text{MeOH}}/\text{mmol}_{\text{Cu}}$ as the pressure

of methane increased from 1 bar to 40 bar. The latter is more than 4 times higher than the value obtained at 1 bar. The promotive effect by further increasing methane pressure from 40 to 60 bar is negligible. Moreover, we observed only minor amounts of CO₂ (2-4 mmol_{CO2}/mol_{Cu}) were observed in the high pressure tests. These results demonstrate that increase methane pressure is an advantageous strategy to improve the methanol productivity for methane oxidation at low temperature. A detailed kinetic and mechanic study on how the methane pressure affect the productivity of methanol and the distribution of products will be provided in separate article.

XANES spectra recorded during CH₄ loading

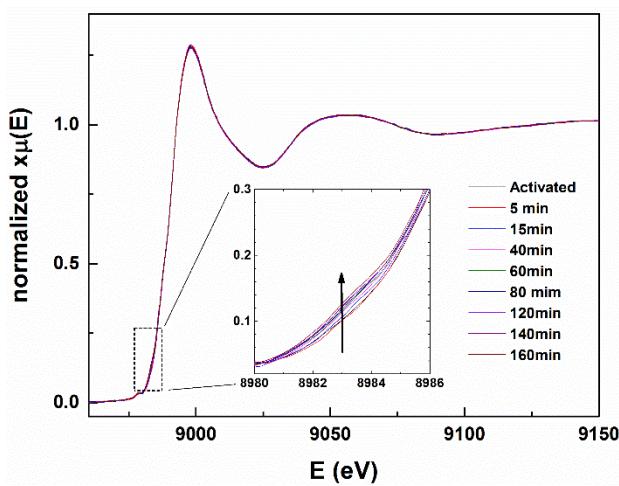


Figure S19. Normalized Cu k-edge XANES spectra recorded during CH₄ loading at 150 °C onto Cu-2.9-NU-1000 after O₂-activation. This figure shows that the overall shape of the XANES curves during CH₄ loading is unchanged,

only a very small increase in the Cu^I 1s→4p transition intensity at ~8983 eV was observed. Linear combination fitting suggests that ~6% of Cu^{II} was reduced to Cu^I upon CH₄ loading.

Fitted result of Cu-2.9-NU-1000 after 1 cycle catalysis

Fitting the used Cu-2.9-NU-1000 (after 1 catalytic cycle) shows similar structure to that of as-synthesized sample. There are still 4 O atoms in the first shell with average Cu-O distance of 1.94 Å. The coordination number of J-T O atom (~ 2.34 Å) is 1.3. The coordination number of Cu-Cu doesn't change, but the distance of Cu-Cu slightly increase to 2.89 Å.

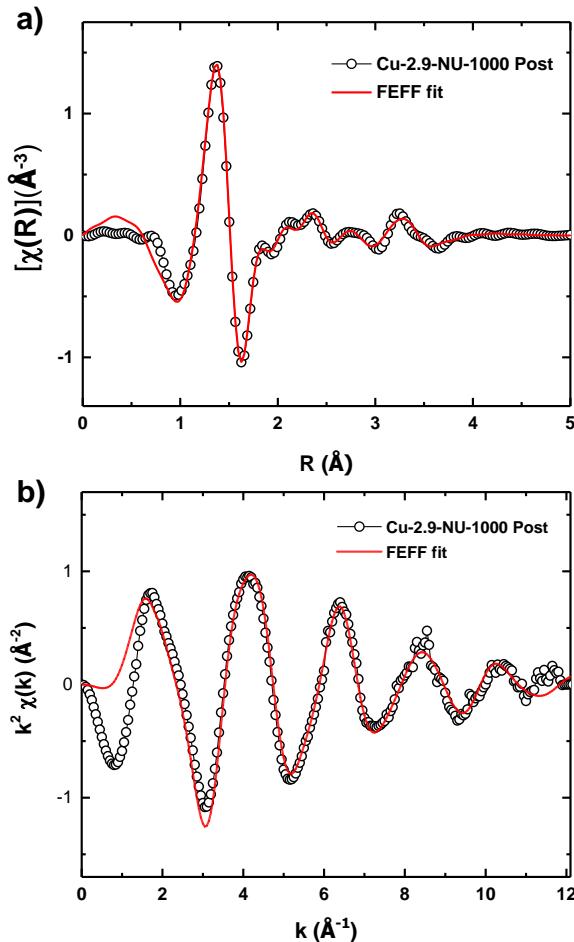


Figure S20. k^2 -weighted Cu K-edge (a) $\text{Im}[\chi(R)]$ and (b) $\chi(k)$ spectra of used Cu-2.9-NU-1000 and the obtained FEFF fits. The color-coding is reported in the legend.

Table S3. The parameters determined from Cu-2.9-NU-1000 after methane oxidation (1 cycle, 1 bar CH₄) by fitting the experimental spectrum with a Cu(OH)₂ model derived using FEFF9. Other parameters: amplitude reduction factor (amp) = 0.83, R-factor = 0.0012, and $E_0 = -7.6 \pm 0.8$.

| Shell | CN | Distance (Å) | DWF |
|----------------------|---------------|-------------------|---------------------|
| Cu-O ₁ SS | 4.1 ± 0.2 | 1.937 ± 0.004 | 0.0059 ± 0.0007 |
| Cu-O ₂ SS | 1.3 ± 0.5 | 2.335 ± 0.015 | 0.0193 ± 0.0065 |
| Cu-Cu SS | 0.9 ± 0.2 | 2.886 ± 0.016 | 0.0096 ± 0.0051 |
| Cu-O MS | -- | 3.874 ± 0.016 | 0.0236 ± 0.0028 |

Fit of k-plots of three samples

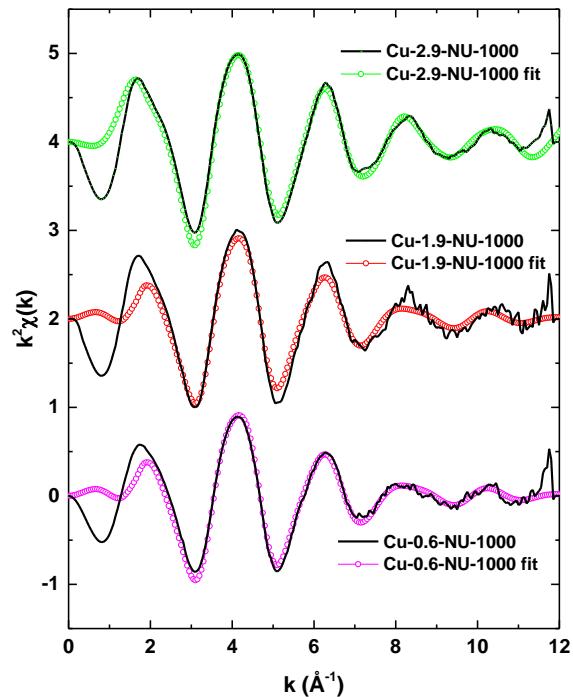


Figure S21. The $k^2\chi(k)$ Cu-EXAFS spectra of the three Cu-NU-1000 samples and the corresponded FEFF fits. The color-coding is reported in the legend.

Mass spectrometer signals of methanol ($m/z = 31$)

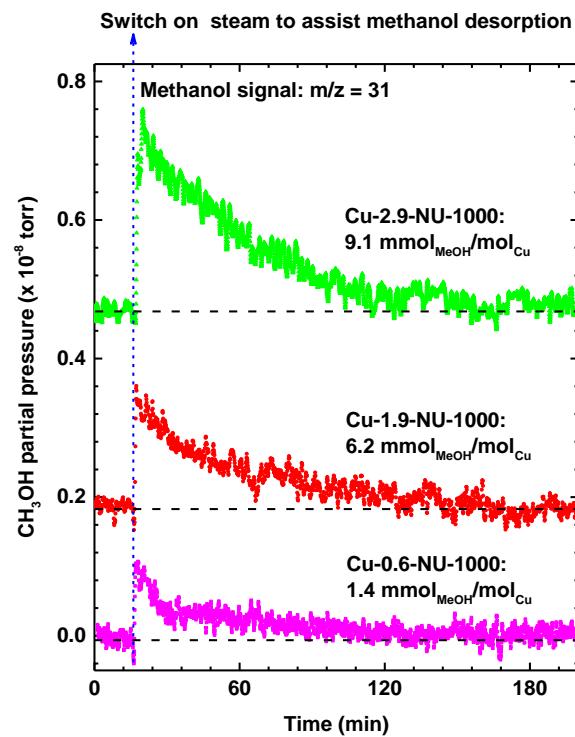


Figure S22. MS signal of methanol ($m/z = 31$) recorded during the products desorption (with steam/He = 10/90) from Cu-2.9-NU-1000 (green), Cu-1.9-NU-1000 (red), and Cu-0.6-NU-1000 (purple). The Cu-exchanged NU-1000 samples (80 mg for each) were activated in 1 bar O₂ at 200 °C for 2 hours. Then they contacted with 1 bar CH₄ at 150 °C for 3 hours. The values of methanol productivity per mole Cu is calculated after subtracting the contribution of NU-1000 MOF.

k¹, k², and k³-weighted EXAFS spectra of dicopper and monocopper samples

Figure S23 shows the k^1 -, k^2 -, and k^3 -weighted Cu-EXAFS $\text{Img}[\chi(R)]$ spectra of (a) Cu-2.9-NU-1000 (dimeric Cu dominated sample) and (b) Cu-0.6-NU-1000 (monomeric Cu dominated sample) after activation in O₂. The Cu-O peak has been scaled so that their amplitudes are approximately equivalent. As the k -weight increases (k^1 , k^2 , k^3) the amplitudes of the features between 2.0 and 2.6 Å increase (Figure S23a), which is indicative of backscattering from a higher-Z atom such as Cu. It confirms the presence of Cu-Cu scattering here. However, this change in Cu-0.6-NU-1000 is minor, indicating that Cu-Cu interaction here is missing or very weak (Figure S23b).

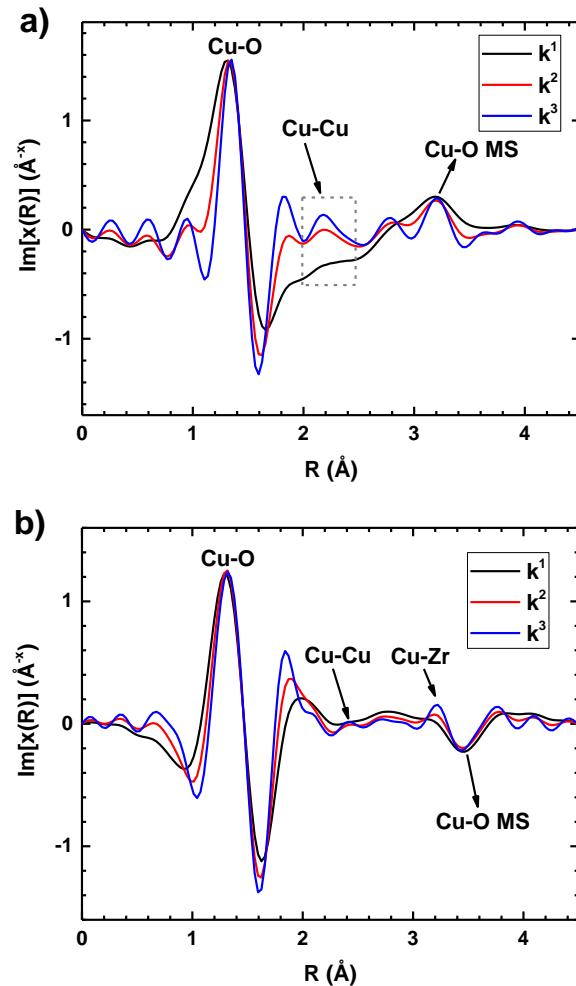


Figure S23. The k^1 -, k^2 -, and k^3 -weighted Cu-EXAFS $\text{Img}[\chi(R)]$ spectra of (a) Cu-2.9-NU-1000, and (b) Cu-0.6-NU-1000

XRD and BET measurements of Cu-NU-1000 after catalysis

Generally, the crystallinity of Cu-NU-1000 is largely the same after methane oxidation. There is very small decrease (< 5 %) in the porosity of the sample after 1 catalytic cycle either with 1 bar or 40 bar methane. The porosity loss slightly increased to ~10% after five catalytic cycles with 1 bar CH₄.

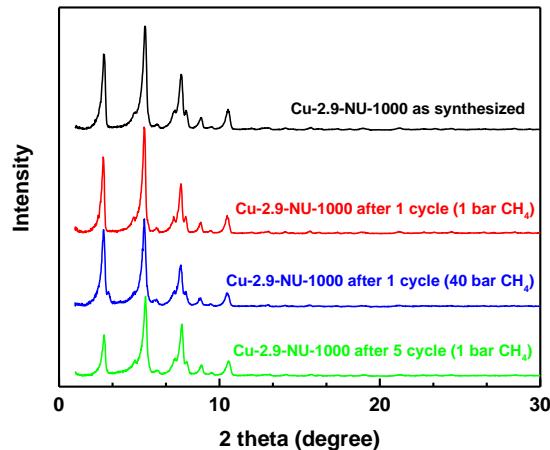


Figure S24. XRD patterns of Cu-2.9-NU-1000 after 1 and 5 cycle catalytic reaction with 1 bar methane, and 1 cycle reaction with 40 bar methane. The freshly prepared Cu-2.9-NU-1000 is used as a reference.

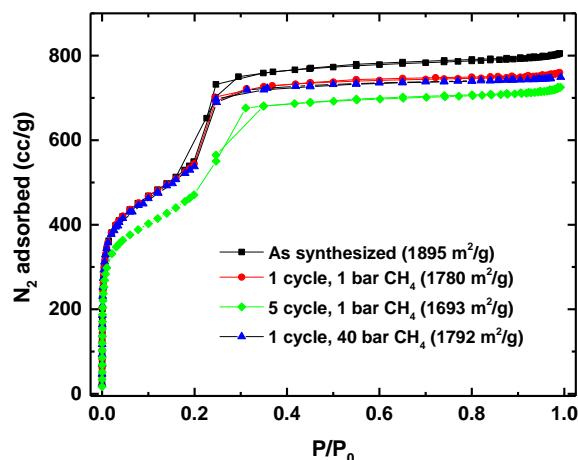


Figure S25. N₂-sorption isotherms of Cu-2.9-NU-1000 after 1 and 5 cycle catalytic reaction with 1 bar methane, and 1 cycle reaction with 40 bar methane. The freshly prepared Cu-2.9-NU-1000 is used as a reference.

DFT structures of mono-Copper NU-1000 nodes

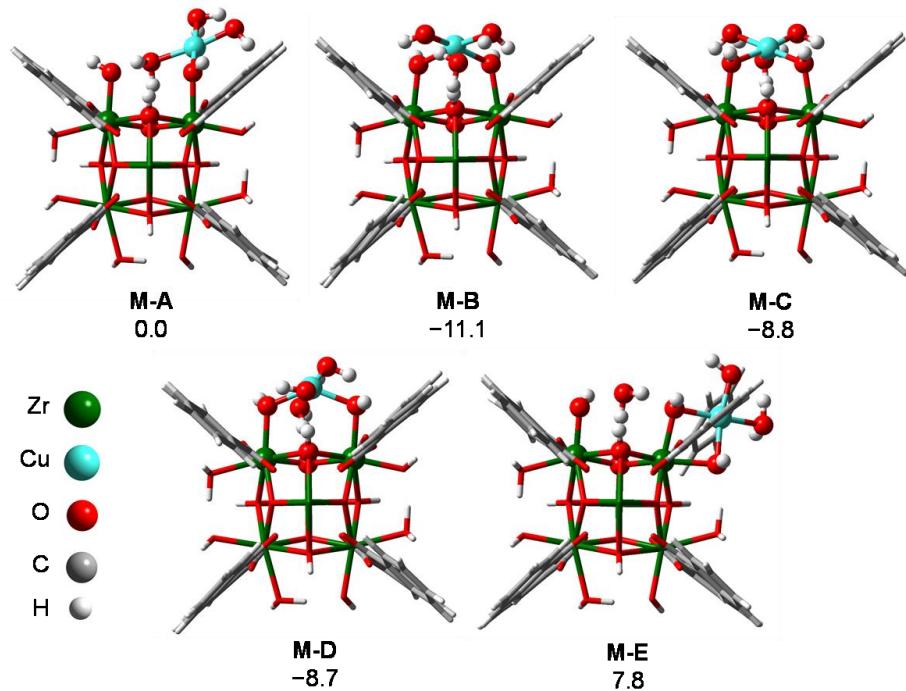


Figure S26. DFT-optimized structures of mono-copper NU-1000 cluster models. Electronic energies in kcal mol⁻¹. All energies are relative to **M-A**.

Additional comparison of simulated and experimental EXAFS for mono-copper models

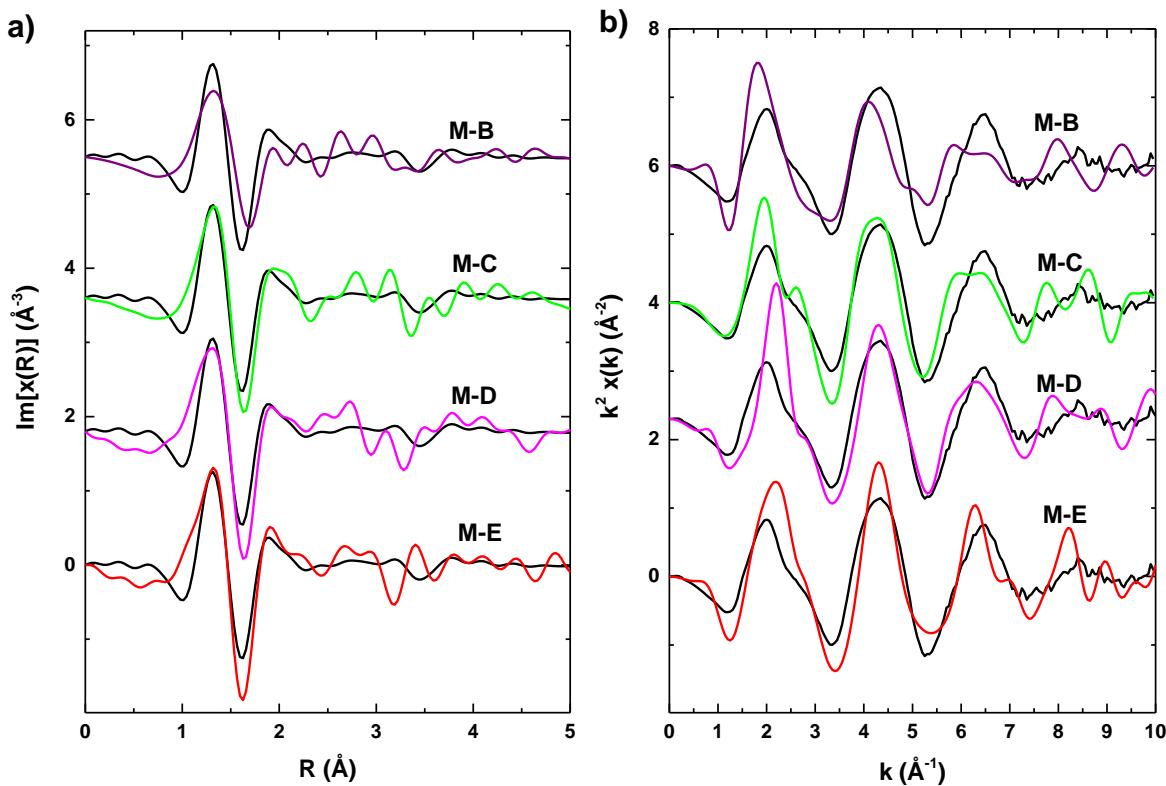


Figure S27. The k^2 -weighted Cu-EXAFS (a) $\text{Im}[\chi(R)]$ and (b) $\chi(k)$ spectra of experimentally measured Cu-0.6-NU-1000 (black curve) and the calculated EXAFS spectra of DFT optimized mono-copper models.

DFT structures of di-copper NU-1000 nodes

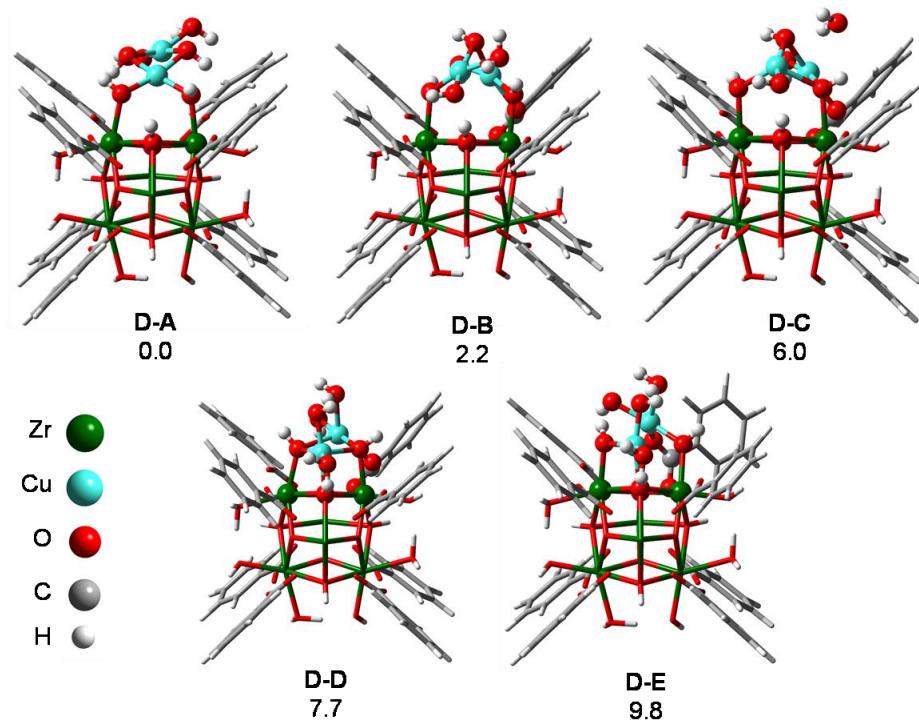


Figure S28. DFT-optimized structures of di-copper NU-1000 cluster models. Electronic energies in kcal mol⁻¹. All energies are relative to **D-A**.

Additional comparison of simulated and experimental EXAFS for di-copper models

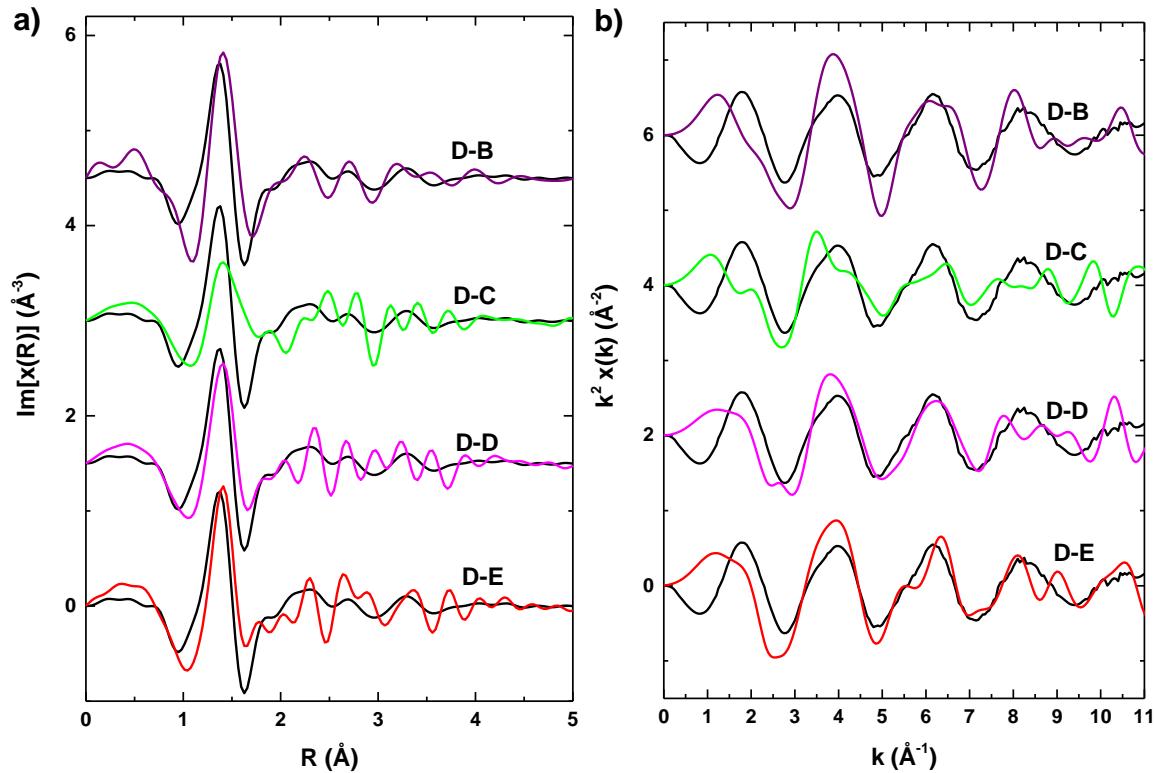


Figure S29. The k^2 -weighted Cu-EXAFS (a) $\text{Im}[\chi(R)]$ and (b) $x(k)$ spectra of experimentally measured Cu-2.9-NU-1000 (black curve) and the calculated EXAFS spectra of DFT optimized di-copper models.

3D drawing of the di-copper species in the large hexagonal pore

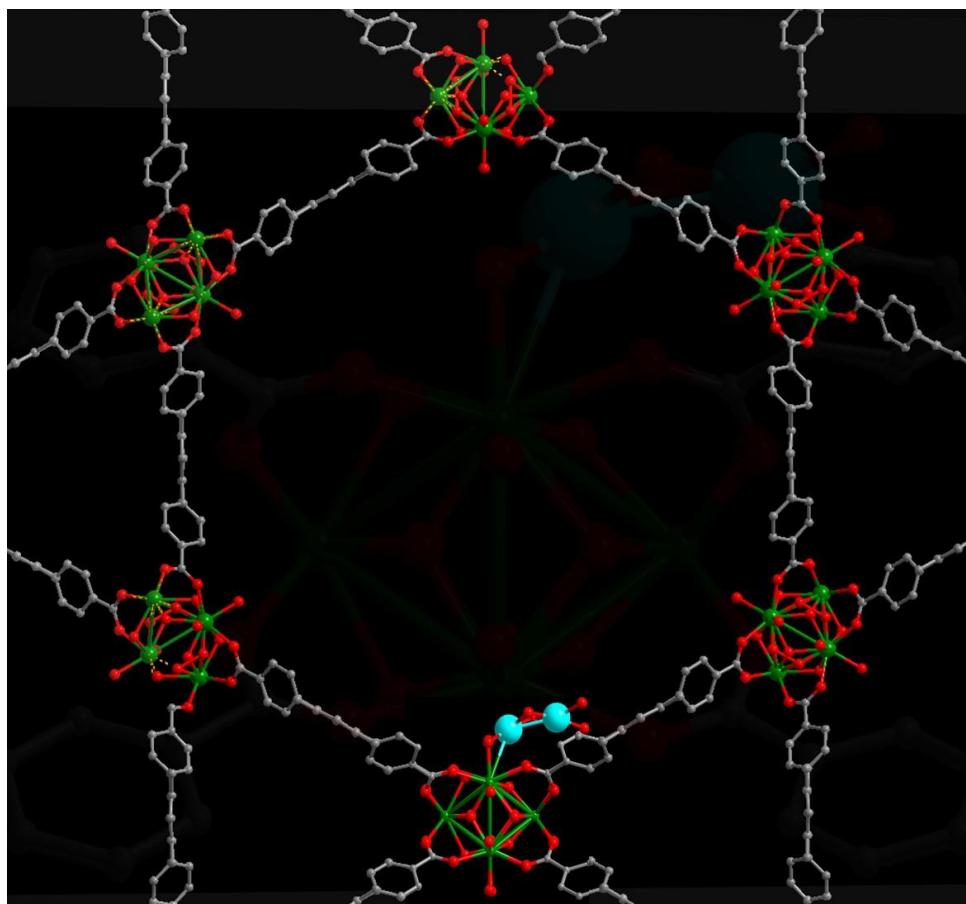


Figure S30. The 3D drawing to show the location of dinuclear copper center in the large pore of NU-1000.

Energies for all the optimized structures

Table S4. Electronic energies for all optimized structures.

| Species | <i>E</i> (a.u.) | Species | <i>E</i> (a.u.) |
|------------|-----------------|------------|-----------------|
| M-A | -5284.539551 | D-A | -5557.192131 |
| M-B | -5284.557270 | D-B | -5557.188600 |
| M-C | -5284.553501 | D-C | -5557.182523 |
| M-D | -5284.553436 | D-D | -5557.179901 |
| M-E | -5284.527085 | D-E | -5557.176565 |

Table S5. The spin state, electronic energy (*E*), enthalpy(*H*), Gibbs free energy(*G*) for the structures involving in the reaction pathways as calculated by density functional theory at 298.15 K and 1 atm.

| Structure | Spin quantum number <i>S</i> | <i>E</i> (a.u.) | <i>H</i> (a.u.) | <i>G</i> (a.u.) |
|--|------------------------------|-----------------|-----------------|-----------------|
| Cu ^{II} (OH) ₂ | 1/2 | -5648.359206 | -5647.718765 | -5647.848803 |
| TSA1 | 1/2 | -5688.830811 | -5688.147550 | -5688.286106 |
| A1 | 1/2 | -5688.836361 | -5688.148283 | -5688.288615 |
| TSA2 | 1/2 | -5688.774625 | -5688.091611 | -5688.228726 |
| A2 | 1/2 | -5688.838975 | -5688.149227 | -5688.287133 |
| Cu ^{II} O | 1/2 | -5571.871000 | -5571.258004 | -5571.383094 |
| TSA3 | 1/2 | -5612.356882 | -5611.699585 | -5611.83028 |
| A3 | 1/2 | -5612.409939 | -5611.747571 | -5611.879665 |
| Cu ^{II} (O·)(OH) | 1 | -5647.687756 | -5647.059474 | -5647.189536 |
| TSA4 | 1 | -5688.197373 | -5687.52586 | -5687.661958 |
| A4 | 0 | -5688.26016 | -5687.580121 | -5687.712793 |
| TSA5 | 0 | -5688.232707 | -5687.553781 | -5687.686802 |
| A5 | 0 | -5688.292305 | -5687.609339 | -5687.743722 |
| Cu ^{II} ₂ (OH) ₄ | 1 | -7440.616073 | -7439.941501 | -7440.082666 |
| TSB1 | 1 | -7481.099591 | -7480.380193 | -7480.526251 |
| B1 | 1 | -7481.126891 | -7480.401894 | -7480.548656 |
| TSB2 | 1 | -7481.046933 | -7480.328304 | -7480.473892 |
| B2 | 1 | -7481.103049 | -7480.379054 | -7480.525264 |
| Cu ^{II} ₂ O(OH) ₂ | 1 | -7364.095827 | -7363.44897 | -7363.585311 |
| TSB3 | 1 | -7404.598227 | -7403.906971 | -7404.049088 |
| B3 | 1 | -7404.668251 | -7403.970767 | -7404.111734 |
| TSB4 | 0 | -7404.603464 | -7403.911721 | -7404.051807 |

| | | | | |
|---|-----|--------------|--------------|--------------|
| B4 | 0 | -7404.693744 | -7403.992966 | -7404.135683 |
| Cu ^{II} ₂ (O·)(OH) ₃ | 3/2 | -7439.94732 | -7439.284361 | -7439.424986 |
| TSB5 | 3/2 | -7480.452888 | -7479.746842 | -7479.894676 |
| B5 | 1/2 | -7480.516805 | -7479.80291 | -7479.946531 |
| TSB6 | 1/2 | -7480.4839 | -7479.770751 | -7479.914587 |
| B6 | 1/2 | -7480.534276 | -7479.818375 | -7479.96373 |

Computational details

Catalyst structure determinations.

The calculations of the structures in Figure 6 were performed by density functional theory using the M06-L density functional³ as implemented in *Gaussian 09*.⁴ The M06-L functional has shown good performance for medium-range electron-correlation effects, transition metal chemistry,⁵ and MOF-supported catalysts.⁶ Numerical integrations were performed with an ultrafine grid. To reduce the computational cost, the automatic density-fitting set generated by the *Gaussian* program was used. The SDD effective core potentials potential and its associated double- ζ basis set was employed for Cu and Zr atoms,⁷ and the 6-31G(d) basis set was used for O, C, and H.⁸

Cluster models have been successfully employed to describe the structure and reactivity of Zr-based MOF nodes⁹ and they predict the same structural parameters than periodic approaches for a related system.¹⁰ Thus, we prepared a neutral cluster model containing one NU-1000 node and eight benzoate linkers. During optimization all atoms were relaxed while the *para* carbon atoms were fixed to mimic the MOF environment. All dinuclear and mononuclear Cu structures were calculated in the high-spin state: triplet and doublet, respectively.

Activated catalyst structure and reaction mechanism calculation.

Unrestricted density calculations were carried out using the M06-L density functional³ implemented in *Gaussian 09*⁴ to study the activated catalyst structures and reaction mechanism. The def2-SVP basis set was employed for C, H and O atoms of the node and linker, while the def2-TZVP basis set was employed for C, H, O, Cu of Cu-oxo cluster and Zr, including the SDD effective core potential for Zr. s,^{7, 11-12}

Cluster models contain one NU-1000 node with four benzoate and four formate linkers as shown in [Figure S31](#). During optimization all atoms were relaxed while the carbon atoms were kept fixed.

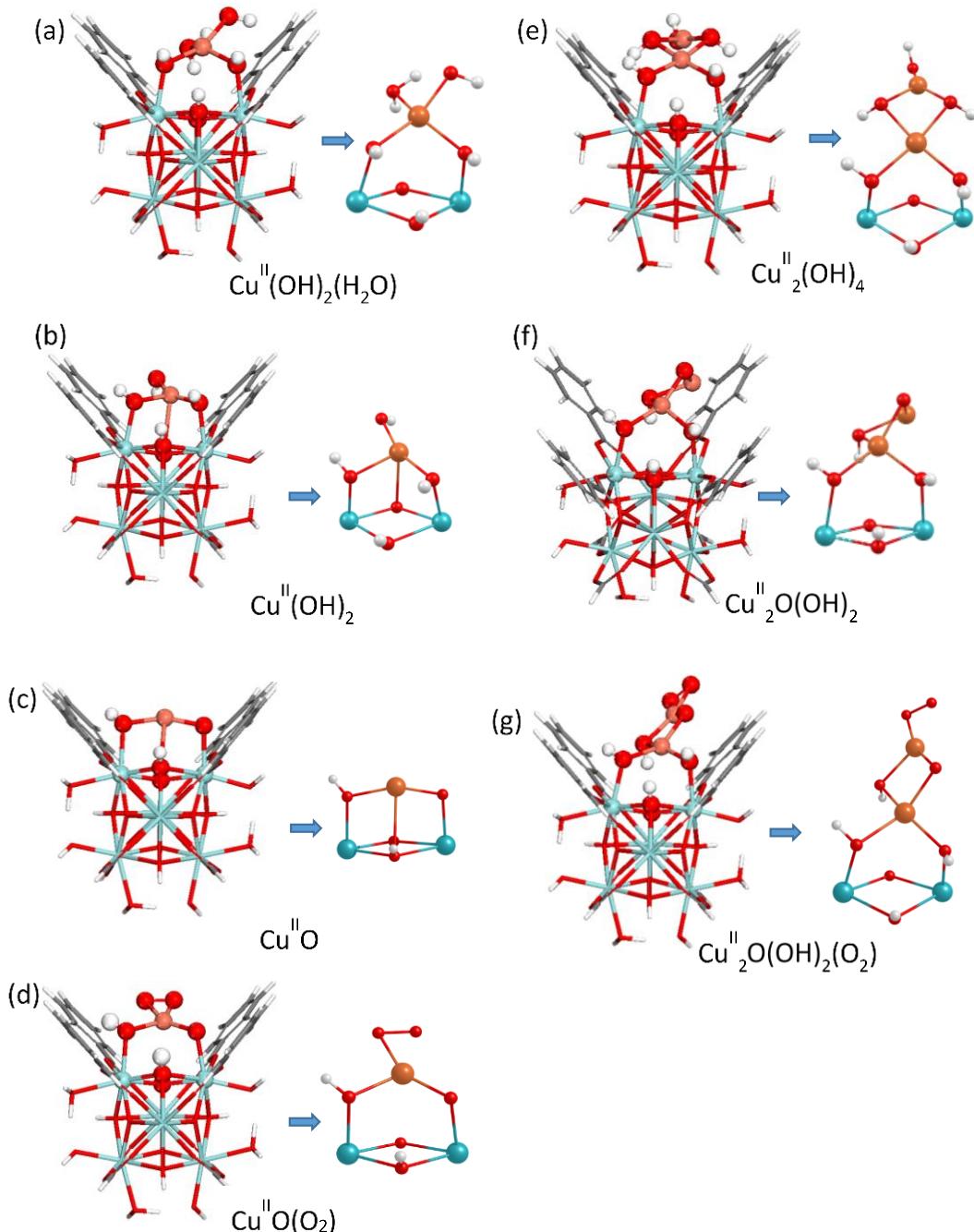
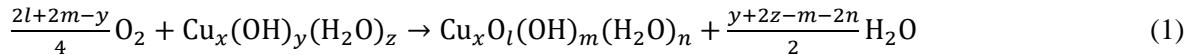


Figure 31. The cluster models for (a) $\text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O})$, (b) $\text{Cu}^{\text{II}}(\text{OH})_2$, (c) $\text{Cu}^{\text{II}}\text{O}$, (d) $\text{Cu}^{\text{II}}\text{O}(\text{O}_2)$, (e) $\text{Cu}^{\text{II}}_2(\text{OH})_4$, (f) $\text{Cu}^{\text{II}}_2\text{O}(\text{OH})_2$ and (g) $\text{Cu}^{\text{II}}_2\text{O}(\text{OH})_2(\text{O}_2)$. The NU-1000 node with the fragment shown in the form of sticks in the left hand column of the figures are ignored to clearly show the structures of copper species in the following sections, which are shown in the right hand column.

Thermodynamic analysis

Thermodynamic analysis was carried out to account for the influence of temperature and the presence of H₂O and O₂ on the relative stability of the Cu complexes in Cu-NU-1000 after O₂ activation. The electronic energies for this analysis are computed by density functional theory with the M06-L exchange-correlation functional. The def2-SVP basis set was employed for C, H and O atoms of the node and linker, while the def2-TZVP basis set was employed for C, H, O, Cu of Cu-oxo cluster, and Zr, including the SDD effective core potential for Zr. We consider the temperature range 298.15 K ≤ T ≤ 773.15 K and a total pressure of 1 atm. The equilibria between species with different chemical compositions were considered in terms of a set of reversible reactions of the form:



The standard-state Gibbs free energy of reaction ΔG(T, P) for this equilibrium is

$$\Delta G = G_{Cu_xO_l(OH)_m(H_2O)_n} - G_{Cu_x(OH)_y(H_2O)_z} + \frac{y+2z-m-2n}{2}\mu_{H_2O}^g - \frac{2l+2m-y}{4}\mu_{O_2}^g \quad (2)$$

We define T₀ as 298.15 K. and P₀ as 1 atm.

For the solids (first two terms on right side of eq 2), we make the approximation that the Gibbs free energies of solids are approximated by their Gibbs free energies at T₀ and P₀ as calculated using *Gaussian 09*.

The chemical potentials of gas-phase O₂ and H₂O are calculated assuming ideal gas-behavior and harmonic vibrations and are given by

$$\mu_{O_2}^g(T, p_{O_2}) = G_{O_2}(T_0, P_0) + \Delta\mu_{O_2}^g(T, p_{O_2}) \quad (3)$$

$$\begin{aligned} \Delta\mu_{O_2}^g(T, p_{O_2}) &= \Delta\mu_{O_2}^g(T, P_0) + RT\ln(\frac{p_{O_2}}{P_0}) \\ &= (H(T, P_0, O_2) - H(T_0, P_0, O_2) - T(S(T, P_0, O_2) \\ &\quad - S(T_0, P_0, O_2)) + RT\ln(\frac{p_{O_2}}{P_0}) \\ &= \int_{T_0}^T C_{P,O_2} dT - T \int_{T_0}^T \frac{C_{P,O_2}}{T} dT + RT\ln(\frac{p_{O_2}}{P_0}) \\ &= (T - T_0)C_{P,O_2} - T[\ln(T/T_0)]C_{P,O_2} + RT\ln\left(\frac{p_{O_2}}{P_0}\right) \end{aligned} \quad (4)$$

$$\begin{aligned} \Delta\mu_{H_2O}^g(T, p_{H_2O}) &= \Delta\mu_{H_2O}^g(T, P_0) + \frac{1}{2}RT\ln(\frac{p_{H_2O}}{P_0}) \\ &= (T - T_0)C_{P,H_2O} - T[\ln(T/T_0)]C_{P,H_2O} + RT\ln\left(\frac{p_{H_2O}}{P_0}\right) \end{aligned} \quad (5)$$

where R is the gas constant, p_{O₂} and p_{H₂O} are partial pressures, p_{H₂O} equals 1 - p_{O₂}, μ_{O₂}^g and μ_{H₂O}^g are chemical potentials of gas-phase O₂ and H₂O, Δμ_{O₂}^g(T, p_{O₂}) and Δμ_{H₂O}^g(T, p_{H₂O}) are the chemical potential changes of gas-phase O₂ and H₂O, and C_{P,O₂} and C_{P,H₂O} are the heat capacities of O₂ and H₂O at constant pressure (1 bar), respectively. We approximate C_P by its value at 298.15 K.

The enthalpy and entropy contributions are calculated from the partition functions using the harmonic oscillator approximation for vibrations. We did not scale the frequencies; frequencies below 50 cm⁻¹ were replaced by 50 cm⁻¹ when computing vibrational partition functions.

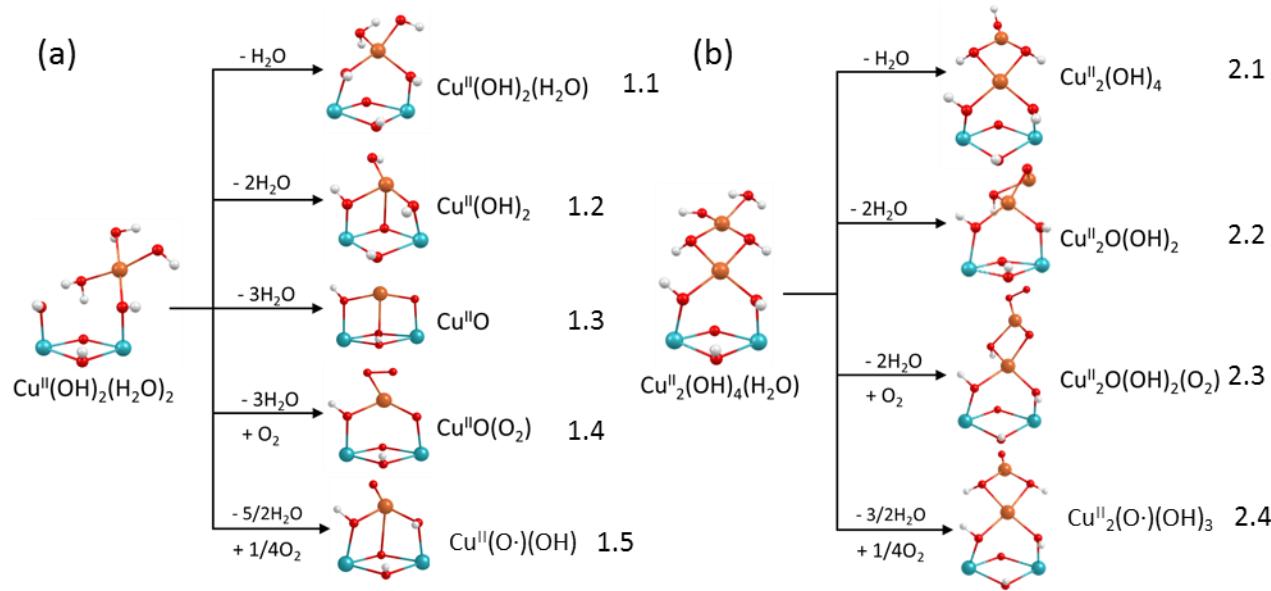


Figure S32. Possible Cu species, $\text{Cu}_x\text{O}_l(\text{OH})_m(\text{H}_2\text{O})_n$, generated under the activation conditions in (a) the mononuclear case and (b) the dinuclear case.

Table S6. Gibbs free energies of reaction (kcal/mol) as calculated by density functional theory at 298.15 K and 1 bar oxygen.

| | Reaction | Gibbs free energy of reaction |
|-----|--|-------------------------------|
| 1.1 | $\text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O})_2 \rightarrow \text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O}) + \text{H}_2\text{O}$ | 11.7 |
| 1.2 | $\text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O})_2 \rightarrow \text{Cu}^{\text{II}}(\text{OH})_2 + 2\text{H}_2\text{O}$ | 10.4 |
| 1.3 | $\text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O})_2 \rightarrow \text{Cu}^{\text{II}}\text{O} + 3\text{H}_2\text{O}$ | 26.4 |
| 1.4 | $\text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O})_2 + \text{O}_2 \rightarrow \text{Cu}^{\text{II}}\text{O}(\text{O}_2) + 3\text{H}_2\text{O}$ | 30.3 |
| 1.5 | $\text{Cu}^{\text{II}}(\text{OH})_2(\text{H}_2\text{O})_2 + 1/4\text{O}_2 \rightarrow \text{Cu}^{\text{II}}(\text{O}\cdot)(\text{OH}) + 5/2 \text{ H}_2\text{O}$ | 32.7 |
| 2.1 | $\text{Cu}^{\text{II}}_2(\text{OH})_4(\text{H}_2\text{O}) \rightarrow \text{Cu}^{\text{II}}_2(\text{OH})_4 + \text{H}_2\text{O}$ | 3.7 |
| 2.2 | $\text{Cu}^{\text{II}}_2(\text{OH})_4(\text{H}_2\text{O}) \rightarrow \text{Cu}^{\text{II}}_2\text{O}(\text{OH})_2 + 2\text{H}_2\text{O}$ | 39.6 |
| 2.3 | $\text{Cu}^{\text{II}}_2(\text{OH})_4(\text{H}_2\text{O}) + \text{O}_2 \rightarrow \text{Cu}^{\text{II}}_2\text{O}(\text{OH})_2(\text{O}_2) + 2\text{H}_2\text{O}$ | 36.4 |
| 2.4 | $\text{Cu}^{\text{II}}_2(\text{OH})_4(\text{H}_2\text{O}) + 1/4\text{O}_2 \rightarrow \text{Cu}^{\text{II}}_2(\text{O}\cdot)(\text{OH})_3 + 3/2 \text{ H}_2\text{O}$ | 25.1 |

Table S7. Heat capacity at constant pressure (1 atm) for O₂ and H₂O in gas phase. *a*, *b*, *c*, *d*, *e*, *f*, and *g* are obtained from the book: C. L. Yaws, *Yaws' Critical Property Data for Chemical Engineers and Chemists*, Knovel: Norwich, NY, 2012.

| $C_p = a + bT + cT^2 + dT^3 + eT^4 + fT^5 + gT^6$ (kcal mol ⁻¹ K ⁻¹) | O ₂ | H ₂ O |
|--|----------------|------------------|
| 298.15 K | 7.0291E-3 | 8.0301E-3 |
| 400 K | 7.2055E-3 | 8.1938E-3 |

| | | |
|-------|-----------|-----------|
| 800 K | 8.0672E-3 | 9.2436E-3 |
|-------|-----------|-----------|

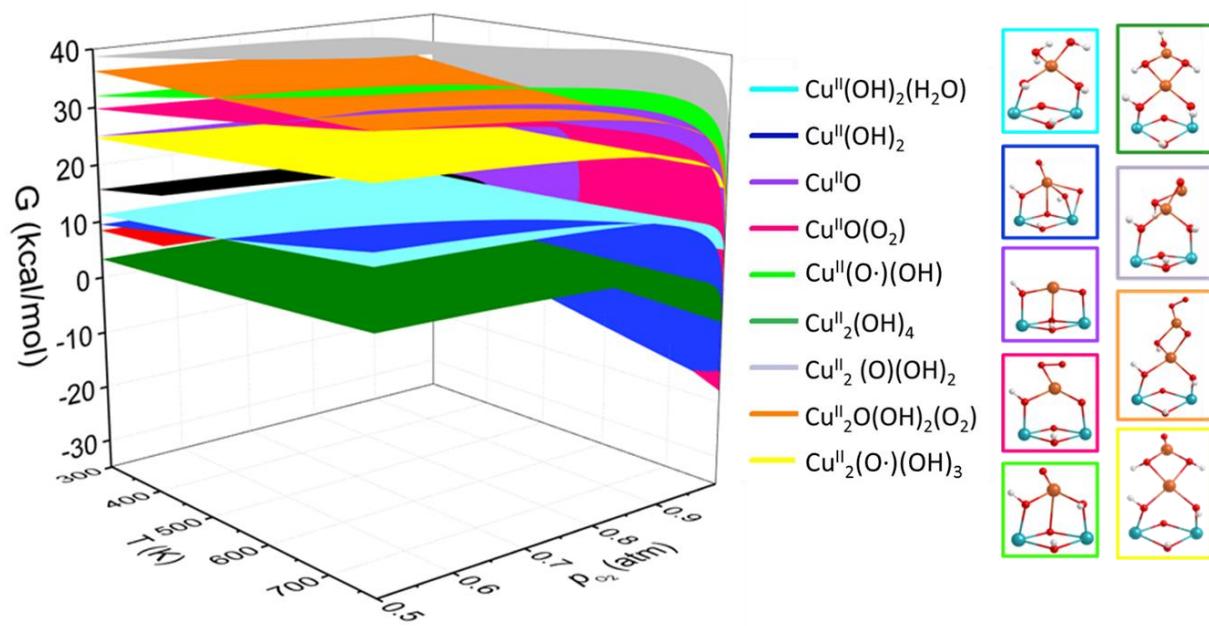


Figure S33. 3D projection for Gibbs free energies (ΔG in kcal/mol) of the formation of $Cu_xO_mH_n$ complexes in Cu-NU-1000 as functions of temperature (T in K) and partial pressure of O_2 (p_{O_2} , atm).

Cartesian coordinates

XYZ coordinates for all DFT-optimized structures. Energies and Gibbs energies in Hartrees.

| M-A E=-5284.539551 | | | | | M-B E=-5284.557270 | | |
|--------------------|-----------|-----------|-----------|----|--------------------|-----------|-----------|
| C | 5.373502 | -0.313586 | 4.167939 | H | 3.059661 | -1.420065 | -5.509410 |
| C | -5.463238 | 4.074858 | -0.234055 | H | -4.705944 | -1.058368 | -7.521276 |
| C | 5.965650 | 2.900307 | 0.277237 | H | 3.877972 | -8.270312 | 0.656212 |
| C | -5.899635 | 1.105855 | 3.562914 | H | -5.784326 | -7.285891 | 0.251887 |
| C | 4.023537 | -0.173428 | 4.513291 | H | 4.902062 | -2.071575 | -7.051926 |
| C | -4.088061 | 4.322427 | -0.157405 | H | -7.741640 | -0.393733 | -4.547395 |
| C | 4.671033 | 3.409088 | 0.119324 | H | 7.115579 | -5.439852 | 0.595728 |
| C | -4.607174 | 0.885280 | 4.054644 | H | -8.282780 | -3.833255 | -0.330415 |
| C | 3.687751 | 0.158210 | 5.830925 | H | 7.686621 | -1.888143 | -3.778626 |
| C | -3.633433 | 5.646524 | -0.145678 | H | 7.702277 | 5.821986 | 0.394841 |
| C | 4.476955 | 4.795921 | 0.062205 | H | -6.610649 | 7.276852 | -0.345231 |
| C | -4.374473 | 0.998281 | 5.430351 | H | 6.319926 | -7.797216 | 0.606262 |
| C | 4.684751 | 0.349625 | 6.783109 | H | 7.221271 | -2.311250 | -6.185594 |
| C | -4.534923 | 6.703316 | -0.212187 | H | -8.038403 | -6.296590 | -0.092274 |
| C | 5.565035 | 5.658878 | 0.155543 | H | -7.514795 | 1.793160 | 4.680225 |
| C | -5.415635 | 1.320360 | 6.296451 | H | -7.105849 | -0.810358 | -6.915584 |
| C | 6.028625 | 0.210020 | 6.433853 | H | 6.806829 | 0.362018 | 7.179900 |
| C | -5.903934 | 6.450426 | -0.291013 | H | -1.693056 | 1.750521 | -2.198394 |
| C | 6.852052 | 5.146385 | 0.315898 | H | 1.926424 | 1.714261 | 2.081291 |
| C | -6.701818 | 1.5040897 | 5.801554 | H | 0.338349 | -4.248281 | 2.463865 |
| C | 6.367556 | -0.125992 | 5.122854 | H | 0.544208 | 0.648202 | -4.687215 |
| C | -6.363964 | 5.133331 | -0.300103 | H | -0.324384 | -3.230236 | -2.669276 |
| C | 7.049759 | 3.766453 | 0.372303 | H | -1.243297 | -4.663702 | -1.339059 |
| C | -6.936921 | 1.434988 | 4.430185 | H | -1.167959 | -2.461534 | -3.769143 |
| C | -5.712120 | -0.409800 | -3.836380 | H | -2.396251 | -1.894491 | 2.253279 |
| C | 5.133444 | -4.606877 | 0.633630 | H | 1.656271 | -2.666013 | -1.598764 |
| C | -6.177227 | -3.450207 | -0.120795 | H | 0.234798 | -1.776115 | 4.639061 |
| C | 5.642207 | -1.417331 | -3.306371 | H | -0.494309 | 4.282723 | -1.739897 |
| C | -4.360294 | -0.552807 | -4.170317 | H | -1.063484 | 2.082167 | 4.018458 |
| C | 3.757414 | -4.866783 | 0.662936 | H | -0.468219 | 4.236606 | 1.606923 |
| C | -4.904428 | -4.002018 | 0.069339 | H | -0.005995 | 2.658389 | 2.979737 |
| C | 4.334589 | -1.281338 | -3.788313 | O | 0.756070 | -1.332885 | 1.304349 |
| C | -4.009451 | -0.789373 | -5.504507 | O | 3.264603 | -2.572422 | 0.470042 |
| C | 3.315825 | -6.194882 | 0.675457 | O | 3.533019 | -0.755800 | -1.632332 |
| C | -4.772418 | -5.388823 | 0.200141 | O | 3.359351 | -0.533449 | 2.282335 |
| C | 4.079401 | -1.518686 | -5.143693 | O | 1.750342 | -0.248162 | 3.842013 |
| C | -4.991652 | -0.880629 | -6.485739 | O | -0.150900 | 1.954681 | 3.706544 |
| C | 4.233840 | -7.241266 | 0.654740 | O | 0.231893 | 0.479191 | 3.583694 |
| C | -5.895498 | -6.208226 | 0.143602 | O | -1.882778 | 3.489648 | -0.083861 |
| C | 5.112831 | -1.886228 | -5.999931 | O | -3.828744 | 0.264982 | 1.917910 |
| C | -6.337650 | -0.739501 | -6.147360 | O | 3.586437 | 2.013043 | -0.143694 |
| C | 5.604067 | -6.977200 | 0.624685 | O | -3.932030 | -1.861203 | 0.099123 |
| C | -7.161156 | -5.653179 | -0.047884 | O | -3.689050 | -0.092804 | -1.954259 |
| C | 6.414173 | -2.021451 | -5.514784 | O | -2.107539 | -0.680311 | -3.455579 |
| C | -6.692985 | -0.505229 | -4.818641 | O | -2.565111 | -3.656435 | 0.233939 |
| C | 6.048519 | -5.654699 | 0.618069 | O | -1.275864 | -1.296190 | -0.859774 |
| C | -7.297459 | -4.271808 | -0.181111 | O | -1.744900 | -1.482691 | 1.667166 |
| C | 6.673903 | -1.783553 | -4.164875 | O | -0.501658 | -1.723946 | 4.012574 |
| C | 3.501994 | 2.486162 | 0.035427 | O | -0.527583 | -3.813249 | 2.381979 |
| C | 2.963491 | -0.337194 | 3.473359 | O | 0.216692 | 3.633816 | -1.650568 |
| C | 2.779246 | -3.736932 | 0.638373 | O | -1.152203 | 0.945214 | 1.061834 |
| C | -3.709811 | -3.110139 | 0.137389 | O | 1.343287 | 1.146851 | 1.556800 |
| C | -3.305806 | -0.440379 | -3.117064 | O | 2.366287 | 3.002358 | -0.206131 |
| C | -3.114496 | 3.190131 | -0.103852 | O | 0.224437 | 3.562007 | 1.657627 |
| C | 3.225011 | -0.919711 | -2.857386 | O | 3.724995 | 1.248147 | 0.205940 |
| C | -3.499635 | 0.520669 | 3.118399 | O | -0.421486 | -4.152112 | -1.313783 |
| C | 5.624422 | -0.567472 | 3.140268 | O | -0.269316 | -2.523760 | -3.400261 |
| C | -5.807233 | 3.042734 | -0.245174 | O | 1.143923 | -1.996783 | -1.122253 |
| C | 6.099825 | 1.821686 | 0.324581 | O | 1.545278 | -4.006818 | 0.759124 |
| C | -6.072394 | 1.021418 | 2.492716 | O | 2.056206 | -0.812022 | -3.338482 |
| C | 2.637724 | 0.276945 | 6.090186 | O | 0.129218 | 0.993334 | -3.882628 |
| C | -2.563254 | 5.834822 | -0.086400 | O | -1.297550 | 1.197640 | -1.508299 |
| C | 3.468285 | 5.186689 | -0.067374 | O | 1.119931 | 0.612210 | -0.970684 |
| C | -3.371646 | 0.813505 | 5.810411 | Zr | -2.654631 | -0.023294 | 0.028486 |
| C | 4.412266 | 0.613574 | 7.803682 | Zr | -0.234977 | -0.118084 | 2.677752 |
| C | -4.168645 | 7.728524 | -0.205265 | Zr | -0.435998 | -2.802513 | 0.301321 |
| C | 5.405521 | 6.735245 | 0.113159 | Zr | -0.018318 | 0.453699 | -2.374427 |
| C | -5.223384 | 1.395913 | 7.365540 | Zr | 2.359901 | -0.543499 | 0.273266 |
| C | 7.413733 | -0.238322 | 4.842606 | Zr | 0.093520 | 2.260257 | 0.001114 |
| C | -7.432047 | 4.930824 | -0.361259 | Cu | 1.959953 | 4.207499 | -2.311028 |
| C | 8.054373 | 3.365348 | 0.495727 | H | -0.533669 | -3.075394 | 3.085605 |
| C | -7.936714 | 1.606652 | 4.034485 | H | 1.881188 | 6.019151 | -1.837117 |
| C | -5.974890 | -0.220528 | -2.797718 | H | 1.436917 | 6.076549 | -0.979575 |
| C | 5.467978 | -3.571834 | 0.618520 | H | 3.785317 | 4.886145 | -3.081611 |
| C | -6.267251 | -2.370541 | -2.017128 | H | 4.511869 | 4.472102 | -2.587871 |
| C | 5.829425 | -1.236075 | -2.250121 | H | 3.593898 | 5.727628 | -2.603596 |
| C | -2.956325 | -0.885589 | -5.760525 | O | 2.293754 | 2.334370 | -3.006112 |
| C | 2.245632 | -6.391648 | 0.682569 | H | 1.448898 | 1.980520 | -3.427757 |
| C | -3.781478 | -5.809885 | 0.356998 | H | 2.324720 | 1.765113 | -2.208550 |

| | | | | | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -3.558701 | 5.043259 | 2.937165 | C | 3.887247 | -4.543653 | -3.280581 | H | 0.980466 | 4.064014 | -1.869554 |
| H | 2.483305 | 5.227510 | 3.488468 | C | -4.214703 | -4.456268 | -2.541735 | H | 2.372814 | 0.369331 | 2.908163 |
| H | -2.802690 | 3.276173 | -4.859858 | C | 4.552129 | -3.715716 | 4.004260 | H | -1.796511 | 2.904952 | 0.086323 |
| H | 5.124565 | 4.582303 | -5.446201 | C | -4.489228 | -4.308821 | 5.488305 | H | -0.188830 | -1.153584 | 4.844559 |
| H | -5.460016 | 6.578322 | 3.403516 | C | 4.847032 | -5.345426 | -3.890008 | H | 0.621512 | -2.090199 | -3.908511 |
| H | 4.208458 | 6.785182 | 4.374178 | C | -5.271406 | -5.268837 | -2.939283 | H | 1.244867 | -4.007934 | 2.277759 |
| H | -4.533791 | 4.366320 | -6.277354 | C | 5.626236 | -4.407551 | 4.557099 | H | 0.804704 | -4.511803 | -0.941681 |
| H | 7.796412 | 3.012880 | -2.462465 | C | -5.845772 | -4.107084 | 2.530741 | H | 0.230730 | -3.966847 | 1.054094 |
| H | -8.151938 | 3.789359 | 1.538583 | C | 6.202717 | -5.052851 | -3.740883 | O | -0.769750 | 0.253638 | 1.798253 |
| H | 7.295771 | 4.271901 | 2.745199 | C | -6.582223 | -4.936591 | -2.595099 | O | -3.342708 | 1.606501 | 1.774055 |
| H | -7.616011 | 2.506243 | -3.922839 | C | 6.914393 | -4.233165 | 4.048859 | O | -3.591595 | 1.259578 | -0.955255 |
| H | -6.858914 | -6.233854 | -3.457997 | C | -6.233744 | -3.164856 | 4.277964 | O | -3.319564 | -1.101681 | 2.150321 |
| H | 7.493877 | -5.809304 | -2.198329 | C | 6.591528 | -3.952927 | -2.975682 | O | -1.663382 | -2.066249 | 3.344912 |
| H | -7.765177 | 5.958417 | 2.698735 | C | -6.827203 | -3.784710 | -1.846944 | O | 0.330513 | -3.764612 | 2.053090 |
| H | -6.946646 | 3.987423 | -5.807169 | C | 7.117797 | -3.357871 | 2.981402 | O | 2.436366 | -2.350329 | 2.749770 |
| H | 6.622528 | 6.310504 | 4.004186 | C | 5.587793 | 2.613303 | -2.969403 | O | 2.022595 | -2.885742 | -2.038674 |
| H | 6.663571 | -3.854976 | 6.344909 | C | -5.301831 | 3.145307 | 2.988572 | O | 3.895714 | -1.193964 | 1.473394 |
| H | 7.425986 | 4.346441 | -4.531526 | C | 6.029698 | 3.141275 | 1.818288 | O | 3.660179 | -1.561671 | -1.216143 |
| H | -7.680473 | -4.266441 | 5.021608 | C | -5.760601 | 2.574919 | -2.053948 | O | 3.855774 | 1.591109 | 1.095509 |
| H | 2.243612 | -0.455125 | -2.187784 | C | 4.226072 | 2.814247 | -3.228835 | O | 3.622751 | 1.226794 | -1.594572 |
| H | -2.085209 | -2.766845 | 0.727035 | C | 3.938104 | 3.404390 | 3.177093 | O | 1.968672 | 2.322015 | -2.678905 |
| H | -1.535127 | 2.492520 | 3.951187 | C | 4.733852 | 3.443825 | 2.254951 | O | 2.415411 | 2.947276 | 2.188110 |
| H | -0.670257 | 0.613052 | -4.349325 | C | -4.452582 | 2.827395 | -2.486582 | O | 1.213221 | 1.521412 | -0.034176 |
| H | -0.123881 | 3.982501 | -0.914570 | C | 3.852557 | 3.708706 | -4.239275 | O | 1.724966 | 0.307657 | 2.191069 |
| H | 0.385572 | 4.739299 | 1.038025 | C | -3.557550 | 4.519697 | 3.932861 | O | 0.535136 | -0.824862 | 4.291702 |
| H | 0.912123 | 3.917953 | -2.118881 | C | 4.541373 | 4.533872 | 3.111532 | O | 0.425761 | 1.807439 | 4.061103 |
| H | 1.550231 | 0.762933 | 3.206978 | C | -4.231490 | 3.808657 | -3.460138 | O | -0.205722 | -1.989101 | -3.417780 |
| H | -2.105027 | 2.829290 | -0.564990 | C | 4.821312 | 4.384620 | -4.976132 | O | 1.219570 | -1.434161 | 0.370796 |
| H | -1.271369 | -0.674771 | 4.806489 | C | -4.521754 | 5.358166 | 4.486169 | O | -1.234380 | -1.999347 | 0.672467 |
| H | -0.668710 | -2.511584 | -3.567866 | C | 5.624911 | 5.304760 | 3.522847 | O | -2.156628 | -2.748787 | -1.734538 |
| H | 0.689157 | -3.701403 | 2.797463 | C | -5.301301 | 4.522759 | -3.990764 | O | 0.071604 | -4.022057 | -0.542289 |
| H | 0.738277 | -4.568121 | -0.397971 | C | 6.176774 | 4.179167 | -4.714452 | O | -3.608794 | -1.425141 | -0.624326 |
| H | -0.126747 | -3.824903 | 1.439431 | C | 5.879642 | 5.096507 | 4.295135 | O | 0.226236 | 4.094691 | 1.124561 |
| O | -1.340335 | 0.403415 | 1.586617 | C | 6.913975 | 4.998940 | 3.0383454 | O | 0.112025 | 3.832990 | -1.500445 |
| O | -3.898185 | 1.636884 | 0.945350 | C | -6.602455 | 4.263126 | -3.559251 | O | -1.244728 | 2.110034 | 0.121146 |
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| O | -0.187021 | -3.526114 | 2.413451 | C | -6.827172 | 3.286940 | -2.588714 | O | 1.363632 | -0.248308 | -1.871140 |
| O | 1.707746 | -1.956533 | 3.344261 | C | -3.320271 | -2.433411 | -1.360759 | O | -1.071514 | -0.158180 | -1.150789 |
| O | 2.179960 | -2.995162 | -1.332222 | C | -2.887669 | -1.875524 | 3.061905 | Zr | 2.650331 | 0.003330 | 0.053324 |
| O | 3.343270 | -0.851521 | 2.249742 | C | -2.910663 | 2.521681 | 3.542317 | Zr | 0.298342 | -1.467620 | 2.299410 |
| O | 3.601398 | -1.521379 | -0.375231 | C | 3.581221 | 2.601643 | 1.813225 | Zr | 0.321543 | 2.090772 | 1.771123 |
| O | 3.306341 | 1.876386 | 1.538560 | C | 3.197478 | 2.070297 | -4.237719 | Zr | -0.036459 | 1.531602 | -1.735424 |
| O | 3.575138 | 1.164090 | -1.106645 | C | 3.241691 | -2.567727 | -1.869476 | Zr | -2.362932 | 0.052025 | 0.490905 |
| O | 2.103747 | 2.195119 | -2.479160 | C | -3.318701 | 2.052373 | -1.910057 | Zr | 0.001799 | -2.043914 | -1.262711 |
| O | 1.658207 | 3.258529 | 2.231071 | C | 3.606823 | -2.076528 | 2.343328 | Cu | -1.421468 | -0.568979 | -4.144415 |
| O | 0.909872 | 1.561124 | 0.001163 | C | -5.563252 | -1.703590 | 2.831623 | H | 0.482110 | 0.805269 | 4.249554 |
| O | 1.046048 | 0.603367 | 2.395784 | C | 5.921959 | -2.286513 | -1.769080 | O | -2.736420 | -1.839713 | -4.501742 |
| O | -0.471614 | -0.366757 | 4.555609 | C | -5.954112 | -2.069825 | -0.864877 | H | -2.398928 | -2.632263 | -4.054919 |
| O | -0.607952 | 2.224161 | 3.823949 | C | 6.194244 | -1.971608 | 1.601847 | O | -2.680589 | 0.872717 | -4.857914 |
| O | 0.214376 | -2.325382 | -3.214171 | C | -2.466961 | -3.736938 | 4.981350 | H | -2.358474 | 1.643331 | -4.351851 |
| O | 0.920434 | -1.335546 | 0.701722 | C | 2.827210 | -4.762045 | -3.393395 | H | -3.543279 | 0.616952 | -4.422697 |
| O | -1.534977 | -1.977701 | 0.617512 | C | -3.188136 | -4.710475 | -2.798416 | O | -4.663427 | -0.308723 | -3.435223 |
| O | -2.006937 | -2.901272 | -1.929993 | C | 3.547463 | -3.837587 | 4.404306 | H | -4.128088 | -1.082446 | -3.767202 |
| O | -0.044018 | -4.045480 | -0.170422 | C | -4.179086 | -5.044625 | 6.228459 | H | -4.445555 | -0.265230 | -2.489447 |
| O | -3.672838 | -1.659352 | -1.051169 | C | 4.536434 | -6.202153 | -4.485664 | | | | |
| O | -0.337996 | 4.198762 | 0.688616 | C | -5.071847 | -6.165821 | -3.523073 | | | | |
| O | 0.000454 | 3.678970 | -1.880898 | C | 5.458078 | -5.084416 | 5.393204 | | | | |
| O | -1.547890 | 2.066172 | -0.352852 | C | -7.290280 | -3.002665 | 4.071006 | | | | |
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| O | -1.974367 | 1.833872 | -3.020788 | C | -7.847479 | -3.516545 | -1.577818 | | | | |
| O | 0.193706 | 0.614642 | -3.909975 | C | 8.118968 | -3.215011 | 2.577793 | | | | |
| O | 0.451987 | -0.371353 | -1.625231 | C | 8.189943 | 1.916772 | -2.182929 | | | | |
| O | -0.106436 | -0.295454 | -1.265405 | C | -5.590593 | 2.280578 | 2.394859 | | | | |
| Zr | 2.337905 | 0.131488 | 0.503737 | C | 6.170236 | 2.289113 | 1.157066 | | | | |
| Zr | -0.331831 | -1.214262 | 2.430982 | C | -5.924447 | 1.807014 | -1.301104 | | | | |
| Zr | -0.304428 | 2.273018 | 1.543101 | C | 2.794536 | 3.862139 | -4.443794 | | | | |
| Zr | -0.017172 | 1.360951 | -1.901789 | C | -2.497620 | 4.727772 | 4.064385 | | | | |
| Zr | -2.663747 | 0.006393 | 0.042126 | C | 3.534467 | 4.759253 | 3.456956 | | | | |
| Zr | 0.023873 | -2.135991 | -1.054354 | C | -3.212716 | 4.012485 | -3.785449 | | | | |
| Cu | 1.336464 | -1.011040 | -4.187770 | C | 4.516748 | 5.074423 | -5.761463 | | | | |
| H | -0.562238 | 1.248453 | 4.131033 | C | -4.211255 | 6.225795 | 5.066182 | | | | |
| O | 2.683360 | 0.107188 | -4.841797 | C | 5.463630 | 6.147359 | 4.193274 | | | | |
| H | 2.280048 | 0.987624 | -4.792170 | C | -5.119342 | 5.285181 | -4.746131 | | | | |
| O | 2.642833 | -2.604416 | -4.233717 | C | 7.608720 | 3.125988 | -3.493051 | | | | |
| H | 2.255169 | -3.127713 | -3.506094 | C | -7.319316 | 3.769582 | 3.389803 | | | | |
| H | 3.468122 | -2.207203 | 3.852142 | C | 8.113025 | 3.669173 | 1.882275 | | | | |
| O | 4.495071 | -0.896967 | -3.180040 | C | -7.840423 | 3.076489 | -2.251222 | | | | |
| H | 4.010695 | -0.281352 | -3.792911 | C | -7.407883 | -5.571326 | -2.910123 | | | | |
| H | 4.484192 | -0.479031 | -2.305712 | C | 6.953520 | -5.680066 | -4.218536 | | | | |
| H | -6.631689 | 5.754879 | 4.726353 | H | -7.438279 | 4.819769 | -3.979696 | | | | |
| H | 7.759899 | 5.604013 | 3.406857 | H | 7.753073 | -4.774961 | 4.482617 | | | | |
| H | 6.932852 | 4.707895 | -5.292042 | H | -6.596522 | -4.682478 | 5.769782 | | | | |
| H | -1.895652 | -0.338695 | -2.671630 | H | 1.895652 | 4.754879 | 4.726353 | | | | |
| H | -1.789442 | -2.784572 | 0.786175 | H | -0.454941 | 2.084126 | 4.367294 | | | | |
| H | 0.621231 | 1.015755 | -4.307768 | H | 0.165815 | 4.040353 | -0.502011 | | | | |
| H | 1.022519 | 4.575211 | 1.394863 | H | </ | | | | | | |

| | | | | | | | | | | | |
|---|-----------|-----------|-----------|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.085091 | 5.442899 | 1.875251 | H | -1.041003 | -0.017666 | -4.419633 | C | -5.683634 | 1.919989 | 3.350177 |
| C | -4.085865 | 2.354228 | -4.840054 | H | 0.069507 | 3.693678 | -1.755819 | C | 4.274855 | 0.996294 | 4.064782 |
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| C | -5.076851 | 6.336376 | 2.163953 | H | 1.008741 | 3.297263 | -2.977566 | C | 4.648636 | 3.241302 | -1.155273 |
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| C | -6.410370 | 5.951000 | 2.015740 | H | 1.216637 | -3.763228 | -2.385113 | C | 4.504071 | 4.366480 | -1.977310 |
| C | 6.440151 | 5.984687 | 1.891850 | H | 0.966466 | -3.002543 | 3.522919 | C | -4.062398 | 2.370921 | 5.080114 |
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| C | -6.729045 | 2.169484 | -3.971969 | O | -3.613968 | 0.822690 | -1.580926 | C | 6.378595 | 1.865077 | 5.701763 |
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| C | -3.251140 | 3.102079 | 1.375288 | O | 0.064656 | -2.878359 | 3.179608 | C | -6.388851 | 2.938204 | 5.426209 |
| C | 3.277968 | 3.173263 | 1.152277 | O | 2.093138 | -1.240600 | 3.540330 | C | 6.648156 | 1.178098 | 4.517553 |
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| C | 3.290441 | -1.080479 | 3.147633 | O | 3.623880 | 2.000649 | 0.815261 | C | -5.867029 | -1.590090 | -3.345900 |
| H | -5.899126 | -0.875847 | 2.799277 | O | 3.605476 | 0.820042 | -1.626087 | C | 5.267949 | -4.327649 | 1.476516 |
| H | 6.023759 | -2.406558 | -0.742282 | O | 2.038533 | 1.450076 | -3.125156 | C | -6.087509 | -3.455176 | 1.023000 |
| H | -5.932078 | -2.491554 | -0.512997 | O | 2.079957 | 3.578728 | 1.299162 | C | 5.529451 | -2.412037 | -3.157562 |
| H | 5.911827 | -1.234708 | 2.551563 | O | 1.077656 | 1.476377 | -0.434796 | C | 4.529827 | -1.749881 | -3.727707 |
| H | -2.951894 | -2.129682 | 5.641659 | O | 1.412372 | 1.065588 | 0.209892 | C | 3.899848 | -4.578379 | 1.643249 |
| H | 3.072917 | -5.482779 | -1.160787 | O | 0.046491 | 0.622140 | 4.354731 | C | -4.796244 | -3.923725 | 1.294882 |
| H | -2.996972 | -5.401606 | -1.633781 | O | -0.048456 | 3.038951 | 3.283016 | C | 4.214681 | -2.304868 | -3.626358 |
| H | 3.101346 | -2.020155 | 5.686352 | O | 0.302234 | -3.432784 | -2.402506 | C | -4.238165 | -2.266191 | -4.995795 |
| H | -4.740167 | -3.079186 | 7.097066 | O | 1.077571 | -1.179127 | 0.907462 | C | 3.484671 | -5.860429 | 2.021561 |
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| H | -7.742909 | -4.163745 | -0.869279 | O | 0.106117 | 3.181830 | -2.635534 | C | 4.881988 | -3.373412 | -5.691347 |
| H | 7.766945 | -2.052839 | 3.997408 | O | -1.362842 | 1.998802 | -0.654588 | C | -6.597956 | -2.457891 | -5.480111 |
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| H | -5.905483 | 2.678534 | 1.207238 | O | -2.074015 | 1.416771 | -3.122974 | C | -7.021589 | -5.561060 | 1.746014 |
| H | 5.921103 | 2.791021 | 0.820193 | O | -0.152406 | -0.164853 | -0.454110 | C | 6.189997 | -3.483736 | -5.218523 |
| H | -5.903306 | 1.299974 | -2.172673 | O | 1.364308 | -0.800135 | -1.620065 | C | -6.893081 | -1.946774 | -4.215634 |
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| H | -3.048911 | 2.424375 | -5.161702 | Zr | 0.047777 | 2.568097 | 1.021391 | C | 3.490632 | 2.338897 | -0.900101 |
| H | 4.825890 | 3.096931 | -6.754299 | Zr | -0.013486 | 0.913346 | -2.156033 | C | 3.163427 | 0.565129 | 3.163988 |
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| | | | | | | | | | | | |
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| C | 7.722935 | 4.115754 | -3.174748 | O | -0.064600 | 2.140680 | 3.363198 | H | 3.098778 | 4.484730 | 2.997779 |
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| C | 7.186124 | -5.192921 | 1.832813 | O | -4.078384 | 3.926480 | 3.431589 | H | -2.207653 | 4.942989 | 4.303181 |
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| C | 8.446183 | -0.234948 | 3.881848 | O | -4.071468 | -3.249670 | 4.878962 | H | 7.190460 | 2.744609 | -5.965798 |
| C | 5.790479 | -1. | | | | | | | | | |

| | | | | | | | | | | | |
|--------------------|-----------|-----------|-----------|---|-----------|-----------|-----------|----|-----------|-----------|-----------|
| H | -0.970279 | -1.154958 | 4.512315 | C | 4.110939 | 1.786729 | -4.870265 | O | 1.339702 | -0.060086 | 2.050805 |
| H | -0.472320 | 2.185303 | 4.067627 | C | -4.970983 | 2.943253 | -5.639582 | O | 2.342220 | 2.534130 | 1.579541 |
| H | -0.000738 | 0.040837 | 4.116369 | C | 4.480369 | -6.256994 | -3.555683 | O | 0.195473 | 1.850486 | 3.486700 |
| O | 1.046551 | -1.917303 | 0.317038 | C | -5.689791 | -5.405116 | -3.494459 | O | 3.727831 | 0.830342 | 1.080937 |
| O | 3.611177 | -2.071702 | -1.067830 | C | 5.153368 | 2.023895 | -5.761928 | O | -0.298137 | -2.779704 | -3.370065 |
| O | 3.588367 | 0.669467 | -1.553174 | C | -6.321379 | 2.756147 | -5.342115 | O | -0.213168 | -0.242636 | -4.117995 |
| O | 3.605047 | -1.625094 | 1.629193 | C | 5.839722 | -5.956434 | -3.451881 | O | 1.204510 | -1.077917 | -1.954241 |
| O | 2.057340 | -2.543260 | 2.994029 | C | -6.963346 | -4.845774 | -3.386424 | O | 1.693126 | -3.795687 | -1.582284 |
| O | -0.057539 | -0.972500 | 4.228651 | C | 6.466802 | 1.702733 | -5.414776 | O | 2.069499 | 1.225477 | -3.022235 |
| O | -2.068735 | -2.279334 | 3.160469 | C | -6.682992 | 2.078380 | -4.177324 | O | 0.100457 | 2.900992 | -2.708053 |
| O | -2.123820 | 2.352368 | 2.237096 | C | 6.240308 | -4.849126 | -2.702747 | O | -1.338530 | 1.658845 | -0.438849 |
| O | -3.631377 | -1.562451 | 1.694835 | C | -7.133494 | -3.639104 | -2.708298 | O | 1.085962 | 0.942981 | -0.317865 |
| O | -3.676724 | 1.108807 | 1.168495 | C | 6.727644 | 1.147368 | -4.161522 | Zr | -2.636143 | -0.248712 | 0.097165 |
| O | -3.624312 | -2.074133 | -1.050540 | C | 3.497414 | 1.962054 | 1.593544 | Zr | -0.188399 | -1.807907 | 2.224469 |
| O | -3.627615 | 0.570255 | -1.591716 | C | 3.010802 | -2.358577 | 2.772326 | Zr | -0.331778 | -2.622806 | -1.272289 |
| O | -2.072128 | 1.384884 | -3.016599 | C | 2.915442 | -3.457737 | -1.524058 | Zr | -0.030025 | 0.839903 | -2.079424 |
| O | -2.085314 | -3.401168 | -2.040272 | C | -3.592847 | -2.857417 | -1.626556 | Zr | 2.391385 | -0.665497 | 0.043277 |
| O | -1.089895 | -0.749590 | -1.406246 | C | -3.297768 | 1.241170 | -2.692573 | Zr | 0.014145 | 1.678624 | 1.399166 |
| O | -1.402249 | -2.521511 | 0.448945 | C | -3.164722 | 2.445371 | 1.843833 | Cu | -0.374714 | 4.328420 | -1.407658 |
| O | -0.025171 | -4.044645 | 2.154349 | C | 3.250043 | 0.911414 | -2.674936 | Cu | 2.051724 | 3.850148 | 0.015256 |
| O | 0.065572 | -6.464766 | -0.426597 | C | -3.467225 | -1.642177 | 2.913686 | H | 1.024160 | 3.026598 | -2.986781 |
| O | -0.007290 | 3.735053 | 1.333426 | H | 5.674683 | -2.333168 | 3.795456 | H | -0.096015 | 4.474172 | 1.312047 |
| O | -1.094133 | -0.214740 | 1.533828 | H | -5.854040 | 2.271958 | 1.677983 | O | 3.645366 | 3.725508 | -0.955284 |
| O | 1.411413 | -0.068611 | 2.070799 | H | 6.019270 | 1.083163 | 1.907483 | H | 4.074044 | 2.869284 | -0.803003 |
| O | 2.218829 | 2.657494 | 1.639915 | H | -6.068614 | -1.008519 | 2.628985 | O | -2.185402 | 4.070543 | -1.171304 |
| O | 0.143581 | 1.5755942 | 3.636781 | H | 2.680957 | -3.399923 | 5.250424 | H | -2.625645 | 4.012602 | -2.032572 |
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| O | 1.359547 | -0.872060 | -1.986986 | H | 4.451128 | -4.128165 | 6.840017 | O | 1.337185 | 5.175214 | -1.327890 |
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| O | 2.033579 | 1.499940 | -2.962699 | H | 5.297184 | 5.584041 | 3.877852 | H | -1.850212 | 2.496666 | -0.644423 |
| O | 0.106963 | 3.138831 | -2.243663 | H | -5.197651 | -3.501181 | 6.828466 | | | | |
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| O | 1.061251 | 1.011845 | -0.226191 | H | -7.548750 | 3.762086 | 2.729668 | | | | |
| Zr | -2.526186 | -0.466000 | 0.074045 | H | 7.897809 | 2.253739 | 3.056452 | | | | |
| Zr | 0.018357 | -1.940948 | 2.127714 | H | -7.949658 | -1.528000 | 4.175924 | | | | |
| Zr | -0.047871 | -2.555395 | -1.411668 | H | -5.972430 | 1.066536 | -2.401729 | | | | |
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| Zr | 2.504747 | -0.480828 | 0.033999 | H | -6.156325 | -2.058636 | -1.601598 | | | | |
| Zr | -0.052533 | 1.600136 | 1.542090 | H | 5.879844 | 0.462399 | -2.294686 | | | | |
| Cu | -0.840720 | 4.480777 | -1.178058 | H | -2.933141 | 2.593624 | -5.004738 | | | | |
| Cu | 1.562797 | 4.049395 | 0.232523 | H | 2.469432 | -5.678889 | -3.012486 | | | | |
| H | 1.065449 | 3.368700 | -2.233183 | H | -3.595623 | -5.193222 | -3.001928 | | | | |
| H | -0.768730 | 4.337278 | 1.326873 | H | 3.083540 | 2.022989 | -5.139876 | | | | |
| O | 2.804029 | 4.002568 | -1.145802 | H | -4.681115 | 3.476945 | -6.543245 | | | | |
| H | 3.487465 | 3.339179 | -0.968279 | H | 4.156361 | -7.115997 | -4.141089 | | | | |
| O | -2.608441 | 3.821276 | -1.301368 | H | -5.552240 | -6.348666 | -4.019993 | | | | |
| H | -2.782577 | 3.566876 | -2.218580 | H | 4.939068 | 2.458422 | -6.736997 | | | | |
| O | -1.945295 | 5.609066 | 0.341208 | H | -7.734899 | 1.930945 | -3.937954 | | | | |
| H | -2.754475 | 5.275772 | -0.111663 | H | 7.297746 | -4.604809 | -2.614895 | | | | |
| H | -1.864987 | 6.556211 | 0.157343 | H | -8.125086 | -3.197826 | -2.621697 | | | | |
| O | 0.694005 | 5.553171 | -0.747732 | H | 7.748790 | 0.896534 | -3.878880 | | | | |
| H | 1.341160 | 5.608535 | -1.473486 | H | 7.532487 | 4.504671 | 4.042851 | | | | |
| H | -2.006071 | 2.334308 | -0.566676 | H | -6.818336 | 5.698858 | 4.112578 | | | | |
| D-C E=-5557.182523 | | | | H | 6.579508 | -6.579503 | -3.951327 | | | | |
| C | 5.420985 | -2.732869 | 3.359105 | H | 7.280017 | 1.886562 | -6.114693 | | | | |
| C | -5.545530 | 3.120340 | 2.285258 | H | -7.820473 | -5.349982 | -3.829759 | | | | |
| C | 5.876340 | 2.067673 | 2.348305 | H | -7.516715 | -2.784707 | 6.280585 | | | | |
| C | -5.891200 | -1.549600 | 3.555990 | H | -7.087909 | 3.139621 | -6.013349 | | | | |
| C | 4.069862 | -2.828571 | 3.715037 | H | 6.848318 | -3.955415 | 6.197273 | | | | |
| C | -4.176932 | 3.355595 | 2.461891 | H | 1.908035 | 0.123125 | 2.813108 | | | | |
| C | 4.613341 | 2.668966 | 2.264116 | H | 0.512620 | -5.025422 | -3.400299 | | | | |
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| C | 3.731508 | -3.337893 | 4.974349 | H | -0.263385 | -1.243964 | -3.939926 | | | | |
| C | -3.774091 | 4.448904 | 3.238016 | H | -1.102979 | -3.212331 | -3.691074 | | | | |
| C | 4.409803 | 3.935446 | 2.825846 | H | -1.093911 | 0.019741 | -4.436150 | | | | |
| C | -4.344879 | -2.648463 | 5.048285 | H | -2.303951 | -3.058608 | 0.821089 | | | | |
| C | 4.726460 | -3.739595 | 5.860915 | H | 1.727510 | -1.320551 | -2.732454 | | | | |
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| C | 5.459197 | 4.593729 | 3.456759 | H | -1.081852 | -0.754927 | 4.559628 | | | | |
| C | -5.395164 | -2.948103 | 5.911581 | H | -0.499607 | 2.417079 | 3.852383 | | | | |
| C | 6.071473 | -3.641914 | 5.502024 | H | -0.023653 | 0.316715 | 4.061832 | | | | |
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| C | 6.712573 | 3.989224 | 3.545024 | O | 3.357993 | -2.397843 | -0.974885 | | | | |
| C | -6.696841 | -2.548823 | 5.604385 | O | 3.560723 | 0.315824 | -1.591532 | | | | |
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| C | -6.487628 | 3.958239 | 2.875765 | O | 1.796863 | -2.517318 | 3.119254 | | | | |
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| C | 5.687204 | 0.905428 | -3.269674 | O | -3.851079 | -1.832093 | -0.925587 | | | | |
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| C | 3.531349 | -5.459707 | -2.921112 | O | -0.398127 | -3.895734 | 2.373353 | | | | |
| C | -4.592301 | -4.762609 | -2.929930 | O | -0.367869 | -4.650768 | -0.165767 | | | | |
| O | -1.154671 | -0.031898 | 1.523897 | O | 0.184564 | 3.784665 | 0.692571 | | | | |
| O | -1.546711 | -0.031898 | 1.523897 | O | -1.154671 | -0.031898 | 1.523897 | | | | |

| | | | | | | | | | | | | |
|---|-----------|-----------|------------|--------------------------|-----------|------------|-----------|----------|-----------|-----------|-----------|-----------|
| H | -5.913925 | -1.367617 | 2.220344 | Cu | -1.463621 | -3.883618 | 0.210980 | H | 5.903546 | -2.357913 | -2.003320 | |
| H | 5.856051 | 1.930488 | 2.378936 | H | -0.324469 | -3.923422 | -2.269350 | H | -5.894283 | -1.934008 | -2.214564 | |
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| H | -3.123523 | -4.439095 | 3.285051 | H | -3.628328 | -3.506364 | -0.605622 | H | 2.965531 | -4.394804 | -4.361359 | |
| H | 2.927469 | 3.982156 | 4.734120 | O | 3.757563 | -3.419479 | -0.244059 | H | -3.107743 | -4.310224 | -4.433912 | |
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| H | 4.725229 | 4.930156 | 6.163943 | O | 1.709039 | -5.372120 | -0.913504 | H | -4.973462 | -5.248090 | -5.788269 | |
| H | -7.820945 | 2.877672 | 3.554849 | H | 2.343182 | -5.806818 | -0.325504 | H | 4.911098 | 4.716732 | -5.413729 | |
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| H | 7.669979 | 2.866291 | 3.803725 | H | -7.774313 | -2.860062 | -3.562643 | H | 7.792209 | 2.321404 | -3.299895 | |
| H | 5.862773 | -0.772360 | -2.388944 | H | 7.080701 | 3.568606 | 5.621443 | H | -7.181319 | 3.874574 | 5.389240 | |
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| H | 4.801642 | 6.089892 | -5.017058 | C | -4.054715 | 3.271925 | 4.183871 | H | -0.005119 | -0.094697 | -4.036787 | |
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| H | -7.695689 | -2.175095 | -3.617378 | C | 5.908868 | 4.214580 | 3.927125 | H | 0.694339 | -4.873551 | 1.658708 | |
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| H | 7.167610 | 5.394765 | -4.684356 | C | -6.501125 | -4.428155 | 4.513420 | O | 3.614400 | -1.881064 | -1.373001 | |
| H | 7.109862 | 4.377844 | 5.702556 | C | 6.631338 | -3.7711694 | 3.467244 | O | 3.665708 | 0.860915 | -1.355995 | |
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| H | -1.989277 | 0.075123 | 2.865479 | C | -6.784002 | -3.450206 | 3.558667 | O | -0.128718 | -1.814745 | 3.951400 | |
| H | -1.081592 | 4.836926 | -1.039208 | C | -5.685417 | 2.063632 | -2.908650 | O | -2.126191 | -2.896983 | 2.589659 | |
| H | -0.125133 | 4.529362 | 0.191796 | C | 5.667846 | -3.012820 | -2.839307 | O | -2.070037 | 1.991331 | 2.680280 | |
| H | 0.038818 | 0.604649 | -4.034512 | C | -5.707330 | -2.657396 | -3.005161 | O | -3.661642 | -1.833254 | 1.311516 | |
| H | 0.677117 | 2.707461 | -4.106192 | C | 5.739779 | 2.069129 | -3.712554 | O | -3.631759 | 0.912588 | 1.452883 | |
| H | 1.023848 | -0.564213 | -4.334579 | C | -4.345712 | 2.441741 | -3.064760 | O | -3.611431 | -1.703074 | -1.488991 | |
| H | 1.911039 | 3.301503 | 3.403262 | C | 4.325906 | -3.330626 | -3.085120 | O | -3.660928 | 1.008852 | -1.326153 | |
| H | -1.954407 | 0.701220 | -2.840593 | C | -4.387506 | -3.058953 | -3.246705 | O | 0.032461 | -4.444388 | -1.380579 | |
| H | -0.850279 | 4.586753 | 2.228060 | C | 4.407932 | 2.450185 | -2.922322 | O | 0.717598 | 3.165710 | 2.008323 | |
| H | 0.913588 | 1.478147 | 4.393243 | C | -4.023646 | 3.491407 | -3.934013 | O | -1.147889 | -0.561092 | 1.508510 | |
| H | 0.623917 | -1.790928 | 4.174614 | C | 4.010619 | -4.164019 | -4.164015 | O | 1.391283 | -0.488166 | 2.068482 | |
| H | -0.048746 | 0.257212 | 4.077563 | C | -4.136396 | -3.994152 | -4.256221 | O | 3.451255 | 2.942371 | 0.769081 | |
| O | -1.110105 | 1.877653 | 0.157591 | C | 4.120853 | 3.413979 | -3.896636 | O | 0.084923 | 0.825197 | 3.889910 | |
| O | -3.683568 | 1.883055 | -1.229323 | C | -5.027787 | 4.148293 | -4.638697 | O | 3.736645 | 0.794071 | 1.397347 | |
| O | -3.594426 | -0.916932 | -1.485154 | C | 5.019026 | -4.668534 | -4.982149 | O | 0.040197 | -1.738754 | -3.933924 | |
| O | -3.666218 | 1.675238 | 1.487566 | C | -5.181461 | -4.517269 | -5.008445 | O | -0.017590 | 0.916526 | -3.930226 | |
| O | -2.133616 | 2.744335 | 2.759035 | C | 5.147285 | 3.972832 | -4.654559 | O | 1.406408 | -0.430469 | -2.043315 | |
| O | 0.001281 | 1.272736 | 4.124834 | C | -6.359086 | 3.757504 | -4.491150 | O | 2.050405 | -3.113069 | -2.434165 | |
| O | 1.990557 | 2.550413 | 2.948076 | C | 6.354689 | -4.346441 | -4.733827 | O | 2.119021 | 2.168250 | -2.357923 | |
| O | 2.135327 | -2.079098 | 2.515971 | C | -6.494403 | -4.112173 | -4.764542 | O | -0.105167 | 3.478130 | -1.416085 | |
| O | 3.560397 | 1.692998 | 1.564852 | C | 6.471341 | 3.579191 | -4.451804 | O | -1.339337 | 1.649022 | 0.047769 | |
| O | 3.680628 | -1.023157 | 1.253101 | C | -6.684928 | 2.714347 | -3.624510 | O | 1.161144 | 1.075039 | 0.086632 | |
| O | 3.555972 | 1.948635 | -1.239415 | C | 6.673547 | -3.520184 | -3.655724 | Zr | -2.510724 | -0.422880 | -0.019795 | |
| O | 3.615611 | -0.753037 | -0.1505629 | C | -6.752212 | -3.179437 | -3.760169 | Zr | -0.012290 | -2.364353 | 1.699462 | |
| O | 2.067809 | -1.683239 | -2.871323 | C | 6.762100 | 2.630093 | -3.471067 | Zr | -0.028670 | -2.186630 | -1.879655 | |
| O | 2.009199 | 3.198521 | -2.318394 | C | 3.923989 | 2.051690 | 1.526328 | Zr | 0.061768 | 1.388637 | -1.653188 | |
| O | 1.051290 | 0.625491 | -1.480639 | C | 3.200491 | -2.807099 | 2.204316 | Zr | 2.552040 | -0.480762 | 0.011630 | |
| O | 1.324358 | 2.539508 | 0.229698 | C | 3.249280 | -2.741253 | -2.232340 | Zr | -0.098333 | 1.187828 | 1.809366 | |
| O | -0.076852 | 4.204044 | 1.792055 | C | -3.274678 | -2.491894 | -2.462434 | Cu | -1.608283 | 3.564944 | -0.110193 | |
| O | -0.171088 | 4.568811 | -0.826968 | C | -3.270865 | 1.741499 | -2.299143 | Cu | 1.759234 | 4.022393 | 0.601737 | |
| O | 0.201630 | -3.606285 | 1.227003 | C | -3.270292 | 1.685446 | 2.398646 | H | 0.667051 | 4.104742 | -1.481219 | |
| O | 1.053356 | 0.351103 | 1.533164 | C | 3.311817 | 1.791103 | -2.148563 | H | 0.465382 | 3.818571 | 2.675292 | |
| O | -1.451211 | 0.207182 | 2.071290 | C | -3.318378 | -2.603036 | 2.264367 | O | 2.192010 | 4.917597 | -0.984407 | |
| O | -2.168218 | -2.609398 | 1.898529 | C | 5.849677 | -2.501291 | 1.901348 | H | 2.951819 | 4.481960 | -1.397215 | |
| O | -0.127961 | -1.363419 | 3.739607 | C | -5.906774 | 1.115793 | 2.330655 | O | -3.689628 | 3.456440 | 0.211393 | |
| O | -3.706989 | -1.091262 | 1.247961 | C | 5.124550 | 0.463092 | 3.361485 | H | -3.906420 | 2.508230 | 0.070443 | |
| O | -0.088403 | 2.260234 | -3.716395 | C | -5.964364 | -2.099995 | 2.079969 | O | 0.800498 | 5.816463 | 1.009850 | |
| O | 0.111899 | -0.372141 | -4.061443 | C | 2.916097 | -4.536227 | -4.267642 | H | 1.230456 | 6.265796 | 0.257330 | |
| O | -1.415468 | 0.652520 | -2.037503 | C | -3.020187 | 3.587115 | 4.305348 | O | -1.635476 | 5.413122 | 0.186288 | |
| O | -2.157418 | 3.329433 | -2.052956 | C | 4.677000 | 4.557315 | 2.183737 | H | -2.308363 | 5.581007 | 0.862509 | |
| O | -2.007541 | -1.839745 | -2.802649 | C | -3.110089 | -4.504820 | 4.177653 | H | -0.176398 | 5.715216 | 0.720646 | |
| O | -0.043631 | -3.292948 | -0.5911350 | C | 4.725625 | -5.591207 | 5.618255 | H | -4.111530 | 3.935062 | -0.520065 | |
| O | 1.364656 | -1.605767 | -0.172928 | C | 4.821755 | 4.608755 | 5.638658 | | | | | |
| O | - | | | | | | | | | | | |

| | | | | | | | | | | | |
|--|--------------|--------------|--------------|--|----------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 120 | | | H | 21.529887000 | 17.478617000 | 3.045435000 | O | 26.174667000 | 16.592746000 | 6.878979000 | |
| Cu^{II}(OH)₄(H₂O) | | | H | 34.797626000 | 16.894133000 | 11.093474000 | O | 30.106420000 | 19.057997000 | 8.293487000 | |
| H | 23.262487000 | 19.259423000 | 2.701551000 | H | 27.738824000 | 12.979274000 | 11.213783000 | O | 33.043666000 | 15.971389000 | 5.945410000 |
| H | 21.918297000 | 15.730475000 | 4.801345000 | H | 25.114727000 | 17.541614000 | 11.266182000 | O | 33.734497000 | 17.846621000 | 6.966009000 |
| H | 24.010404000 | 15.753515000 | 6.154017000 | H | 32.001252000 | 21.748586000 | 11.051258000 | O | 29.022733000 | 16.673027000 | 6.832940000 |
| H | 28.340217000 | 18.222636000 | 12.637783000 | H | 25.338680000 | 19.273091000 | 4.069308000 | O | 32.997948000 | 16.057013000 | 10.766456000 |
| H | 36.517838000 | 15.238317000 | 2.664688000 | H | 29.373128000 | 12.254211000 | 4.067426000 | O | 33.723702000 | 17.926791000 | 9.742680000 |
| H | 38.025227000 | 18.622880000 | 4.888070000 | H | 34.491176000 | 15.209436000 | 4.104997000 | O | 31.098456000 | 18.011736000 | 10.408379000 |
| H | 35.982234000 | 18.582892000 | 6.313535000 | H | 30.440558000 | 22.219414000 | 4.084112000 | O | 29.745829000 | 14.767202000 | 8.378038000 |
| H | 29.745065000 | 17.525602000 | 12.392250000 | Zr | 29.064714000 | 18.736494000 | 6.503908000 | O | 28.037395000 | 20.717290000 | 6.991574000 |
| H | 27.921200000 | 20.801907000 | 8.012899000 | Zr | 29.005932000 | 18.898123000 | 10.063442400 | O | 29.227983000 | 18.409427000 | 12.296732000 |
| H | 30.227605000 | 15.443497000 | 12.736612000 | Zr | 30.757728000 | 15.781697000 | 10.170224000 | O | 27.949812000 | 20.635161000 | 9.608577000 |
| H | 28.274699000 | 21.433411000 | 10.066725000 | Zr | 30.879294000 | 15.641060000 | 6.564284000 | O | 26.950383000 | 18.335087000 | 10.996671000 |
| H | 28.622620000 | 21.425575000 | 6.741507000 | Zr | 27.743411000 | 16.013108000 | 8.317095000 | O | 26.092214000 | 16.690659000 | 9.724361000 |
| H | 31.572439000 | 18.256135000 | 11.207208000 | Zr | 32.105735000 | 18.519952000 | 8.326698000 | O | 29.340807000 | 14.168047000 | 10.970025000 |
| H | 26.803469000 | 18.773290000 | 8.289956000 | H | 28.708286000 | 18.921196000 | 3.826505000 | O | 27.457300000 | 14.313766000 | 9.739135000 |
| H | 31.468446000 | 23.992389000 | 2.671959000 | H | 31.584514000 | 16.324732000 | 4.051802000 | O | 31.577015000 | 16.536139000 | 8.370045000 |
| H | 35.141099000 | 6.2362516000 | 4.918751000 | O | 30.809060000 | 15.899390000 | 4.427993000 | O | 30.381761000 | 20.581655000 | 10.772838000 |
| H | 34.093780000 | 21.848786000 | 6.318493000 | O | 29.351029000 | 18.452842000 | 4.373046000 | O | 32.334366000 | 20.311685000 | 9.685038000 |
| H | 31.974835000 | 13.772694000 | 8.657978000 | Cu | 29.11672424000 | 16.592424000 | 3.703785000 | O | 28.977734000 | 16.772658000 | 9.793090000 |
| H | 28.307649000 | 10.457655000 | 2.710754000 | O | 28.789290000 | 14.953689000 | 2.726255000 | O | 30.402902000 | 20.492589000 | 5.852613000 |
| H | 24.585512000 | 11.100025000 | 4.808689000 | H | 29.160443000 | 14.223112000 | 3.234062000 | O | 32.344381000 | 20.261969000 | 6.954233000 |
| H | 25.666582000 | 12.911866000 | 6.142203000 | O | 27.375962000 | 17.018533000 | 2.941174000 | O | 31.145097000 | 17.913973000 | 6.244976000 |
| H | 32.684870000 | 13.707707000 | 6.608929000 | H | 26.790866000 | 17.486417000 | 3.547964000 | O | 27.691661000 | 18.357079000 | 8.291599000 |
| H | 32.848283000 | 14.022420000 | 9.959700000 | O | 26.383708000 | 13.342378000 | 1.620364000 | O | 30.580926000 | 16.180457000 | 12.234424000 |
| H | 31.536089000 | 18.242715000 | 5.442542000 | H | 26.504073000 | 12.565408000 | 2.183466000 | O | 31.940233000 | 13.873203000 | 9.712122000 |
| H | 29.646293000 | 13.821607000 | 8.341437000 | H | 25.453751000 | 13.635315000 | 1.740801000 | O | 31.859492000 | 13.825778000 | 7.116496000 |
| C | 26.061288000 | 17.496867000 | 5.997004000 | Cu | 26.867169000 | 15.148033000 | 2.584133000 | O | 29.368481000 | 14.161036000 | 5.674880000 |
| C | 24.806452000 | 17.506245000 | 5.189863000 | O | 25.004520000 | 15.171221000 | 2.622608000 | O | 27.496939000 | 14.290970000 | 6.905370000 |
| C | 24.586153000 | 18.494812000 | 4.217597000 | H | 24.614368000 | 16.048207000 | 2.570970000 | H | 38.310373000 | 16.957132000 | 3.033855000 |
| C | 23.418415000 | 18.485764000 | 3.457276000 | | | | | H | 33.844237000 | 24.702442000 | 3.061945000 |
| C | 22.440167000 | 17.489247000 | 3.647444000 | | | | | H | 25.894596000 | 9.876779000 | 3.056240000 |
| C | 22.661967000 | 16.513834000 | 4.638703000 | 116 | | | | H | 21.528339000 | 17.479647000 | 3.047645000 |
| C | 23.829506000 | 16.519280000 | 5.398176000 | Cu^{II}O(OH)₂(O₂) | | | | H | 34.801573000 | 16.894177000 | 11.087279000 |
| C | 33.868496000 | 16.903694000 | 6.130205000 | H | 23.262476000 | 19.258261000 | 2.700212000 | H | 27.740233000 | 12.974300000 | 11.207621000 |
| C | 35.111026000 | 16.894750000 | 5.299725000 | H | 21.912574000 | 15.736910000 | 4.808880000 | H | 25.115078000 | 17.541884000 | 11.266561000 |
| C | 35.273600000 | 15.953348000 | 4.269735000 | H | 24.003085000 | 15.759476000 | 6.162848000 | H | 31.999753000 | 21.748667000 | 11.052844000 |
| C | 36.411260000 | 15.974755000 | 3.465064000 | H | 28.338934000 | 18.236298000 | 12.635661000 | H | 25.345556000 | 19.264153000 | 4.065432000 |
| C | 37.420943000 | 16.937187000 | 3.666012000 | H | 36.517358000 | 15.238593000 | 2.664408000 | H | 29.364368000 | 12.280498000 | 4.050199000 |
| C | 37.253514000 | 17.869762000 | 4.709702000 | H | 38.025574000 | 18.622420000 | 4.888550000 | H | 34.490793000 | 15.209482000 | 4.105030000 |
| C | 36.114989000 | 17.853118000 | 5.512676000 | H | 35.982252000 | 18.583299000 | 6.313155000 | H | 30.440984000 | 22.218644000 | 4.083457000 |
| C | 33.836780000 | 16.959033000 | 10.535640000 | H | 29.742529000 | 17.536220000 | 12.397096000 | Zr | 29.058955000 | 18.706591000 | 6.484527000 |
| C | 26.050712000 | 17.527364000 | 10.664687000 | H | 27.941874000 | 20.792959000 | 8.000385000 | Zr | 29.009166000 | 18.895301000 | 10.058402000 |
| C | 28.183345000 | 13.821282000 | 10.638080000 | H | 30.220945000 | 15.409535000 | 12.751590000 | Zr | 30.759924000 | 15.781364000 | 10.186564000 |
| C | 31.573370000 | 20.879064000 | 10.504638000 | H | 28.266233000 | 21.426357000 | 10.059614000 | Zr | 30.911038000 | 15.614257000 | 6.595218000 |
| C | 31.605394000 | 20.824081000 | 6.099571000 | H | 28.056260000 | 21.407150000 | 6.737478000 | Zr | 27.749913000 | 16.006622000 | 8.325679000 |
| C | 32.203651000 | 12.926578000 | 5.289666000 | H | 31.573914000 | 18.263037000 | 11.209155000 | Zr | 32.103901000 | 18.519445000 | 8.321620000 |
| C | 31.468250000 | 22.541467000 | 4.263264000 | H | 26.816633000 | 18.763493000 | 8.268906000 | H | 28.324039000 | 18.464142000 | 3.985679000 |
| C | 32.051055000 | 23.530716000 | 3.473051000 | H | 31.468106000 | 23.996209000 | 2.672377000 | H | 31.617573000 | 16.307036000 | 4.042460000 |
| C | 33.385415000 | 23.937235000 | 3.684991000 | H | 35.141313000 | 23.622908000 | 4.918380000 | O | 30.912277000 | 15.799207000 | 4.451698000 |
| C | 34.107728000 | 23.321906000 | 4.729973000 | H | 34.093727000 | 21.849616000 | 6.319085000 | O | 29.164620000 | 18.185657000 | 4.373451000 |
| C | 33.528856000 | 22.330809000 | 5.518577000 | H | 31.983031000 | 13.750879000 | 8.700105000 | Cu | 29.090307000 | 16.190964000 | 3.895934000 |
| C | 28.201363000 | 13.798772000 | 5.970288000 | H | 28.304324000 | 10.467076000 | 10.270340000 | O | 29.014789000 | 14.921717000 | 2.492591000 |
| C | 27.574726000 | 12.706285000 | 5.169919000 | H | 24.584299000 | 11.103346000 | 4.806103000 | H | 26.887192000 | 15.670798000 | 4.825416000 |
| C | 28.317316000 | 12.007707000 | 4.205567000 | H | 25.663605000 | 12.907636000 | 6.145783000 | O | 27.134020000 | 15.973656000 | 3.939858000 |
| C | 27.719353000 | 19.095860000 | 3.458178000 | H | 32.6704094000 | 13.637512000 | 6.631215000 | Cu | 27.213869000 | 14.447424000 | 2.702050000 |
| C | 26.365102000 | 10.659929000 | 3.653220000 | H | 32.851582000 | 14.018049000 | 10.000769000 | O | 25.457095000 | 13.630612000 | 2.263697000 |
| C | 25.634743000 | 11.351840000 | 4.637583000 | H | 31.566035000 | 18.220267000 | 5.438807000 | O | 26.358203000 | 13.103790000 | 1.496382000 |
| C | 26.230612000 | 12.363560000 | 5.386025000 | H | 29.662455000 | 13.806091000 | 8.365987000 | | | | |
| O | 26.960268000 | 18.339963000 | 5.696876000 | C | 26.016567000 | 17.496086000 | 5.996859000 | | | | |
| O | 26.146363000 | 16.641102000 | 6.921455000 | C | 24.806491000 | 17.506324000 | 17.506324000 | | | | |
| O | 30.103747000 | 19.075982000 | 8.303720000 | C | 24.586192000 | 18.494784000 | 4.217548000 | | | | |
| O | 33.016240000 | 16.002475000 | 5.900038000 | C | 23.418409000 | 18.485760000 | 3.457286000 | | | | |
| O | 33.751271000 | 17.819852000 | 6.994087000 | C | 22.440174000 | 17.489258000 | 3.647451000 | | | | |
| O | 29.006978000 | 16.701682000 | 6.819475000 | C | 22.661600000 | 16.513841000 | 4.638695000 | | | | |
| O | 33.000160000 | 16.050826000 | 10.751223000 | C | 23.894424000 | 16.519355000 | 5.983816000 | | | | |
| O | 33.722652000 | 17.937369000 | 9.751268000 | C | 33.868135000 | 16.904232000 | 6.130650000 | | | | |
| O | 31.097463000 | 18.010559000 | 10.404334000 | C | 35.110958000 | 16.894629000 | 5.299625000 | | | | |
| O | 29.737137000 | 14.781819000 | | | | | | | | | |

| | | | | | | | | | | | |
|---|--------------|---------------|--------------|---|--------------|--------------|--------------|------------|--------------|--------------|---------------|
| C | 22.661958000 | 16.513843000 | 4.638698000 | H | 24.005863000 | 15.761396000 | 6.163837000 | H | 25.335944000 | 19.275381000 | 4.068962000 |
| C | 23.829435000 | 16.519366000 | 5.398327000 | H | 28.343797000 | 18.213943000 | 12.642860000 | H | 29.370599000 | 12.263923000 | 4.062427000 |
| C | 33.868194000 | 16.904267000 | 6.130662000 | H | 36.517941000 | 15.238133000 | 2.664866000 | H | 34.490756000 | 15.210081000 | 4.104608000 |
| C | 35.110961000 | 16.894613000 | 5.299629000 | H | 38.025123000 | 18.623046000 | 4.887885000 | H | 30.440320000 | 22.219988000 | 4.084142000 |
| C | 35.273563000 | 15.953402000 | 4.269678000 | H | 35.982469000 | 18.582546000 | 6.313903000 | Zr | 29.070343000 | 18.745720000 | 6.516114000 |
| C | 36.411229000 | 15.974751000 | 3.465070000 | H | 29.749078000 | 17.518121000 | 12.393137000 | Zr | 29.007226000 | 18.895696000 | 10.070401000 |
| C | 37.420943000 | 16.937186000 | 3.666012000 | H | 27.915989000 | 20.802482000 | 8.022407000 | Zr | 30.760360000 | 15.778935000 | 10.166118000 |
| C | 37.253511000 | 17.869769000 | 4.709696000 | H | 30.233125000 | 15.438028000 | 12.733519000 | Zr | 30.871219000 | 15.644438000 | 6.553127000 |
| C | 36.115041000 | 17.853046000 | 5.512754000 | H | 28.277393000 | 21.431264000 | 10.073816000 | Zr | 27.745629000 | 16.012177000 | 8.317631000 |
| C | 33.837141000 | 16.958907000 | 10.535584000 | H | 28.609230000 | 21.430802000 | 6.748733000 | Zr | 32.108318000 | 18.517618000 | 8.327466000 |
| C | 26.050620000 | 17.523797000 | 10.664602000 | H | 31.574178000 | 18.252534000 | 11.208537000 | H | 28.853468000 | 19.020683000 | 3.804030000 |
| C | 28.183404000 | 13.821192000 | 10.638016000 | H | 26.802493000 | 18.777362000 | 8.301717000 | H | 31.516945000 | 16.354107000 | 4.037592000 |
| C | 31.573527000 | 20.879172000 | 10.504557000 | H | 31.468522000 | 23.992273000 | 2.671833000 | O | 30.748309000 | 15.919594000 | 4.418836000 |
| C | 31.605436000 | 20.823687000 | 6.099611000 | H | 35.141037000 | 23.623667000 | 4.918869000 | O | 29.416747000 | 18.506786000 | 4.395405000 |
| C | 32.203608000 | 21.926571000 | 5.289625000 | H | 34.093778000 | 21.848569000 | 6.318352000 | Cu | 29.071386000 | 16.675709000 | 3.699716000 |
| C | 31.468280000 | 22.541415000 | 4.263212000 | H | 31.975336000 | 13.776531000 | 8.647085000 | O | 28.562377000 | 15.093801000 | 2.70795000 |
| C | 32.051053000 | 23.530720000 | 3.473055000 | H | 28.305573000 | 10.461969000 | 2.706422000 | H | 28.746947000 | 14.28332600 | 3.196408000 |
| C | 33.385414000 | 23.937235000 | 3.684992000 | H | 24.585825000 | 11.091812200 | 4.810123000 | O | 27.458905000 | 17.374468000 | 2.857377000 |
| C | 34.107730000 | 23.321902000 | 4.729968000 | H | 25.669100000 | 12.905723000 | 6.148982000 | H | 26.914388000 | 17.838666000 | 3.504777000 |
| C | 33.528819000 | 22.330887000 | 5.518658000 | H | 32.684312000 | 13.714292000 | 6.598686000 | Cu | 26.728511000 | 15.623387000 | 2.330016000 |
| C | 28.200767000 | 13.799517000 | 5.970316000 | H | 32.848966000 | 14.018745000 | 9.950550000 | O | 24.920326000 | 16.086114000 | 1.654557000 |
| C | 27.574833000 | 12.706325000 | 5.169772000 | H | 31.522636000 | 18.249463000 | 5.447619000 | H | 24.329733000 | 16.229778000 | 2.406475000 |
| C | 28.317315000 | 12.007738000 | 4.205536000 | H | 29.642948000 | 13.824781000 | 8.330819000 | C | 25.982989000 | 13.689652000 | 1.716934000 |
| C | 27.719336000 | 10.995847000 | 3.458195000 | C | 26.061597000 | 17.496055000 | 5.996863000 | H | 26.776946000 | 13.495365000 | 0.998424000 |
| C | 26.365101000 | 10.659934000 | 3.653216000 | C | 24.806514000 | 17.506303000 | 5.189713000 | H | 26.228370000 | 13.234061000 | 2.673331000 |
| C | 25.634739000 | 11.351846000 | 4.637578000 | C | 24.586187000 | 18.494793000 | 4.217558000 | H | 25.077336000 | 13.199289000 | 1.353777000 |
| C | 26.230658000 | 12.363451000 | 5.386136000 | C | 23.418409000 | 18.485760000 | 3.457286000 | H | 25.253470000 | 14.869263000 | 1.642777000 |
| O | 26.965935000 | 18.334407000 | 5.690931000 | C | 22.440175000 | 17.489256000 | 3.647450000 | | | | |
| O | 26.146253000 | 16.643895000 | 6.923426000 | C | 22.661958000 | 16.513843000 | 4.638698000 | | | | |
| O | 30.103186000 | 19.078580000 | 8.305412000 | C | 23.829435000 | 16.519366000 | 5.398327000 | 122 | | | |
| O | 33.011998000 | 16.007970000 | 5.893846000 | C | 33.868194000 | 16.904267000 | 6.130662000 | B1 | | | |
| O | 33.753523000 | 17.816815000 | 6.998374000 | C | 35.110961000 | 16.894613000 | 5.299629000 | H | 23.254351000 | 19.268540000 | 2.711250000 |
| O | 29.006295000 | 16.705251000 | 6.814431000 | C | 35.273563000 | 15.953402000 | 4.269678000 | H | 21.913263000 | 15.736347000 | 4.807342000 |
| O | 33.000423000 | 16.050688000 | 10.750363000 | C | 36.411229000 | 15.974751000 | 3.465070000 | H | 24.007862000 | 15.759178000 | 6.161060000 |
| O | 33.722738000 | 17.934535000 | 9.752169000 | C | 37.420943000 | 16.937186000 | 3.666012000 | H | 28.343768000 | 18.213283000 | 12.642395000 |
| O | 31.097488000 | 18.010006000 | 10.404508000 | C | 37.253511000 | 17.869769000 | 4.709696000 | H | 36.517961000 | 15.238003000 | 2.664993000 |
| O | 29.738062000 | 14.782908000 | 8.359970000 | C | 36.115041000 | 17.853046000 | 5.512754000 | H | 38.025201000 | 18.622961000 | 4.887963000 |
| O | 28.004366000 | 20.729081000 | 7.005098000 | C | 33.887141000 | 16.958907000 | 10.355854000 | H | 35.982573000 | 18.582409000 | 6.314052000 |
| O | 29.228726000 | 18.397370000 | 12.299724000 | C | 26.050620000 | 17.523797000 | 10.664602000 | H | 29.749240000 | 17.517409000 | 12.392152000 |
| O | 27.950517000 | 20.643242000 | 9.619989000 | C | 28.183404000 | 13.821192000 | 10.638016000 | H | 27.915086000 | 20.799406000 | 8.018903000 |
| O | 26.949054000 | 18.336887000 | 10.998443000 | C | 31.573527000 | 20.879172000 | 10.504457000 | H | 30.232746000 | 15.438841000 | 12.732835000 |
| O | 26.094217000 | 16.6889854000 | 9.726652000 | C | 31.605436000 | 20.823687000 | 6.099611000 | H | 28.278811000 | 21.430854000 | 10.0668642000 |
| O | 29.345868000 | 14.163003000 | 10.960435000 | C | 32.203608000 | 21.926571000 | 5.289625000 | H | 28.610785000 | 21.427210000 | 6.747075000 |
| O | 27.456739000 | 14.317697000 | 9.742014000 | C | 31.468280000 | 22.541215000 | 4.632312000 | H | 31.573719000 | 18.252706000 | 11.208421000 |
| O | 31.562581000 | 16.543065000 | 8.356056000 | C | 32.051053000 | 23.530720000 | 3.473050000 | H | 26.804028000 | 18.778388000 | 8.303433000 |
| O | 30.385821000 | 20.576375000 | 10.784951000 | C | 33.385414000 | 23.932735000 | 3.684992000 | H | 31.468629000 | 23.992561000 | 2.6711882000 |
| O | 32.328891000 | 20.318068000 | 9.675600000 | C | 34.107730000 | 23.321902000 | 4.729968000 | H | 35.141036000 | 23.623660000 | 4.918821000 |
| O | 28.974764000 | 16.777951000 | 9.718919000 | C | 33.528819000 | 23.330887000 | 5.518658000 | H | 34.093690000 | 21.848408000 | 6.318310000 |
| O | 30.385431000 | 20.541925000 | 5.903703000 | C | 28.200767000 | 13.799517000 | 5.970316000 | H | 31.976695000 | 13.777022000 | 8.648281000 |
| O | 32.359876000 | 20.237745000 | 6.926211100 | C | 27.574833000 | 12.706325000 | 5.169772000 | H | 28.305850000 | 10.462490000 | 2.706276000 |
| O | 31.148965000 | 17.936904000 | 6.273406000 | C | 28.317315000 | 12.007738000 | 4.205536000 | H | 24.584248000 | 11.101711000 | 4.806129000 |
| O | 27.681801000 | 18.375089000 | 8.294653000 | C | 27.719336000 | 10.995847000 | 3.458195000 | H | 25.666521000 | 12.910395000 | 6.143781000 |
| O | 30.583795000 | 16.175798000 | 12.221690000 | C | 26.365101000 | 16.059934000 | 3.653216000 | H | 32.689283000 | 13.715191000 | 6.602662000 |
| O | 31.936197000 | 13.878697000 | 9.673437000 | C | 25.634739000 | 11.351846000 | 4.637578000 | H | 32.848045000 | 14.015619000 | 9.954369000 |
| O | 31.860309000 | 13.863003000 | 7.077044000 | C | 26.230658000 | 12.363451000 | 5.386136000 | H | 31.521238000 | 18.248152000 | 5.448568000 |
| O | 29.372285000 | 14.156197000 | 5.674539000 | O | 26.963564000 | 18.331671000 | 5.686510000 | H | 29.641602000 | 13.825318000 | 8.327030000 |
| O | 27.504552000 | 14.299199000 | 6.907580000 | O | 26.137716000 | 16.646474700 | 6.925663000 | C | 26.061613000 | 17.495840000 | 5.996824000 |
| H | 38.310527000 | 16.956963000 | 3.034058000 | O | 30.104133000 | 19.081075000 | 8.310701000 | C | 24.806499000 | 17.506411000 | 5.189738000 |
| H | 33.844138000 | 24.702454000 | 3.061896000 | O | 33.004953000 | 16.016804000 | 5.882881000 | C | 24.586187000 | 18.494794000 | 4.217558000 |
| H | 25.896796000 | 9.871692000 | 3.060726000 | O | 33.758530000 | 17.809231000 | 7.005674000 | C | 23.418405000 | 18.485764000 | 3.457292000 |
| H | 21.528336000 | 17.480980000 | 3.047456000 | O | 29.001048000 | 16.709175000 | 6.162818000 | C | 22.440178000 | 17.489252000 | 3.647445000 |
| H | 34.798129000 | 11.093095000 | 3.0301979000 | O | 33.001979000 | 16.048080000 | 10.745847000 | C | 22.661967000 | 16.513831000 | 4.638684000 |
| H | 27.739197000 | 12.978187000 | 1.1221246000 | O | 33.722598000 | 17.936411000 | 7.954926000 | C | 23.829422000 | 16.519383000 | 5.398347000 |
| H | 25.114169000 | 17.542468000 | 11.265224000 | O | 31.090661000 | 18.008360000 | 10.405315000 | C | 33.868220000 | 16.904203000 | 6.130727000 |
| H | 29.004779000 | 17.214939000 | 10.067214000 | O | 29.347180000 | 14.160539000 | 10.956991000 | C | 33.837137000 | 16.958911000 | 10.353593000 |
| H | 30.757109000 | 15.780115000 | 10.170300000 | O | 27.455729000 | 14.317315000 | 9.742156000 | | | | |

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|-------------|---------------|---------------|--------------|-------------|--------------|--------------|--------------|--------------|
| O | 29.001425000 | 16.710936000 | 6.814573000 | C | 22.440178000 | 17.489252000 | 3.647445000 | |
| O | 33.001832000 | 16.048267000 | 10.745451000 | C | 22.661967000 | 16.513831000 | 4.638684000 | |
| O | 33.723067000 | 17.936881000 | 9.755407000 | C | 23.829422000 | 16.519383000 | 5.398347000 | |
| O | 31.099125000 | 18.008464000 | 10.404731000 | C | 33.868220000 | 16.904203000 | 6.130727000 | |
| O | 29.735393000 | 14.785191000 | 8.356909000 | C | 35.110945000 | 16.894653000 | 5.299604000 | |
| O | 27.994874000 | 20.727391000 | 7.006195000 | C | 35.273562000 | 15.953406000 | 4.269675000 | |
| O | 29.230720000 | 18.391430000 | 12.300961000 | C | 36.411225000 | 15.974756000 | 3.465064000 | |
| O | 27.950490000 | 20.641988000 | 9.621890000 | C | 37.420945000 | 16.937182000 | 3.666015000 | |
| O | 26.949273000 | 18.335857000 | 10.999395000 | C | 37.253518000 | 17.867959000 | 4.707905000 | |
| O | 26.092696000 | 16.690718000 | 9.725536000 | C | 36.115032000 | 17.853059000 | 5.512743000 | |
| O | 29.346744000 | 14.616202000 | 10.957781000 | C | 33.837137000 | 16.958911000 | 10.535593000 | |
| O | 27.455969000 | 14.318131000 | 9.742337000 | C | 26.050609000 | 17.523852000 | 10.664620000 | |
| O | 31.558748000 | 16.543726000 | 8.353824000 | C | 28.183386000 | 13.821231000 | 10.638013000 | |
| O | 30.386824000 | 20.574397000 | 10.788580000 | C | 31.573529000 | 20.879186000 | 10.504559000 | |
| O | 32.327487000 | 20.319898000 | 9.673438000 | C | 31.605411000 | 20.823560000 | 6.099453000 | |
| O | 28.974867000 | 16.777208000 | 9.783303000 | C | 32.203616000 | 21.926616000 | 5.289694000 | |
| O | 30.380012000 | 20.558968000 | 5.923005000 | C | 31.468276000 | 22.541427000 | 4.623223000 | |
| O | 32.364794000 | 20.229239000 | 6.916135000 | C | 32.051051000 | 23.530724000 | 3.473058000 | |
| O | 31.154274000 | 17.939073000 | 6.284880000 | C | 33.385417000 | 23.932728000 | 3.684985000 | |
| O | 27.680703000 | 18.376158000 | 8.295855000 | C | 34.107734000 | 23.321891000 | 4.729958000 | |
| O | 30.587192000 | 16.173090000 | 12.218449000 | C | 33.528808000 | 22.330912000 | 5.518633000 | |
| O | 31.935987000 | 13.877607000 | 9.6648472000 | C | 28.200842000 | 13.799446000 | 5.970377000 | |
| O | 31.863192000 | 13.872509000 | 7.072761000 | C | 27.574786000 | 12.706392000 | 5.169698000 | |
| O | 29.375138000 | 14.145140000 | 5.686279000 | C | 28.317352000 | 12.007676000 | 4.205600000 | |
| O | 27.497220000 | 14.309093000 | 6.900233000 | C | 27.719380000 | 10.995810000 | 3.458196000 | |
| H | 38.310510000 | 16.956983000 | 3.034048000 | C | 26.365079000 | 10.660416000 | 4.265966000 | |
| H | 33.844189000 | 24.702264000 | 3.061702000 | C | 25.634756000 | 11.351454000 | 4.637917000 | |
| H | 25.895242000 | 9.875079000 | 3.058095000 | C | 26.230653000 | 12.363536000 | 5.386037000 | |
| H | 21.525425000 | 17.483571000 | 3.051924000 | O | 26.963680000 | 18.336904000 | 5.690989000 | |
| H | 34.796788000 | 16.893636000 | 11.095385000 | O | 26.143703000 | 16.643689000 | 6.923608000 | |
| H | 27.738228000 | 12.979767000 | 11.213831000 | O | 30.104058000 | 19.077025000 | 8.310620000 | |
| H | 25.114133000 | 17.542639000 | 11.265511000 | O | 33.011102000 | 16.008457000 | 5.189131000 | |
| H | 32.001017000 | 21.750172000 | 11.049287000 | O | 33.754526000 | 17.816149000 | 6.998542000 | |
| H | 25.333617000 | 17.2976962000 | 4.0766422000 | O | 29.001517000 | 17.605317000 | 6.816533000 | |
| H | 29.370087000 | 12.264187000 | 4.059554000 | O | 33.002002000 | 16.048535000 | 10.747832000 | |
| H | 34.490824000 | 15.210030000 | 4.104626000 | O | 33.722999000 | 17.933850000 | 9.751751000 | |
| H | 30.440067000 | 22.220405000 | 4.084686000 | O | 31.098848000 | 18.005623000 | 10.403919000 | |
| Zr | 29.077444000 | 17.484624000 | 6.517561000 | O | 29.733446000 | 14.779579000 | 8.3555304000 | |
| Zr | 29.007209000 | 18.894904000 | 10.069986000 | O | 28.006308000 | 20.731763000 | 7.012920000 | |
| Zr | 30.760742000 | 15.778009000 | 10.165469000 | O | 29.232092000 | 18.389595000 | 12.301937000 | |
| Zr | 30.870147000 | 15.641466000 | 6.549580000 | O | 27.950066000 | 20.640882000 | 9.628271000 | |
| Zr | 27.746923000 | 16.009878000 | 8.316747000 | O | 26.950159000 | 18.334274000 | 11.001249000 | |
| Zr | 32.109920000 | 18.515380000 | 8.328049000 | O | 26.092905000 | 16.689940000 | 9.726802000 | |
| H | 28.925611000 | 19.062249000 | 3.789739000 | O | 29.347034000 | 14.160995000 | 10.957600000 | |
| H | 31.509178000 | 16.356061000 | 4.034875000 | O | 27.454863000 | 14.316419000 | 9.743098000 | |
| H | 30.738483000 | 15.925132000 | 4.416420000 | O | 31.560353000 | 16.539635000 | 8.352114000 | |
| O | 29.443435000 | 18.517625000 | 4.394283000 | O | 30.386760000 | 20.574514000 | 10.787463000 | |
| Cu | 29.065488000 | 16.698362000 | 3.685803000 | O | 32.329255000 | 20.317099000 | 9.676759000 | |
| O | 28.486524000 | 15.100197000 | 2.809283000 | O | 28.975095000 | 16.774585000 | 9.783099000 | |
| H | 28.709073000 | 14.310676000 | 3.315865000 | O | 30.385184000 | 20.546783000 | 5.509192000 | |
| O | 27.436397000 | 17.482307000 | 2.878829000 | O | 32.360672000 | 20.236686000 | 6.925629000 | |
| H | 27.042144000 | 17.924325000 | 3.643358000 | O | 31.147301000 | 17.936255000 | 6.277843000 | |
| Cu | 26.600998000 | 15.645819000 | 2.540240000 | O | 27.679783000 | 18.374918000 | 8.298295000 | |
| H | 25.326492000 | 16.962911000 | 1.268899900 | O | 30.588474000 | 16.169552000 | 12.218886000 | |
| H | 25.925240000 | 17.672326000 | 1.563893000 | O | 31.937068000 | 13.875294000 | 9.662378000 | |
| C | 25.537364000 | 14.029621000 | 2.356977000 | O | 31.850567000 | 13.858629000 | 7.064693000 | |
| H | 24.786795000 | 13.996000000 | 3.149637000 | O | 29.365084000 | 14.162303000 | 5.667791000 | |
| H | 25.043214000 | 14.072928000 | 3.185587000 | O | 27.502267000 | 14.294274000 | 6.910465000 | |
| H | 26.165337000 | 13.143372000 | 2.412772000 | H | 38.310518000 | 16.957102000 | 3.033993000 | |
| H | 24.507585000 | 17.110904000 | 1.759957000 | H | 33.844237000 | 24.702328000 | 3.061750000 | |
| H | 25.899673000 | 9.857971000 | 3.078115000 | H | 21.528497000 | 17.480577000 | 3.047330000 | |
| H | 24.7790700600 | 16.895380000 | 11.095461000 | H | 34.797006000 | 16.895380000 | 11.095461000 | |
| H | 27.739476000 | 12.979439000 | 11.214784000 | H | 26.136220000 | 16.641300000 | 5.691854800 | |
| 122 TSB2 | H | 23.263356000 | 19.258323000 | 2.700641000 | H | 25.113036000 | 17.544814000 | 11.263853000 |
| H | 21.912537000 | 15.736861000 | 4.810018000 | H | 32.000184000 | 21.751726000 | 11.047606000 | |
| H | 24.005258000 | 15.760356000 | 6.163212000 | H | 25.335893000 | 19.275452000 | 4.069210000 | |
| H | 28.344501000 | 18.211539000 | 12.641843000 | H | 29.372215000 | 12.263062000 | 4.068747000 | |
| H | 36.517996000 | 15.238203000 | 2.664744000 | H | 34.490589000 | 15.210055000 | 4.101569000 | |
| H | 38.025289000 | 18.622875000 | 4.888031000 | H | 30.440340000 | 22.197310000 | 4.084566000 | |
| H | 35.982100000 | 18.582596000 | 6.313800000 | Zr | 29.068047000 | 18.741347000 | 6.515102000 | |
| H | 29.749897000 | 17.515393000 | 12.392503000 | Zr | 29.065953000 | 18.892703000 | 10.070252000 | |
| H | 27.921176000 | 20.802542000 | 8.024531000 | Zr | 30.759001000 | 15.776375000 | 10.165048000 | |
| H | 30.232356000 | 15.433569000 | 12.732015000 | Zr | 30.867082000 | 15.637172000 | 6.552360000 | |
| H | 28.279267000 | 21.428270000 | 10.077288000 | Zr | 27.743314000 | 16.009164000 | 3.814773000 | |
| H | 28.625246000 | 21.429510000 | 10.675666000 | Zr | 32.105844000 | 18.515240000 | 8.326863600 | |
| H | 31.575104000 | 18.250158000 | 11.206304000 | H | 28.839576000 | 19.899889000 | 3.805133000 | |
| H | 26.802071000 | 18.775176000 | 8.297888000 | H | 31.564972000 | 16.372470000 | 4.073801000 | |
| H | 31.468399000 | 23.992531000 | 2.672023000 | O | 30.781175000 | 15.924550000 | 4.405337000 | |
| H | 35.141118000 | 23.623597000 | 4.918742000 | O | 29.406622000 | 18.491245000 | 4.398071000 | |
| H | 34.093487000 | 21.848529000 | 6.318564000 | Cu | 29.133750000 | 16.667760000 | 3.638190000 | |
| H | 31.973371000 | 13.771672000 | 8.646764000 | O | 28.642030000 | 15.219255000 | 2.436533000 | |
| H | 28.309683000 | 14.057079000 | 2.716963000 | H | 28.789788000 | 14.353472000 | 2.837051000 | |
| H | 24.587361000 | 11.094969000 | 4.813661000 | O | 27.475592000 | 17.405285000 | 2.903123000 | |
| H | 25.669908000 | 12.902703000 | 6.151178000 | H | 26.980736000 | 17.831576000 | 3.613315000 | |
| H | 32.675458000 | 13.703428000 | 6.591744000 | Cu | 26.719283000 | 15.770067000 | 2.197019000 | |
| H | 32.849751000 | 14.018114000 | 9.947568000 | O | 26.109163000 | 14.174269000 | 1.323362000 | |
| H | 31.524443000 | 18.247953000 | 5.447350000 | H | 25.302552000 | 16.309290000 | 2.068050000 | |
| H | 29.639604000 | 18.319830000 | 8.329499000 | C | 26.970093000 | 12.875924000 | 2.042852000 | |
| H | 26.061613000 | 17.495840000 | 5.996824000 | H | 27.192181000 | 13.476228000 | -0.626754000 | |
| C | 24.806499000 | 17.506411000 | 5.189738000 | H | 27.786853000 | 12.647450000 | 0.907190000 | |
| C | 24.586187000 | 18.494794000 | 4.217558000 | H | 26.183765000 | 12.145997000 | 1.040336000 | |
| C | 23.418405000 | 18.485764000 | 4.357292000 | H | 25.280264000 | 14.292017000 | 0.840982000 | |

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|---|--------------|---------------|--------------|----|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 25.897035000 | 9.871261000 | 3.061201000 | C | 26.230705000 | 12.363298000 | 5.386144000 | C | 23.829438000 | 16.519362000 | 5.398321000 |
| H | 21.530066000 | 17.481920000 | 3.047544000 | O | 26.932534000 | 18.377200000 | 5.747062000 | C | 33.868245000 | 16.904208000 | 6.130639000 |
| H | 34.798252000 | 16.893674000 | 11.093063000 | O | 26.169211000 | 16.604580000 | 6.891846000 | C | 35.110970000 | 16.894616000 | 5.299643000 |
| H | 27.740367000 | 12.976034000 | 11.210295000 | O | 30.105289000 | 19.058229000 | 8.285569000 | C | 35.273567000 | 15.953397000 | 4.269684000 |
| H | 25.117054000 | 17.538794000 | 11.270323000 | O | 33.043207000 | 15.973290000 | 5.940976000 | C | 36.411230000 | 15.974750000 | 3.465071000 |
| H | 32.000675000 | 21.748169000 | 11.052818000 | O | 33.735901000 | 17.844939000 | 6.967288000 | C | 37.420942000 | 16.937187000 | 3.666011000 |
| H | 25.342378000 | 19.268921000 | 4.067923000 | O | 29.011986000 | 16.675325000 | 6.825690000 | C | 37.253510000 | 17.869771000 | 4.709694000 |
| H | 29.372821000 | 12.254924000 | 4.065994000 | O | 32.999638000 | 16.052725000 | 10.757537000 | C | 36.115037000 | 17.853052000 | 5.512748000 |
| H | 34.491087000 | 15.209497000 | 4.104802000 | O | 33.724752000 | 17.927360000 | 9.743370000 | C | 33.837139000 | 16.958910000 | 10.535586000 |
| H | 30.440768000 | 22.218915000 | 4.083832000 | O | 31.099525000 | 18.012559000 | 10.39926000 | C | 26.050620000 | 17.523803000 | 10.664603000 |
| Zr | 29.071503000 | 18.730336000 | 6.498591000 | O | 29.738514000 | 14.773860000 | 8.368148000 | C | 28.183405000 | 13.821217000 | 10.638011000 |
| Zr | 29.007909000 | 18.896745000 | 10.059474000 | O | 28.030491000 | 20.715571000 | 6.979052000 | C | 31.573520000 | 20.879169000 | 10.504555000 |
| Zr | 30.759765000 | 15.780635000 | 10.170675000 | O | 29.229429000 | 18.409193000 | 12.287906000 | C | 31.605413000 | 20.823709000 | 6.099625000 |
| Zr | 30.879763000 | 15.633861000 | 6.562257000 | O | 27.949714000 | 20.639749000 | 9.600315000 | C | 32.203604000 | 21.926576000 | 5.289629000 |
| Zr | 27.748630000 | 16.007144000 | 8.317726000 | O | 26.948437000 | 18.338773000 | 10.991918000 | C | 31.468277000 | 22.541420000 | 4.263217000 |
| Zr | 32.107186000 | 18.517251000 | 8.326238000 | O | 26.091636000 | 16.688854000 | 9.725999000 | C | 32.051052000 | 23.530721000 | 3.473056000 |
| H | 28.694343000 | 18.879877000 | 3.820211000 | O | 29.343028000 | 14.166154000 | 10.963343000 | C | 33.385414000 | 23.932734000 | 3.684991000 |
| H | 31.595753000 | 16.313648000 | 4.049987000 | O | 27.455835000 | 14.310828000 | 9.737889000 | C | 34.107731000 | 23.321900000 | 4.729966000 |
| O | 30.821507000 | 15.894057000 | 4.434497000 | O | 31.571921000 | 16.539959000 | 8.356058000 | C | 33.528822000 | 22.330882000 | 5.518652000 |
| O | 29.334990000 | 18.419132000 | 4.375244000 | O | 30.380388000 | 20.583440000 | 10.769967000 | C | 28.200796000 | 13.799505000 | 5.970296000 |
| Cu | 29.121494000 | 16.546322000 | 3.679929000 | O | 32.333724000 | 20.313211000 | 9.683748000 | C | 27.574827000 | 12.706326000 | 5.169755000 |
| O | 28.908938000 | 14.941711000 | 2.636193000 | O | 28.975292000 | 16.775850000 | 9.791636000 | C | 28.317316000 | 12.007734000 | 4.205540000 |
| H | 29.241039000 | 14.191980000 | 3.145163000 | O | 30.400708000 | 20.501311000 | 5.859538000 | C | 27.719337000 | 10.995846000 | 3.458196000 |
| O | 27.370728000 | 19.6597000 | 2.930257000 | O | 32.347235000 | 16.286800000 | 6.950189000 | C | 26.365101000 | 10.659934000 | 3.653216000 |
| H | 26.845125000 | 17.439234000 | 3.574854000 | O | 31.140686000 | 17.918106000 | 6.237496000 | C | 25.634739000 | 11.351847000 | 4.637577000 |
| Cu | 26.948947000 | 15.035504000 | 2.508298000 | O | 27.689797000 | 18.361156000 | 8.287335000 | C | 26.230656000 | 12.363455000 | 5.386132000 |
| O | 24.903357000 | 15.530011000 | 2.224337000 | O | 30.583490000 | 16.180800000 | 12.221502000 | O | 26.975153000 | 18.316952000 | 5.669434000 |
| H | 24.616237000 | 16.294808000 | 2.742984000 | O | 31.937757000 | 13.876747000 | 9.685992000 | O | 26.122005000 | 16.669954000 | 6.942466000 |
| C | 23.950099000 | 14.478848000 | 2.361764000 | O | 31.851577000 | 13.840498000 | 7.094463000 | O | 30.104899000 | 19.088356000 | 8.314114000 |
| H | 23.887615000 | 14.122621000 | 3.392380000 | O | 29.376746000 | 14.132434000 | 5.678222000 | O | 32.993016000 | 16.032194000 | 5.863649000 |
| H | 22.965938000 | 14.811987000 | 2.027915000 | O | 27.493793000 | 14.289892000 | 6.897571000 | O | 33.766517000 | 17.975440000 | 7.019332000 |
| H | 24.299969000 | 13.662278000 | 1.737241000 | H | 38.310284000 | 16.957162000 | 3.033730000 | O | 28.999114000 | 16.712516000 | 6.815864000 |
| H | 26.643845000 | 13.570810000 | 2.160221000 | H | 33.844304000 | 24.702345000 | 3.061836000 | O | 33.000667000 | 16.050646000 | 10.74884000 |
| 114 Cu^{II}O(OH)₂ | | | | | | | | | | | |
| H | 23.262841000 | 19.257919000 | 2.699836000 | H | 27.739435000 | 12.978606000 | 11.213777000 | H | 27.993586000 | 20.726992000 | 9.757357000 |
| H | 21.912089000 | 15.737195000 | 4.809114000 | H | 25.116773000 | 17.539791000 | 11.269466000 | O | 29.227494000 | 18.393394000 | 12.304245000 |
| H | 24.005402000 | 15.758890000 | 6.161498000 | H | 25.345071000 | 19.264427000 | 4.064968000 | O | 27.950568000 | 20.643969000 | 9.622897000 |
| H | 28.398000000 | 18.233915000 | 12.624110000 | H | 29.395079000 | 12.187263000 | 4.139819000 | O | 26.947522000 | 18.338086000 | 10.998873000 |
| H | 36.517560000 | 15.238562000 | 2.664433000 | H | 34.492546000 | 15.207427000 | 4.105788000 | O | 26.093140000 | 16.688800000 | 9.727746000 |
| H | 38.025488000 | 18.622575000 | 4.888325000 | H | 30.441263000 | 22.217891000 | 4.083186000 | O | 29.341205000 | 14.168762000 | 10.967351000 |
| H | 35.981716000 | 18.583344000 | 6.313007000 | Zr | 29.058167000 | 18.706776000 | 6.4707637000 | O | 31.553462000 | 16.542820000 | 8.358801000 |
| H | 29.743980000 | 17.5354045000 | 12.384910000 | Zr | 29.010320000 | 18.900985000 | 10.049430000 | O | 30.386961000 | 20.575173000 | 10.790522000 |
| H | 27.937842000 | 20.792449000 | 7.987429000 | Zr | 30.762385000 | 15.783096000 | 10.171543000 | O | 32.326924000 | 20.319211000 | 9.673599000 |
| H | 30.222100000 | 15.450347000 | 12.736281000 | Zr | 30.893299000 | 15.630025000 | 6.565985000 | O | 28.971638000 | 16.779273000 | 9.784138000 |
| H | 28.266560000 | 21.431791000 | 10.049495000 | Zr | 27.747942000 | 16.015234000 | 8.328336000 | O | 30.379883000 | 20.558949000 | 5.920736000 |
| H | 28.660962000 | 21.403124000 | 6.723556000 | Zr | 32.103149000 | 18.519702000 | 8.321122000 | O | 32.364053000 | 20.228276000 | 6.915214000 |
| H | 31.574681000 | 18.261793000 | 11.200791000 | H | 28.332138000 | 18.547996000 | 3.973936000 | O | 31.157855000 | 17.933237000 | 6.296955000 |
| H | 26.813789000 | 18.765576000 | 8.269468000 | H | 31.738131000 | 16.147851000 | 4.024324000 | O | 27.680228000 | 18.378569000 | 8.297292000 |
| H | 31.468235000 | 23.992282000 | 2.672073000 | O | 30.932719000 | 15.808461000 | 4.438559000 | O | 30.586040000 | 16.177922000 | 12.224086000 |
| H | 35.141341000 | 23.629879000 | 4.918335000 | O | 29.173840000 | 18.257578000 | 4.349561000 | O | 31.929875000 | 13.876595000 | 9.684603000 |
| H | 34.093648000 | 21.849369000 | 6.318993000 | Cu | 29.207671000 | 16.360444000 | 3.625991000 | O | 31.896575000 | 13.886115000 | 7.100252000 |
| H | 31.976614000 | 13.765945000 | 8.670441000 | O | 29.063870000 | 15.072163000 | 2.281122000 | O | 29.405668000 | 14.078099000 | 5.768537000 |
| H | 28.312585000 | 10.451325000 | 2.720433000 | H | 27.169272000 | 15.738503000 | 4.958949000 | O | 27.470386000 | 14.349828000 | 6.861184000 |
| H | 24.587073000 | 11.097722000 | 4.813894000 | O | 27.243412000 | 15.786120000 | 3.995732000 | H | 38.310653000 | 16.957001000 | 3.034159000 |
| H | 25.669954000 | 12.912690000 | 6.143806000 | Cu | 27.988861000 | 14.057512000 | 3.365104000 | H | 33.844105000 | 24.702405000 | 3.061803000 |
| H | 32.677844000 | 13.682461000 | 6.624347000 | H | 25.898320000 | 14.057512000 | 3.365104000 | H | 25.896332000 | 9.869348000 | 3.063644000 |
| H | 32.849755000 | 14.020965000 | 9.972808000 | H | 21.526611000 | 17.482874000 | 3.050372000 | H | 21.526611000 | 17.482874000 | 3.050372000 |
| H | 31.545447000 | 18.197465000 | 5.408567000 | H | 21.972200000 | 17.399215000 | 16.890909000 | H | 11.091144000 | 11.091144000 | 11.091144000 |
| H | 29.658907000 | 13.812631000 | 8.362230000 | H | 20.799425000 | 12.976937000 | 11.210831000 | H | 27.739245000 | 11.210831000 | 11.210831000 |
| C | 26.061563000 | 17.496077000 | 5.996881000 | H | 23.258957000 | 19.263999000 | 2.707111000 | H | 25.114006000 | 17.542681000 | 11.265635000 |
| C | 24.806500000 | 17.506312000 | 5.189735000 | H | 21.911857000 | 15.737846000 | 4.810215000 | H | 32.001484000 | 21.750988000 | 11.047947000 |
| C | 24.586192000 | 18.494785000 | 4.217549000 | H | 24.008632000 | 15.760275000 | 6.162512000 | H | 25.323355000 | 19.288999000 | 4.081725000 |
| C | 23.418410000 | 18.485758000 | 3.457284000 | H | 28.340218000 | 18.212910000 | 12.643685000 | H | 29.358559000 | 12.293355000 | 4.044037000 |
| C | 22.440174000 | 17.489258000 | 3.647452000 | H | 36.518020000 | 15.237884000 | 2.665604000 | H | 34.489690000 | 15.211422000 | 4.104499000 |
| C | 22.661958000 | 16.513843000 | 4.638698000 | H | 38.025145000 | 16.623100000 | 4.887814000 | H | 30.439478000 | 22.221805000 | 4.085420000 |
| | | | | | | | | | | | |

| | | | | | | | | | | | |
|---|---------------|--------------|--------------|-------------|--------------|----------------|--------------|----|--------------|--------------|--------------|
| H | 21.915664000 | 15.733114000 | 4.804694000 | H | 32.001515000 | 21.747616000 | 11.052779000 | O | 33.724614000 | 17.930487000 | 9.747458000 |
| H | 24.008373000 | 15.756702000 | 6.158755000 | H | 25.340177000 | 19.271479000 | 4.069441000 | O | 31.097027000 | 18.013552000 | 10.396697000 |
| H | 28.337375000 | 18.229261000 | 12.635263000 | H | 29.374155000 | 12.248479000 | 4.069370000 | O | 29.730853000 | 14.798151000 | 8.344210000 |
| H | 36.517850000 | 15.238264000 | 2.664744000 | H | 34.491363000 | 15.209123000 | 4.105136000 | O | 27.989840000 | 20.751789000 | 7.014956000 |
| H | 38.025335000 | 18.622749000 | 4.888184000 | H | 30.440666000 | 22.219227000 | 4.083965000 | O | 29.226529000 | 18.406895000 | 12.286545000 |
| H | 35.982191000 | 18.582817000 | 6.313586000 | Zr | 29.064990000 | 18.729445000 | 6.498077000 | O | 27.949241000 | 20.653935000 | 9.628953000 |
| H | 29.742159000 | 17.531687000 | 12.392748000 | Zr | 29.005170000 | 18.899176000 | 10.060722000 | O | 26.947316000 | 18.338575000 | 10.995300000 |
| H | 27.923942000 | 20.799102000 | 8.004815000 | Zr | 30.756363000 | 15.783252000 | 17.057478000 | O | 26.091423000 | 16.690828000 | 9.724465000 |
| H | 30.223403000 | 15.449032000 | 12.741471000 | Zr | 30.883655000 | 15.636970000 | 6.573865000 | O | 29.349506000 | 14.158427000 | 10.953479000 |
| H | 28.273877000 | 21.434409000 | 10.058152000 | Zr | 27.743537000 | 16.011148000 | 8.317734000 | O | 27.458662000 | 14.314062000 | 9.737607000 |
| H | 28.626779000 | 21.420544000 | 6.733062000 | Zr | 32.105084000 | 8.520629000 | 8.327588000 | O | 31.560962000 | 16.549074000 | 8.352184000 |
| H | 31.571016000 | 18.259703000 | 11.207869000 | H | 28.652427000 | 18.868163000 | 3.835280000 | O | 30.383361000 | 20.581372000 | 10.778316000 |
| H | 26.804652000 | 18.772541000 | 8.285802000 | H | 31.609951000 | 16.322364000 | 4.064711000 | O | 32.331294000 | 20.317452000 | 9.678586000 |
| H | 31.468382000 | 19.295231000 | 2.672087000 | O | 30.834245000 | 15.895834000 | 4.438350000 | O | 28.973482000 | 16.781331000 | 9.777379000 |
| H | 35.141140000 | 23.623412000 | 4.918686000 | O | 29.319718000 | 18.414152000 | 4.361729000 | O | 30.392160000 | 20.538611000 | 5.881446000 |
| H | 34.093648000 | 21.849035000 | 6.318752000 | Cu | 29.128660000 | 16.540016000 | 3.698848000 | O | 32.354876000 | 20.249244000 | 6.935579000 |
| H | 31.975566000 | 13.770147000 | 8.669291000 | O | 28.941572000 | 14.846239000 | 2.764117000 | O | 31.137787000 | 17.933491000 | 6.247169000 |
| H | 28.307799000 | 10.458285000 | 2.710866000 | H | 29.415384000 | 14.230086000 | 3.336160000 | O | 27.674127000 | 18.379156000 | 8.293657000 |
| H | 24.585084000 | 11.100492000 | 4.808405000 | O | 27.361349000 | 16.839311000 | 9.293484000 | O | 30.580345000 | 16.179034000 | 12.213077000 |
| H | 25.667279000 | 12.911122000 | 6.144043000 | Cu | 27.011220000 | 14.882770000 | 2.833292000 | O | 31.933091000 | 13.886858000 | 9.636974000 |
| H | 32.687476000 | 13.701057000 | 6.620145000 | H | 26.739408000 | 17.304029000 | 3.505498000 | O | 31.848223000 | 13.872421000 | 7.032803000 |
| H | 32.847302000 | 14.023042000 | 9.971408000 | C | 25.104562000 | 14.665685000 | 2.722609000 | O | 29.385453000 | 14.123358000 | 5.683771000 |
| H | 31.542595000 | 18.237983000 | 5.442784000 | H | 24.624471000 | 15.602935000 | 2.444306000 | O | 27.496747000 | 14.298488000 | 6.894009000 |
| C | 26.061556000 | 17.496070000 | 5.996871000 | H | 24.898593000 | 13.907489000 | 1.963297000 | H | 38.310658000 | 16.957131000 | 3.043077000 |
| C | 24.806508000 | 17.506299000 | 5.189723000 | H | 24.714867000 | 14.327108000 | 3.682950000 | H | 33.844048000 | 24.702937000 | 3.062317000 |
| C | 24.586184000 | 18.494779000 | 4.217563000 | | | | | H | 25.900652000 | 9.867041000 | 3.0464632000 |
| C | 23.418408000 | 18.485761000 | 3.457287000 | | | | | H | 21.527779000 | 17.479956000 | 3.048282000 |
| C | 22.440175000 | 17.489255000 | 3.647449000 | | | | | H | 34.794732000 | 16.897228000 | 11.099699000 |
| | | | | 119 | | | | H | 27.735765000 | 12.985743000 | 11.221119000 |
| | | | | TsB4 | | | | H | 25.116275000 | 17.537902000 | 11.269331000 |
| C | 22.661959000 | 16.513842000 | 4.638697000 | H | 23.262830000 | 19.258276000 | 2.700176000 | H | 32.002163000 | 21.746363000 | 11.054864000 |
| C | 23.829438000 | 16.519362000 | 5.398321000 | H | 21.911581000 | 15.737916000 | 4.810033000 | H | 25.353332000 | 19.256567000 | 4.063969000 |
| C | 33.868245000 | 16.904208000 | 6.130639000 | H | 24.002637000 | 15.762400000 | 6.165972000 | H | 29.405420000 | 12.134397000 | 4.186899000 |
| C | 35.110970000 | 16.894616000 | 5.299643000 | H | 28.334601000 | 18.227629000 | 12.614659000 | H | 34.486328000 | 15.215099000 | 4.104244000 |
| C | 35.273567000 | 15.953397000 | 4.269684000 | H | 36.517959000 | 15.238863000 | 2.663691000 | H | 30.438765000 | 22.222180000 | 4.086790000 |
| C | 36.411230000 | 15.974750000 | 3.465071000 | H | 38.025641000 | 18.622581000 | 4.888172000 | H | 29.037510000 | 18.774719000 | 6.469731000 |
| C | 37.420942000 | 16.937187000 | 3.666011000 | H | 35.981606000 | 18.582888000 | 6.313439000 | Zr | 29.008993000 | 18.904040000 | 10.047121000 |
| C | 37.253510000 | 17.869771000 | 4.709694000 | H | 29.741096000 | 17.533051000 | 12.380631000 | Zr | 30.756858000 | 15.784951000 | 10.161202000 |
| C | 36.115037000 | 17.853052000 | 5.512748000 | H | 27.925020000 | 20.827725000 | 8.026566000 | Zr | 30.869167000 | 15.669747000 | 6.545652000 |
| C | 33.837139000 | 16.958910000 | 10.535586000 | H | 30.220988000 | 15.445610000 | 12.724984000 | Zr | 30.757430000 | 16.027208000 | 8.307577000 |
| C | 26.050620000 | 17.525803000 | 10.664603000 | H | 28.281874000 | 21.436160000 | 10.083867000 | Zr | 32.099570000 | 18.522946000 | 8.318151000 |
| C | 28.183405000 | 18.321217000 | 10.638011000 | H | 28.569493000 | 21.470406000 | 6.728878000 | H | 29.939498000 | 18.958980000 | 3.998849000 |
| C | 31.573520000 | 20.879169000 | 5.104555000 | H | 31.570655000 | 18.261851000 | 11.199357000 | H | 30.824238000 | 15.279153000 | 3.843429000 |
| C | 31.605413000 | 20.823709000 | 6.099625000 | H | 26.794371000 | 18.775122000 | 8.295877000 | O | 30.753307000 | 16.055105000 | 4.418988000 |
| C | 32.468277000 | 22.541420000 | 4.263217000 | H | 35.141114000 | 22.632708000 | 4.918667000 | O | 29.117456000 | 18.649770000 | 4.390916000 |
| C | 32.051052000 | 23.530721000 | 3.473056000 | H | 34.093105000 | 21.848304000 | 6.318715000 | Cu | 28.837478000 | 16.484981000 | 4.008739000 |
| C | 33.385414000 | 23.937234000 | 3.684991000 | H | 31.958213000 | 13.788562000 | 8.620309000 | O | 29.443730000 | 14.607123000 | 2.364993000 |
| C | 34.107731000 | 23.321900000 | 4.729966000 | H | 28.317433000 | 10.442308000 | 2.728292000 | H | 29.552022000 | 14.267163000 | 1.467842000 |
| C | 33.528822000 | 22.330882000 | 5.518652000 | H | 24.587907000 | 11.095753000 | 4.816449000 | O | 27.114203000 | 15.689277000 | 3.557907000 |
| C | 28.200796000 | 13.799505000 | 5.970296000 | H | 25.670464000 | 12.910538000 | 6.146786000 | Cu | 27.934238000 | 13.918561000 | 3.449322000 |
| C | 27.574827000 | 12.706326000 | 5.169775000 | H | 32.720922000 | 13.804636000 | 6.628140000 | H | 26.403292000 | 15.847229000 | 4.183982000 |
| C | 28.317316000 | 12.007734000 | 4.205540000 | H | 32.848148000 | 14.035793000 | 9.911447000 | C | 29.175798000 | 16.612782000 | 1.808935000 |
| C | 27.719387000 | 10.995846000 | 3.458196000 | H | 31.599873000 | 18.084367000 | 5.414621000 | H | 28.748193000 | 17.504601000 | 2.271672000 |
| C | 26.365101000 | 16.659934000 | 3.653216000 | H | 29.636529000 | 13.838549000 | 8.318382000 | H | 30.230584000 | 16.673765000 | 1.591935000 |
| C | 25.634739000 | 11.351847000 | 4.637577000 | C | 26.061546000 | 17.496086000 | 5.996840000 | H | 28.541934000 | 16.218800000 | 1.031725000 |
| C | 26.230656000 | 12.363455000 | 5.386132000 | C | 24.806505000 | 17.506321000 | 5.189728000 | | | | |
| O | 26.959438000 | 18.338692000 | 5.696256000 | C | 24.586178000 | 18.494807000 | 4.217574000 | | | | |
| O | 26.145429000 | 16.639361000 | 9.620598000 | C | 23.418408000 | 18.485760000 | 3.457287000 | | | | |
| O | 30.103637000 | 19.074307000 | 8.300295000 | C | 22.440177000 | 17.489252000 | 3.647445000 | | | | |
| O | 33.021637000 | 15.996237000 | 5.910033000 | C | 22.661600000 | 16.515841000 | 4.638696000 | | | | |
| O | 33.748143000 | 17.826071000 | 6.988499000 | C | 23.829434000 | 16.519368000 | 5.398327000 | | | | |
| O | 29.010160000 | 16.698573000 | 6.822597000 | C | 23.886217000 | 16.904252000 | 6.130584000 | | | | |
| O | 32.998734000 | 16.053505000 | 10.756162000 | C | 35.110964000 | 16.894627000 | 5.299634000 | | | | |
| O | 33.7231229000 | 9.749377000 | 4.794377000 | C | 35.273567000 | 15.953397000 | 4.269684000 | | | | |
| O | 31.096439000 | 18.012676000 | 10.405209000 | C | 36.411228000 | 15.974530000 | 3.465068000 | | | | |
| O | 29.738229000 | 14.780253000 | 8.366693000 | C | 37.420942000 | 16.937187000 | 3.666011000 | | | | |
| O | 28.008693000 | 20.723518000 | 6.993583000 | C | 37.253513000 | 17.869767000 | 4.709699000 | | | | |
| O | 29.225821000 | 12.405151000 | 5.302936000 | C | 36.115043000 | 17.853044000 | 5.512757000 | | | | |
| O | 27.949956000 | 20.644337000 | 9.610403000 | C | 33.837127000 | 16.958906000 | 10.535555000 | | | | |
| O | 26.947425000 | 20.339773000 | 10.994538000 | C | 26.050618000 | 17.523810000</ | | | | | |

| | | | | | | | | | | | |
|----|--------------|--------------|--------------|---|--------------|--------------|--------------|-------------|--------------|--------------|--------------|
| C | 35.273550000 | 15.953417000 | 4.269661000 | H | 36.518034000 | 15.238013000 | 2.665005000 | H | 34.491080000 | 15.209610000 | 4.104905000 |
| C | 36.411225000 | 15.974759000 | 3.465064000 | H | 38.025263000 | 18.622829000 | 4.888106000 | H | 30.440033000 | 22.220701000 | 4.084761000 |
| C | 37.420938000 | 16.937192000 | 3.666005000 | H | 35.982593000 | 18.582512000 | 6.313955000 | Zr | 29.067485000 | 18.740850000 | 6.513081000 |
| C | 37.253512000 | 17.869770000 | 4.709696000 | H | 29.746952000 | 17.522339000 | 12.393801000 | Zr | 29.005032000 | 18.896032000 | 10.068888000 |
| C | 36.115079000 | 17.852994000 | 5.512807000 | H | 27.918849000 | 20.802393000 | 8.019516000 | Zr | 30.757769000 | 15.779588000 | 10.169870000 |
| C | 33.837220000 | 16.958862000 | 10.535584000 | H | 30.230073000 | 15.442094000 | 12.737081000 | Zr | 30.877048000 | 15.640012000 | 6.561213000 |
| C | 26.050659000 | 17.523698000 | 10.664616000 | H | 28.274096000 | 21.431779000 | 10.071189000 | Zr | 27.742754000 | 16.010571000 | 8.315770000 |
| C | 28.183460000 | 13.821152000 | 10.638023000 | H | 28.619692000 | 21.430254000 | 6.749900000 | Zr | 32.106607000 | 18.517950000 | 8.328750000 |
| C | 31.573568000 | 20.879219000 | 10.504540000 | H | 31.573259000 | 18.255135000 | 11.207259000 | H | 28.820320000 | 19.010150000 | 3.803646000 |
| C | 31.605408000 | 20.823747000 | 6.099713000 | H | 26.802991000 | 18.773951000 | 8.292395000 | H | 31.541779000 | 16.366205000 | 4.047512000 |
| C | 32.203580000 | 19.219654600 | 5.289569000 | H | 31.468383000 | 23.992835000 | 6.276260000 | O | 30.777976000 | 15.912889000 | 4.415850000 |
| C | 31.468297000 | 22.541372000 | 4.263171000 | H | 35.141015000 | 23.623647000 | 4.9187474000 | O | 29.384753000 | 18.473765000 | 4.371629000 |
| C | 32.051062000 | 23.530704000 | 3.473042000 | H | 34.093674000 | 21.848907000 | 6.318642000 | Cu | 29.076855000 | 16.622755000 | 3.734148000 |
| C | 33.385409000 | 23.932745000 | 3.685001000 | H | 31.976014000 | 13.773013000 | 8.656673000 | O | 28.601532000 | 14.958370000 | 2.861866000 |
| C | 34.107721000 | 23.321925000 | 4.729991000 | H | 28.307152000 | 10.459790000 | 2.709194000 | H | 28.996033000 | 14.224229000 | 3.349180000 |
| C | 33.528818000 | 22.330886000 | 5.518653000 | H | 24.583499000 | 11.106115200 | 4.804084000 | O | 27.335511000 | 17.081564000 | 2.977192000 |
| C | 28.200367000 | 13.800062000 | 5.970259000 | H | 25.664076000 | 12.913161000 | 6.139868000 | H | 26.838456000 | 17.683064000 | 3.545446000 |
| C | 27.574958000 | 12.706456000 | 5.170289000 | H | 32.688910000 | 13.709138000 | 6.607530000 | Cu | 26.699974000 | 15.237999000 | 3.057552000 |
| C | 28.317520000 | 12.007419000 | 4.205514000 | H | 32.847649000 | 14.018015000 | 9.960537000 | O | 25.182212000 | 14.404780000 | 3.195581000 |
| C | 27.719166000 | 10.996016000 | 3.458134000 | H | 31.534479000 | 18.251004000 | 5.448917000 | | | | |
| C | 26.365062000 | 10.659976000 | 3.653133000 | H | 29.643471000 | 13.823619000 | 8.332406000 | | | | |
| C | 25.634706000 | 11.351921000 | 4.637531000 | C | 26.061597000 | 17.496055000 | 5.996863000 | 121 | | | |
| C | 26.230716000 | 12.363230000 | 5.386000000 | C | 24.806514000 | 17.506303000 | 5.189713000 | TSB5 | | | |
| O | 26.937291000 | 18.363866000 | 5.730446000 | C | 24.586187000 | 18.494793000 | 4.217558000 | H | 23.261639000 | 19.260838000 | 2.703070000 |
| O | 26.153549000 | 16.616480000 | 6.901719000 | C | 23.418409000 | 18.485760000 | 3.457286000 | H | 21.918918000 | 15.729703000 | 4.803079000 |
| O | 30.100700000 | 19.085588000 | 8.289625000 | C | 22.440175000 | 17.489256000 | 3.647450000 | H | 24.011863000 | 15.748716000 | 6.148752000 |
| O | 33.029780000 | 15.992501000 | 5.916552000 | C | 22.661958000 | 16.513843000 | 4.638698000 | H | 28.341319000 | 18.220512000 | 12.640127000 |
| O | 33.741171000 | 17.841110000 | 6.973103000 | C | 23.894350000 | 16.519366000 | 5.398327000 | H | 36.518034000 | 15.238021000 | 2.664984000 |
| O | 29.003127000 | 16.718692000 | 6.818568000 | C | 33.868194000 | 16.904267000 | 6.130662000 | H | 38.025296000 | 18.622806000 | 4.888118000 |
| O | 33.004073000 | 16.044766000 | 10.739908000 | C | 35.110961000 | 16.894613000 | 5.299629000 | H | 35.982415000 | 18.582556000 | 6.313881000 |
| O | 33.725653000 | 17.931610000 | 9.747842000 | C | 35.273563000 | 15.953402000 | 4.269678000 | H | 29.746215000 | 17.523373000 | 12.392988000 |
| O | 31.099563000 | 18.008423000 | 10.389528000 | C | 36.411229000 | 15.974751000 | 3.465070000 | H | 27.919791000 | 20.801012000 | 8.016446000 |
| O | 29.781289000 | 14.788370000 | 8.341869000 | C | 37.420943000 | 16.937186000 | 3.666012000 | H | 30.227862000 | 15.442727000 | 12.736503000 |
| O | 28.000789000 | 20.742299000 | 7.017757000 | C | 37.255311000 | 17.869769000 | 4.709696000 | H | 28.275886000 | 21.431745000 | 10.068361000 |
| O | 29.234912000 | 18.391166000 | 12.287835000 | C | 36.115041000 | 17.853046000 | 5.512754000 | H | 28.622994000 | 21.427093000 | 6.747602000 |
| O | 27.951404000 | 20.650419000 | 9.632213000 | C | 33.837141000 | 16.958907000 | 10.535584000 | H | 31.572870000 | 18.255640000 | 11.206847000 |
| O | 26.949366000 | 18.335444000 | 10.998816000 | C | 26.050620000 | 20.523797000 | 10.664602000 | H | 26.803359000 | 18.772790000 | 8.290689000 |
| O | 26.090647000 | 16.692801000 | 9.723143000 | C | 28.183404000 | 13.821192000 | 10.638016000 | H | 31.468381000 | 23.992824000 | 2.672237000 |
| O | 29.352356000 | 14.153393000 | 10.946705000 | C | 31.573527000 | 20.879172000 | 10.504557000 | H | 35.141042000 | 23.623629000 | 4.918832000 |
| O | 27.454622000 | 14.316651000 | 9.742456000 | C | 31.605436000 | 20.823687000 | 6.099611000 | H | 34.093607000 | 21.848855000 | 6.318660000 |
| O | 31.562927000 | 16.544437000 | 8.335957000 | C | 32.203608000 | 21.926571000 | 5.289625000 | H | 31.975911000 | 13.772021000 | 8.658563000 |
| O | 30.385442000 | 20.576471000 | 10.784314000 | C | 31.468280000 | 22.541415000 | 4.263212000 | H | 28.307626000 | 10.459306000 | 2.709855000 |
| O | 32.330121000 | 20.316252000 | 9.678666000 | C | 32.051053000 | 23.530720000 | 3.473055000 | H | 24.583420000 | 11.106495000 | 4.804697000 |
| O | 28.973608000 | 16.778963000 | 9.781857000 | C | 33.385414000 | 23.932735000 | 3.684992000 | H | 25.662549000 | 12.917144000 | 6.135294000 |
| O | 30.398596000 | 20.525049000 | 5.867981000 | C | 34.107730000 | 23.321902000 | 6.332190000 | H | 32.688101000 | 23.992842000 | 12.736503000 |
| O | 32.352344000 | 20.247091000 | 6.935878000 | C | 33.528819000 | 22.330887000 | 5.518658000 | H | 32.848269000 | 14.019852000 | 9.961304000 |
| O | 31.138769000 | 17.935830000 | 6.231739000 | C | 28.200767000 | 13.799517000 | 5.970316000 | H | 31.534013000 | 18.247253000 | 5.446105000 |
| O | 27.675884000 | 18.381568000 | 8.297001000 | C | 27.574833000 | 12.706325000 | 5.169772000 | H | 29.643466000 | 13.822667000 | 8.333998000 |
| O | 30.589982000 | 16.170016000 | 12.199876000 | C | 28.317315000 | 12.007738000 | 4.205536000 | C | 26.061597000 | 17.496055000 | 5.996863000 |
| O | 31.936387000 | 13.881306000 | 9.628630000 | C | 27.719336000 | 10.995847000 | 3.458195000 | C | 24.806514000 | 17.506303000 | 5.189713000 |
| O | 31.837615000 | 13.864298000 | 7.039641000 | C | 26.365101000 | 16.659934000 | 6.353216000 | C | 24.586187000 | 18.494793000 | 4.217558000 |
| O | 29.372641000 | 14.138816000 | 5.660490000 | C | 25.634739000 | 11.351846000 | 4.637578000 | C | 23.418409000 | 18.485760000 | 3.457286000 |
| O | 27.503633000 | 14.288716000 | 6.904437000 | C | 26.230635000 | 12.363451000 | 5.386136000 | C | 22.440175000 | 17.489256000 | 3.647450000 |
| H | 38.310670000 | 16.956695000 | 3.034214000 | O | 26.964536000 | 18.336103000 | 5.692508000 | C | 22.661598000 | 16.513843000 | 4.638698000 |
| H | 33.843898000 | 24.703030000 | 3.062394000 | O | 26.145885000 | 16.642709000 | 6.922301000 | C | 23.829435000 | 16.519366000 | 5.398327000 |
| H | 25.900467000 | 9.867053000 | 3.064644000 | O | 30.103092000 | 19.079070000 | 8.306514000 | C | 33.868194000 | 16.904267000 | 6.130662000 |
| H | 21.527747000 | 17.480447000 | 3.048387000 | O | 33.009512000 | 16.010810000 | 5.890276000 | C | 35.110616000 | 16.894613000 | 5.299629000 |
| H | 34.791600000 | 16.901070000 | 11.105480000 | O | 33.754490000 | 17.814723000 | 7.000663000 | C | 35.273563000 | 15.953402000 | 4.269678000 |
| H | 27.735648000 | 12.987491000 | 11.223782000 | O | 29.007430000 | 16.706389000 | 6.812560000 | C | 36.411229000 | 15.974751000 | 3.465070000 |
| H | 25.115540000 | 17.539836000 | 11.268009000 | O | 33.000641000 | 16.050137000 | 10.749124000 | C | 37.420943000 | 16.937186000 | 3.666012000 |
| H | 31.999694000 | 21.751211000 | 11.049166000 | O | 33.722607000 | 17.934891000 | 9.752650000 | C | 37.253511000 | 17.869769000 | 4.709696000 |
| H | 25.350753000 | 19.260121000 | 4.065343000 | O | 31.097749000 | 18.009581000 | 10.404660000 | C | 36.115041000 | 17.853046000 | 5.512754000 |
| H | 29.406659000 | 12.110729000 | 4.210216000 | O | 29.737328000 | 14.783583000 | 8.358447000 | C | 33.871410000 | 16.958907000 | 10.535584000 |
| H | 34.490846000 | 15.208659000 | 4.106988000 | O | 28.003940000 | 20.730040000 | 7.007449000 | C | 26.050620000 | 17.523797000 | 10.664602000 |
| H | 30.438186000 | 22.223823000 | 4.087157000 | O | 29.229562000 | 18.396212000 | 12.300426000 | C | 28.183404000 | 13.821192000 | 10.638016000 |
| Zr | 29.046283000 | 18.757699000 | 6.485852000 | O | 27.950300000 | 20.642698000 | 9.62156100 | | | | |

| | | | | | | | | | | | |
|------------|--------------|--------------|--------------|---|--------------|--------------|--------------|---|--------------|--------------|--------------|
| O | 26.949217000 | 18.336742000 | 10.998379000 | C | 36.115041000 | 17.853046000 | 5.512754000 | H | 35.982124000 | 18.582615000 | 6.313781000 |
| O | 26.094105000 | 16.689814000 | 9.726654000 | C | 33.837141000 | 16.958907000 | 10.535584000 | H | 29.749757000 | 17.517066000 | 12.391248000 |
| O | 29.345993000 | 14.162781000 | 10.960173000 | C | 26.050620000 | 17.523797000 | 10.664602000 | H | 27.915879000 | 20.803902000 | 8.024619000 |
| O | 27.456654000 | 14.317711000 | 9.742074000 | C | 28.183404000 | 13.821192000 | 10.638016000 | H | 30.231973000 | 15.435928000 | 12.729352000 |
| O | 31.562694000 | 16.542592000 | 8.355887000 | C | 31.573527000 | 20.879172000 | 10.504557000 | H | 28.278802000 | 21.430862000 | 10.077786000 |
| O | 30.385721000 | 20.576375000 | 10.784702000 | C | 31.605436000 | 20.823687000 | 6.099611000 | H | 28.614566000 | 21.430583000 | 6.753875000 |
| O | 32.328929000 | 20.317991000 | 9.675690000 | C | 32.203608000 | 21.926571000 | 5.289625000 | H | 31.574858000 | 18.251998000 | 11.207931000 |
| O | 28.974954000 | 16.777622000 | 9.781733000 | C | 31.468280000 | 22.541415000 | 4.263212000 | H | 26.801904000 | 18.777529000 | 8.302997000 |
| O | 30.385554000 | 20.541642000 | 5.903275000 | C | 32.051053000 | 23.530720000 | 3.473055000 | H | 31.468610000 | 23.991992000 | 2.671577000 |
| O | 32.359674000 | 20.237868000 | 6.926424000 | C | 33.385414000 | 23.932735000 | 3.684992000 | H | 35.141068000 | 23.623698000 | 4.918837000 |
| O | 31.149754000 | 17.935585000 | 6.273297000 | C | 34.107730000 | 23.321902000 | 4.729968000 | H | 34.093727000 | 21.848265000 | 6.318205000 |
| O | 27.682138000 | 18.374587000 | 8.294410000 | C | 33.528819000 | 22.330887000 | 5.518658000 | H | 31.974686000 | 13.779999000 | 8.641188000 |
| O | 30.583454000 | 16.175672000 | 12.221397000 | C | 28.200767000 | 13.799517000 | 5.970316000 | H | 28.306964000 | 10.458913000 | 2.709642000 |
| O | 31.936232000 | 13.878317000 | 9.673322000 | C | 27.574833000 | 12.706325000 | 5.169772000 | H | 24.586642000 | 11.094852000 | 4.812801000 |
| O | 31.860286000 | 13.862404000 | 7.077053000 | C | 28.317315000 | 12.007738000 | 4.205536000 | H | 25.670923000 | 12.905933000 | 6.150521000 |
| O | 29.372237000 | 14.155980000 | 5.674991000 | C | 27.719336000 | 10.995847000 | 3.458195000 | H | 32.687679000 | 13.725616000 | 6.598818000 |
| O | 27.503637000 | 14.299709000 | 6.906896000 | C | 26.365101000 | 10.659934000 | 3.653216000 | H | 32.849065000 | 14.021841000 | 9.944645000 |
| H | 38.310256000 | 16.956955000 | 3.034057000 | C | 25.634739000 | 11.351846000 | 4.637578000 | H | 31.517242000 | 18.249099000 | 5.442939000 |
| H | 33.844131000 | 24.702458000 | 3.061897000 | C | 26.230658000 | 12.363451000 | 5.386136000 | H | 29.643744000 | 13.825647000 | 8.331144000 |
| H | 25.896643000 | 9.871897000 | 3.060633000 | O | 26.967821000 | 18.331030000 | 5.688303000 | C | 26.061597000 | 17.496055000 | 5.996863000 |
| H | 21.529122000 | 17.479745000 | 3.045853000 | O | 26.144564000 | 16.645663000 | 6.925730000 | C | 24.806514000 | 17.506303000 | 5.189713000 |
| H | 34.797982000 | 16.893885000 | 11.093370000 | O | 30.103817000 | 19.078803000 | 3.8083823000 | C | 24.586187000 | 18.494793000 | 4.217558000 |
| H | 27.739115000 | 12.978359000 | 11.212438000 | O | 33.008221000 | 16.012191000 | 5.888597000 | C | 23.418409000 | 18.485760000 | 3.457286000 |
| H | 25.114152000 | 17.542690000 | 11.265193000 | O | 33.755484000 | 17.813222000 | 7.002071000 | C | 22.440175000 | 17.489256000 | 3.647450000 |
| H | 32.001352000 | 21.749347000 | 11.050202000 | O | 29.04031000 | 16.707124000 | 6.816394000 | C | 22.661958000 | 16.513843000 | 4.638698000 |
| H | 25.335689000 | 19.276616000 | 4.071436000 | O | 33.001472000 | 16.048829000 | 10.747280000 | C | 23.829435000 | 16.519366000 | 5.398327000 |
| H | 29.374052000 | 12.251666000 | 4.067116000 | O | 33.722494000 | 17.935389000 | 9.753406000 | C | 33.868194000 | 16.904267000 | 6.130662000 |
| H | 34.491176000 | 15.209424000 | 4.105065000 | O | 31.098451000 | 18.008365000 | 4.209055000 | C | 35.110961000 | 16.894613000 | 5.299629000 |
| H | 30.440128000 | 22.220407000 | 4.084750000 | O | 29.737432000 | 14.783329000 | 8.356713000 | C | 35.273563000 | 15.953402000 | 4.269678000 |
| Zr | 29.07803000 | 18.738059000 | 6.509721000 | O | 27.999804000 | 20.729785000 | 7.010077000 | C | 36.411229000 | 15.974751000 | 3.465070000 |
| Zr | 29.005002000 | 18.895896000 | 10.066890000 | O | 29.230364000 | 18.393583000 | 12.301474000 | C | 37.420943000 | 16.937186000 | 3.666012000 |
| Zr | 30.757324000 | 15.779796000 | 10.170031000 | O | 27.951428000 | 20.642920000 | 9.624858000 | C | 37.253511000 | 17.869769000 | 4.709696000 |
| Zr | 30.879743000 | 15.638574000 | 6.562317000 | O | 26.949893000 | 18.335130000 | 10.999943000 | C | 36.115041000 | 17.853046000 | 5.512754000 |
| Zr | 27.742461000 | 16.009889000 | 8.315109000 | O | 26.094034000 | 16.689841000 | 9.726508000 | C | 33.837141000 | 16.958907000 | 10.535584000 |
| Zr | 32.106168000 | 18.517825000 | 8.328160000 | O | 29.347524000 | 14.160456000 | 10.957014000 | C | 26.050620000 | 17.523797000 | 10.664602000 |
| H | 28.068000000 | 18.991263000 | 3.804804000 | O | 27.456039000 | 14.317981000 | 9.742666000 | C | 28.183404000 | 13.821192000 | 10.638016000 |
| H | 31.570313000 | 16.347031000 | 4.051699000 | O | 31.561941000 | 16.543011000 | 8.354224000 | C | 31.573527000 | 20.879172000 | 10.504557000 |
| O | 29.78382000 | 15.904937000 | 4.416399000 | O | 30.386931000 | 20.574564000 | 10.787895000 | C | 31.605436000 | 20.823687000 | 6.099611000 |
| O | 29.385041000 | 18.466701000 | 4.370205000 | O | 32.327982000 | 20.318637000 | 9.674404000 | C | 32.203608000 | 21.926571000 | 5.289625000 |
| Cu | 29.103444000 | 16.611276000 | 3.719241000 | O | 28.975112000 | 16.776934000 | 9.782895000 | C | 31.468280000 | 22.541415000 | 4.263212000 |
| O | 28.665105000 | 14.942120000 | 2.828722000 | O | 30.383317000 | 20.547859000 | 5.911984000 | C | 32.051053000 | 23.530720000 | 3.473050000 |
| H | 29.076198000 | 14.234882000 | 3.342263000 | O | 32.361998000 | 20.233983000 | 6.922425000 | C | 33.385414000 | 23.932735000 | 3.684992000 |
| O | 27.346860000 | 17.053951000 | 2.992924000 | O | 31.148421000 | 17.938501000 | 6.275152000 | C | 34.107730000 | 23.321902000 | 4.729968000 |
| H | 26.859734000 | 17.628866000 | 3.596917000 | O | 27.680936000 | 18.476268000 | 8.297522000 | C | 33.528819000 | 22.330887000 | 5.518658000 |
| Cu | 26.772953000 | 15.184434000 | 3.089213000 | O | 30.585839000 | 16.172733000 | 12.219887000 | C | 28.200767000 | 13.799517000 | 5.970316000 |
| O | 25.144678000 | 14.524907000 | 3.360620000 | O | 31.937463000 | 13.878487000 | 9.664968000 | C | 27.574833000 | 12.706325000 | 5.169772000 |
| C | 23.820505000 | 14.777560000 | 1.252222000 | O | 31.853231000 | 13.863326000 | 7.066771000 | C | 28.317315000 | 12.007738000 | 4.205636000 |
| H | 22.790306000 | 14.590188000 | 1.533204000 | O | 29.363699000 | 14.165186000 | 5.661643000 | C | 27.719336000 | 10.995847000 | 3.458195000 |
| H | 24.230127000 | 14.049700000 | 0.562435000 | O | 27.505993000 | 14.289383000 | 6.913727000 | C | 26.365101000 | 10.659934000 | 3.653216000 |
| H | 24.478189000 | 14.600896000 | 2.401443000 | H | 38.310486000 | 16.957014000 | 3.034016000 | C | 25.634739000 | 11.351846000 | 4.637580000 |
| H | 24.019850000 | 15.807604000 | 0.978648000 | H | 33.844161000 | 24.702376000 | 3.061824000 | C | 26.230658000 | 12.363451000 | 5.386136000 |
| | | | | H | 25.896232000 | 9.872359000 | 3.060520000 | O | 26.956483000 | 18.341912000 | 5.698904000 |
| | | | | H | 21.531282000 | 17.477312000 | 3.043892000 | O | 26.139718000 | 16.639776000 | 6.919848000 |
| 121 | | | | H | 34.797103000 | 16.889440000 | 11.094849000 | O | 30.104031000 | 19.081537000 | 8.310471000 |
| B5 | | | | H | 27.738430000 | 12.980180000 | 11.214606000 | O | 33.005742000 | 16.016559000 | 5.882944000 |
| H | 23.260748000 | 19.260824000 | 2.703123000 | H | 25.113353000 | 17.543802000 | 11.263881000 | O | 33.759027000 | 17.809330000 | 7.006313000 |
| H | 21.916037000 | 15.733066000 | 4.803777000 | H | 32.001128000 | 21.750448000 | 11.048527000 | O | 29.000343000 | 16.710403000 | 6.818151000 |
| H | 24.006943000 | 15.758053000 | 6.159957000 | H | 25.335534000 | 19.277371000 | 4.072908000 | O | 33.002779000 | 16.046816000 | 10.744491000 |
| H | 28.432800000 | 18.216943000 | 12.643512000 | H | 29.372826000 | 12.258386000 | 4.066253000 | O | 33.722615000 | 17.936706000 | 9.755491000 |
| H | 36.518033000 | 15.238066000 | 2.664952000 | H | 34.491091000 | 15.209611000 | 4.104861000 | O | 31.099729000 | 18.008312000 | 10.404625000 |
| H | 38.025190000 | 18.622921000 | 4.888018000 | H | 30.440338000 | 22.219962000 | 4.084234000 | O | 29.734175000 | 14.785804000 | 8.354935000 |
| H | 35.982513000 | 18.582581000 | 6.313875000 | H | 29.066945000 | 18.473804000 | 6.515080000 | O | 27.996215000 | 20.732872000 | 7.012883000 |
| H | 29.747875000 | 17.519754000 | 12.393953000 | H | 29.005888000 | 18.895763000 | 10.072949000 | O | 29.231573000 | 18.390910000 | 12.301307000 |
| H | 27.917742000 | 20.803560000 | 8.022141000 | H | 30.758765000 | 15.779023000 | 10.168095000 | O | 27.949176000 | 20.642857000 | 9.630588000 |
| H | 30.232313000 | 15.439052000 | 12.735625000 | H | 30.874125000 | 15.643392000 | 4.595044000 | O | 26.949915000 | 18.333471000 | 11.001512000 |
| H | 28.276233000 | 21.431764000 | 10.074164000 | H | 27.743069000 | 16.011728000 | 8.316863000 | | | | |

| | | | | | | | | | | | |
|------------|---------------|--------------|--------------|-------|--------------|---------------|--------------|----|--------------|--------------|--------------|
| Zr | 29.067649000 | 18.748326000 | 6.511263000 | O | 27.999086000 | 20.728764000 | 7.000799000 | C | 36.411218000 | 15.974769000 | 3.465052000 |
| Zr | 29.008408000 | 18.896045000 | 10.068763000 | O | 29.229279000 | 18.396492000 | 12.296861000 | C | 37.420946000 | 16.937185000 | 3.666016000 |
| Zr | 30.761103000 | 15.779507000 | 10.163240000 | O | 27.948414000 | 20.643304000 | 9.620235000 | C | 37.253525000 | 17.869750000 | 4.709718000 |
| Zr | 30.869521000 | 15.648765000 | 6.548321000 | O | 26.948431000 | 18.336316000 | 10.997920000 | C | 36.114989000 | 17.853115000 | 5.512672000 |
| Zr | 27.746858000 | 16.014903000 | 8.317295000 | O | 26.090001000 | 16.691444000 | 9.724158000 | C | 33.836793000 | 16.959027000 | 10.535668000 |
| Zr | 32.107180000 | 18.518530000 | 8.325460000 | O | 29.346184000 | 14.161390000 | 10.958892000 | C | 26.050708000 | 17.523765000 | 10.664703000 |
| H | 28.836080000 | 19.014954000 | 3.800803000 | O | 27.455010000 | 14.316687000 | 9.742373000 | C | 28.183361000 | 13.821281000 | 10.638044000 |
| H | 31.519923000 | 16.343695000 | 4.035290000 | O | 31.562758000 | 16.544770000 | 8.355096000 | C | 31.573361000 | 20.879072000 | 10.054654000 |
| O | 30.747684000 | 15.919956000 | 4.420861000 | O | 30.385293000 | 20.577260000 | 10.784567000 | C | 31.605373000 | 20.824073000 | 6.099579000 |
| O | 29.414886000 | 18.527835000 | 4.400910000 | O | 32.328913000 | 20.319760000 | 9.675056000 | C | 32.203646000 | 21.926567000 | 5.289647000 |
| Cu | 29.063560000 | 16.690481000 | 3.692578000 | O | 28.973458000 | 16.776904000 | 9.787333000 | C | 31.468256000 | 22.541451000 | 4.263248000 |
| O | 28.524110000 | 15.057751000 | 2.793970000 | O | 30.382418000 | 20.555007000 | 5.9186484000 | C | 32.051063000 | 23.530702000 | 3.473038000 |
| H | 28.855640000 | 14.302708000 | 3.303804000 | O | 32.364951000 | 20.232729000 | 6.919197000 | C | 33.385414000 | 23.932738000 | 3.684995000 |
| O | 27.459525000 | 17.390716000 | 2.875068000 | O | 31.150015000 | 17.939280000 | 6.274758000 | C | 34.107721000 | 23.321922000 | 4.729989000 |
| H | 26.977279000 | 17.903895000 | 3.533064000 | O | 27.679754000 | 18.373810000 | 8.294356000 | C | 33.528853000 | 22.330812000 | 5.518578000 |
| Cu | 26.663280000 | 15.469388000 | 2.586808000 | O | 30.586201000 | 16.174443000 | 12.219097000 | C | 28.201403000 | 13.798792000 | 5.970318000 |
| O | 24.841329000 | 15.470685000 | 2.132812000 | O | 31.936750000 | 13.879085000 | 9.666039000 | C | 27.574692000 | 12.706317000 | 5.169898000 |
| C | 25.503846000 | 13.755685000 | 2.126431000 | O | 31.857906000 | 13.867362000 | 7.074635000 | C | 28.317304000 | 12.007744000 | 4.205530000 |
| H | 25.543141000 | 13.645850000 | 1.051855000 | O | 29.373995000 | 14.143308000 | 5.681952000 | C | 27.719329000 | 10.995873000 | 3.458164000 |
| H | 24.600906000 | 13.341607000 | 2.554853000 | O | 27.498156000 | 14.299332000 | 6.903590000 | C | 26.365105000 | 10.659922000 | 3.653229000 |
| H | 24.357640000 | 15.519539000 | 2.971879000 | H | 38.310382000 | 16.957192000 | 3.033804000 | C | 25.634748000 | 11.351827000 | 4.637597000 |
| H | 26.380809000 | 13.322617000 | 2.620077000 | H | 33.844352000 | 24.702119000 | 3.061560000 | C | 26.230607000 | 12.363572000 | 5.386012000 |
| 121 | | | | | | | | | | | |
| B6 | | | | | | | | | | | |
| H | 23.263063000 | 19.257460000 | 2.699944000 | H | 25.115457000 | 17.540388000 | 11.268212000 | O | 33.741693000 | 17.830768000 | 6.979655000 |
| H | 21.907067000 | 15.742975000 | 4.816459000 | H | 32.001504000 | 21.748335000 | 11.052090000 | O | 28.979763000 | 16.702834000 | 6.769417000 |
| H | 24.008651000 | 15.761353000 | 6.163621000 | H | 25.341968000 | 19.268247000 | 4.065921000 | O | 32.999119000 | 16.051362000 | 10.755271000 |
| H | 28.340087000 | 18.215922000 | 12.631165000 | H | 29.371377000 | 12.257472000 | 12.063134000 | O | 33.721117000 | 17.931175000 | 9.748717000 |
| H | 36.517738000 | 15.238368000 | 2.664584000 | H | 34.490650000 | 15.210078000 | 4.104753000 | O | 31.096156000 | 18.013588000 | 10.401455000 |
| H | 38.025151000 | 18.623085000 | 4.887822000 | H | 30.440988000 | 22.218122000 | 4.083616000 | O | 29.734376000 | 14.796344000 | 8.350720000 |
| H | 35.981877000 | 18.582721000 | 6.313632000 | Zr | 29.069259000 | 18.741087000 | 6.498953000 | O | 27.991281000 | 20.757586000 | 7.027216000 |
| H | 29.746961000 | 17.522845000 | 12.388598000 | Zr | 29.009339000 | 18.897437000 | 10.061298000 | O | 29.226202000 | 18.412983000 | 12.290685000 |
| H | 27.7919478000 | 20.800349000 | 8.012347000 | Zr | 30.761199000 | 15.780908000 | 10.165688000 | O | 27.945985000 | 20.653615000 | 9.641660000 |
| H | 30.226833000 | 15.440597000 | 12.730445000 | Zr | 30.873301000 | 15.645330000 | 6.553050000 | O | 26.949332000 | 18.334129000 | 10.990504000 |
| H | 28.279013000 | 21.431615000 | 10.066181000 | H | 27.749647000 | 16.013086000 | 8.317757000 | O | 26.091628000 | 16.692005000 | 9.722895000 |
| H | 28.622445000 | 21.422169000 | 6.742038000 | Zr | 32.106814000 | 18.519018000 | 8.324155000 | O | 29.348687000 | 14.159725000 | 10.956302000 |
| H | 31.573494000 | 18.255409000 | 11.207153000 | H | 28.766051000 | 18.944811000 | 3.799933000 | O | 27.457354000 | 14.320090000 | 9.742592000 |
| H | 26.804017000 | 18.777944000 | 8.301380000 | H | 31.561438000 | 16.314240000 | 4.039577000 | O | 31.569409000 | 16.544238000 | 8.359359000 |
| H | 31.468696000 | 23.991850000 | 2.671407000 | O | 30.782702000 | 15.909318000 | 4.431011000 | O | 30.584805000 | 20.580359000 | 10.780642000 |
| H | 35.141176000 | 23.623505000 | 4.918628000 | O | 29.379739000 | 18.494752000 | 4.394877000 | O | 32.330357000 | 20.317965000 | 9.676576000 |
| H | 34.093667000 | 18.484192000 | 6.318208000 | Cu | 29.088622000 | 16.628140000 | 3.661218000 | O | 28.976673000 | 16.781172000 | 9.778130000 |
| H | 31.974875000 | 17.778107000 | 8.648843000 | O | 28.791953000 | 14.928100000 | 2.753648000 | O | 30.390079000 | 20.547757000 | 5.893638000 |
| H | 28.306643000 | 10.460035000 | 2.708811000 | H | 29.192985000 | 14.282465000 | 3.347955000 | O | 32.359935000 | 20.238769000 | 6.923636500 |
| H | 24.587768000 | 11.091615000 | 4.816667000 | O | 27.430727000 | 17.265444000 | 2.881541000 | O | 31.133782000 | 17.931475000 | 6.250532000 |
| H | 25.670649000 | 12.906174000 | 6.150418000 | H | 26.991365000 | 17.767988000 | 3.576528000 | O | 27.677499000 | 18.377562000 | 8.298039000 |
| H | 32.688990000 | 13.717603000 | 6.607252000 | Cu | 26.916867000 | 15.135496000 | 2.773836000 | O | 30.577103000 | 16.179750000 | 12.222128000 |
| H | 32.848942000 | 14.023173000 | 9.952194000 | O | 24.968735000 | 15.162272000 | 2.545116000 | O | 31.933386000 | 13.885376000 | 9.660699000 |
| H | 31.520741000 | 18.237388000 | 5.436083000 | C | 24.078849000 | 20.1448443000 | 2.515477000 | O | 31.835891000 | 13.864748000 | 7.058820000 |
| H | 29.644908000 | 13.824250000 | 3.835434000 | H | 24.546060000 | 13.201929000 | 3.019524000 | O | 29.357112000 | 14.183715000 | 5.638650000 |
| C | 26.458176000 | 17.496055000 | 5.996863000 | H | 23.871759000 | 13.780062000 | 1.478673000 | O | 27.521149000 | 14.272097000 | 6.924391000 |
| C | 24.806514000 | 17.506303000 | 5.189713000 | H | 24.535306000 | 15.929131000 | 2.939587000 | H | 38.310366000 | 16.956727000 | 3.033904000 |
| C | 24.586187000 | 18.494793000 | 4.217558000 | H | 23.143589000 | 14.289935000 | 3.016590000 | H | 33.844015000 | 24.702778000 | 3.062180000 |
| C | 23.418409000 | 18.485760000 | 3.457286000 | H | 22.475286000 | 17.487480000 | 2.086028000 | H | 25.896861000 | 9.869028000 | 3.064186000 |
| C | 22.440175000 | 17.489256000 | 3.647450000 | H | 21.527615000 | 17.480515000 | 1.7480404000 | H | 21.527615000 | 17.480404000 | 3.048420000 |
| C | 22.661958000 | 16.513843000 | 4.638698000 | H | 24.798530000 | 16.893996000 | 11.092030000 | H | 27.738429000 | 12.980090000 | 11.214463000 |
| C | 23.829435000 | 16.519366000 | 5.398327000 | H | 23.263080000 | 19.258031000 | 2.699812000 | H | 25.114550000 | 17.539327000 | 11.266232000 |
| C | 33.868194000 | 16.904267000 | 6.130662000 | H | 21.911261000 | 15.738094000 | 4.810146000 | H | 32.003183000 | 21.746448000 | 11.053348000 |
| C | 35.110961000 | 16.894613000 | 5.299629000 | H | 24.003542000 | 15.761584000 | 6.164339000 | H | 25.351700000 | 19.258426000 | 4.064641000 |
| C | 35.273563000 | 15.953402000 | 4.269678000 | H | 28.335326000 | 18.237874000 | 12.623949000 | H | 29.365322000 | 12.272914000 | 4.041621000 |
| C | 36.411229000 | 15.974751000 | 4.365070000 | H | 36.518086000 | 15.238152000 | 2.664911000 | H | 34.495420000 | 15.204547000 | 4.106333000 |
| C | 37.2420943000 | 16.937186000 | 3.666012000 | H | 38.025482000 | 18.622504000 | 4.888428000 | H | 30.438348000 | 22.223340000 | 4.084650000 |
| C | 37.253511000 | 17.867969000 | 4.709669000 | H | 35.981493000 | 18.582799000 | 6.313474000 | Zr | 29.034146000 | 18.786432000 | 6.462990000 |
| C | 36.115041000 | 17.853046000 | 5.512754000 | H | 29.739222000 | 17.539924000 | 12.388980000 | Zr | 29.007149000 | 18.906058000 | 10.050460000 |
| C | 33.837141000 | 16.958907000 | 10.535584000 | H | 27.925175000 | 20.833681000 | 8.037623000 | Zr | 30.756131000 | 15.785120000 | 10.174420000 |
| C | 26.050620000 | 17.523797000 | 10.664620000 | H | 24.316730000 | 23.993324000 | 2.672961000 | Zr | 30.874062000 | 15.667418000 | 6.573937000 |
| C | 28.183404000 | 13.821192000 | 10.638016000 | H</td | | | | | | | |

| | | | | | | | | | | | |
|---|--------------|--------------|--------------|--|--------------|--------------|--------------|--|--------------|--------------|--------------|
| H | 35.982550000 | 18.582278000 | 6.314147000 | Zr | 29.044644000 | 18.731357000 | 6.490053000 | O | 27.458432000 | 14.316707000 | 9.740134000 |
| H | 29.742913000 | 17.538857000 | 12.395824000 | Zr | 29.002171000 | 18.898268000 | 10.060814000 | O | 31.558538000 | 16.555424000 | 8.359083000 |
| H | 27.940126000 | 20.809468000 | 8.023320000 | Zr | 30.752760000 | 15.780986000 | 10.182720000 | O | 30.386102000 | 20.576834000 | 10.785824000 |
| H | 30.220728000 | 15.455793000 | 12.749607000 | Zr | 30.886467000 | 15.627185000 | 6.579552000 | O | 32.329152000 | 20.316938000 | 9.676299000 |
| H | 28.266193000 | 21.429684000 | 10.080129000 | Zr | 27.742604000 | 16.012442000 | 8.317604000 | O | 28.973757000 | 16.781283000 | 9.783808000 |
| H | 28.626027000 | 21.445601000 | 6.746095000 | Zr | 32.093715000 | 18.512710000 | 8.336507000 | O | 30.383504000 | 20.548142000 | 5.912230000 |
| H | 31.570810000 | 18.265007000 | 11.203999000 | H | 29.878783000 | 18.834268000 | 3.919034000 | O | 32.361068000 | 20.228065000 | 6.918701000 |
| H | 26.802253000 | 18.769487000 | 8.278933000 | H | 31.662145000 | 16.261908000 | 4.057660000 | O | 31.115352000 | 17.914649000 | 6.200720000 |
| H | 31.467372000 | 23.994320000 | 2.673940000 | O | 30.881831000 | 15.844578000 | 4.431446000 | O | 27.683552000 | 18.384167000 | 8.300075000 |
| H | 35.141062000 | 23.623354000 | 4.918785000 | O | 29.176376000 | 18.359684000 | 4.372701000 | O | 30.577723000 | 16.179476000 | 12.228626000 |
| H | 34.092997000 | 21.850174000 | 6.319969000 | Cu | 29.107050000 | 16.460564000 | 3.776218000 | O | 31.933839000 | 13.881894000 | 9.693541000 |
| H | 31.972532000 | 13.765145000 | 8.684942000 | O | 28.921346000 | 15.043603000 | 2.580660000 | O | 31.868613000 | 13.842793000 | 7.099563000 |
| H | 28.305775000 | 10.461911000 | 2.706652000 | H | 29.655547000 | 14.441618000 | 2.740313000 | O | 29.382127000 | 14.145111000 | 5.696641000 |
| H | 24.586108000 | 11.098202000 | 4.811181000 | O | 27.049421000 | 15.896958000 | 4.019864000 | O | 27.502283000 | 14.302646000 | 6.905026000 |
| H | 25.665707000 | 12.903791000 | 6.148285000 | H | 26.858644000 | 15.529236000 | 4.896626000 | H | 38.310257000 | 16.957738000 | 3.033587000 |
| H | 32.677086000 | 13.677462000 | 6.631376000 | H | 27.311865000 | 15.138158000 | 3.452514000 | H | 33.844435000 | 24.702033000 | 3.061570000 |
| H | 32.843709000 | 14.026075000 | 9.984984000 | H | | | | H | 25.896186000 | 9.871091000 | 3.061873000 |
| H | 31.651309000 | 18.213306000 | 5.509550000 | H | | | | H | 21.528219000 | 17.480263000 | 3.047772000 |
| H | 29.645172000 | 13.818843000 | 8.344151000 | 111. | | | | H | 34.798980000 | 16.893336000 | 11.091054000 |
| C | 26.061275000 | 17.496920000 | 5.997028000 | Cu^{II}O(O₂) | | | | H | 27.740657000 | 12.974851000 | 11.208634000 |
| C | 24.806461000 | 17.506200000 | 5.189825000 | H | 23.261642000 | 19.259000000 | 2.701143000 | H | 25.115076000 | 17.539820000 | 11.266744000 |
| C | 24.586181000 | 18.494778000 | 4.217556000 | H | 21.912851000 | 15.736606000 | 4.808842000 | H | 32.001379000 | 21.750502000 | 11.048323000 |
| C | 23.418428000 | 18.485748000 | 3.457259000 | H | 24.005249000 | 15.760141000 | 6.162443000 | H | 25.344370000 | 19.265766000 | 4.065548000 |
| C | 22.440165000 | 17.489262000 | 3.647457000 | H | 28.335622000 | 18.228063000 | 12.640664000 | H | 29.363565000 | 12.279425000 | 4.049927000 |
| C | 22.661944000 | 16.513853000 | 4.638726000 | H | 36.516250000 | 15.239851000 | 2.663068000 | H | 34.484483000 | 15.217705000 | 4.101109000 |
| C | 23.829524000 | 16.519260000 | 5.398168000 | H | 38.025141000 | 18.623065000 | 4.887967000 | H | 30.441424000 | 22.216991000 | 4.083095000 |
| C | 33.868484000 | 16.903665000 | 6.130203000 | H | 35.982606000 | 18.583896000 | 6.312727000 | Zr | 29.055785000 | 18.757993000 | 6.521590000 |
| C | 35.111019000 | 16.894766000 | 5.299714000 | H | 29.740744000 | 17.529288000 | 12.399626000 | Zr | 29.008994000 | 18.896151000 | 10.069356000 |
| C | 35.273586000 | 15.953359000 | 4.269719000 | H | 27.921331000 | 20.820858000 | 8.029501000 | Zr | 30.754628000 | 15.785786000 | 10.178816000 |
| C | 36.411218000 | 15.974769000 | 3.465052000 | H | 30.221832000 | 15.445921000 | 12.743015000 | Zr | 30.891093000 | 15.618030000 | 6.583450000 |
| C | 37.420946000 | 16.937185000 | 3.666016000 | H | 28.248679000 | 21.432400000 | 10.080497000 | Zr | 27.741032000 | 16.012448000 | 8.312499000 |
| C | 37.253525000 | 17.869750000 | 4.709718000 | H | 28.612884000 | 21.445603000 | 6.749148000 | Zr | 32.113520000 | 18.520444000 | 8.322692000 |
| C | 36.114989000 | 17.853151000 | 5.512672000 | H | 31.570789000 | 18.260509000 | 11.214452000 | H | 28.382719000 | 18.923672000 | 3.951660000 |
| C | 33.638602000 | 16.959021000 | 10.535666000 | H | 26.806145000 | 18.785621000 | 8.295698000 | O | 30.759288000 | 15.898925000 | 4.440359000 |
| C | 26.050704000 | 17.523762000 | 10.664700000 | H | 31.468647000 | 23.991775000 | 2.671456000 | O | 29.194479000 | 18.585686000 | 4.349031000 |
| C | 28.183366000 | 13.821273000 | 10.638049000 | H | 35.141246000 | 23.623117000 | 4.918485000 | Cu | 29.153354000 | 16.649123000 | 4.016297000 |
| C | 31.573363000 | 20.879063000 | 5.104657000 | H | 34.094351000 | 21.848131000 | 6.317722000 | O | 27.840126000 | 15.320598000 | 3.212552000 |
| C | 31.605373000 | 20.824080000 | 6.099571000 | H | 31.977994000 | 17.363557000 | 8.680123000 | O | 27.296641000 | 16.477366000 | 3.207693000 |
| C | 32.203651000 | 21.926567000 | 5.289650000 | H | 28.305983000 | 10.461639000 | 2.706756000 | | | | |
| C | 31.468257000 | 22.541451000 | 4.263247000 | H | 24.585891000 | 11.098238000 | 4.810702000 | | | | |
| C | 32.501063000 | 23.530702000 | 3.470330800 | H | 25.667045000 | 12.905845000 | 6.147192000 | 112. | | | |
| C | 33.385414000 | 23.932738000 | 3.684995000 | H | 32.702935000 | 13.695566000 | 6.640035000 | Cu^{II}(OH)₂ | | | |
| C | 34.107721000 | 23.321922000 | 4.729989000 | H | 32.845257000 | 14.019640000 | 9.985198000 | H | 23.263893000 | 19.256782000 | 2.698556000 |
| C | 33.528853000 | 22.330813000 | 5.518579000 | H | 31.567967000 | 18.199911000 | 5.397269000 | H | 21.912741000 | 15.736761000 | 4.809112000 |
| C | 28.201396000 | 13.798781000 | 5.970339000 | H | 29.643584000 | 13.824251000 | 8.345039000 | H | 24.003048000 | 15.759768000 | 6.163033000 |
| C | 27.574696000 | 12.706313000 | 5.169901000 | C | 26.061855000 | 17.495929000 | 5.996937000 | H | 28.339668000 | 18.227392000 | 12.641835000 |
| C | 28.317304000 | 12.007744000 | 4.205530000 | C | 24.806520000 | 17.506263000 | 6.189732000 | H | 36.517544000 | 15.238547000 | 2.664471000 |
| C | 27.719329000 | 10.995873000 | 3.458164000 | C | 24.586194000 | 18.494771000 | 4.217542000 | H | 38.025467000 | 18.622517000 | 4.888458000 |
| C | 26.365105000 | 10.659922000 | 3.653228000 | C | 23.418409000 | 18.485768000 | 3.457289000 | H | 35.982570000 | 18.583151000 | 6.313360000 |
| C | 25.634748000 | 11.351827000 | 4.637597000 | C | 22.440175000 | 17.489251000 | 3.647442000 | H | 29.743724000 | 17.528960000 | 12.401720000 |
| C | 26.230607000 | 12.363572000 | 5.386012000 | C | 22.661964000 | 16.513826000 | 4.638695000 | H | 27.933270000 | 20.807621000 | 8.028070000 |
| O | 26.931182000 | 18.376754000 | 5.762754000 | C | 23.829415000 | 16.519403000 | 5.398340000 | H | 30.223907000 | 15.443924000 | 12.748792000 |
| O | 26.169292000 | 16.589234000 | 6.879550000 | C | 33.868100000 | 16.903979000 | 6.130282000 | H | 28.270583000 | 21.424441000 | 10.084911000 |
| O | 30.097690000 | 19.074412000 | 8.294191000 | C | 35.110976000 | 16.894714000 | 5.299648000 | H | 28.648437000 | 21.432919000 | 6.763485000 |
| O | 33.031996000 | 15.984267000 | 5.924620000 | C | 35.273560000 | 15.953407000 | 4.269673000 | H | 31.573156000 | 18.258300000 | 11.210946000 |
| O | 33.739867000 | 17.838567000 | 6.974372000 | C | 36.411230000 | 15.974749000 | 3.465071000 | H | 26.810600000 | 18.768674000 | 8.280547000 |
| O | 29.012427000 | 16.697880000 | 6.814691000 | C | 37.420943000 | 16.937187000 | 3.666012000 | H | 31.468181000 | 23.992365000 | 2.672216000 |
| O | 32.997215000 | 16.057256000 | 10.764916000 | C | 37.253507000 | 17.869770000 | 4.709692000 | H | 35.141146000 | 23.623230000 | 4.918698000 |
| O | 33.722571000 | 17.921878000 | 9.744346000 | C | 36.115041000 | 17.853047000 | 5.512757000 | H | 34.093984000 | 21.849385000 | 6.318744000 |
| O | 31.093787000 | 18.013170000 | 10.404378000 | C | 33.836918000 | 16.958977000 | 5.053573900 | H | 31.981240000 | 13.751125000 | 8.691630000 |
| O | 29.732806000 | 14.779357000 | 8.368894000 | C | 26.050656000 | 17.523799000 | 10.664655000 | H | 28.305748000 | 10.462347000 | 2.706208000 |
| O | 28.094800000 | 20.734147000 | 7.013042000 | C | 28.183429000 | 13.821093000 | 10.638036000 | H | 24.585550000 | 11.099490000 | 4.809885000 |
| O | 29.227252000 | 18.412022000 | 12.976050000 | C | 31.573388000 | 20.879258000 | 10.504626000 | H | 25.666001000 | 12.904431000 | 6.147892000 |
| O | 27.944260000 | 20.643258000 | 9.624870000 | C | 31.605581000 | 20.823626000 | 6.099570000 | H | 32.661815000 | 13.632937000 | 6.608800000 |
| O | 26.949643000 | 18.334705000 | 10.999732000 | C | 32.203589000 | 21.926587000 | 5.289635000 | H | 32.855512000 | 14.027579000 | 9.984705000 |
| O | 26.092456000 | 16.690700000 | 9.724964000 | C | 31.468282000 | 22.541411000 | 4.263208000 | H | 31.572578000 | 18.258611000 | 5.459836000 |
| O | 29.341550000 | 14.168264000 | 10.9688 | | | | | | | | |

| | | | | | | | | | | | |
|----|--------------|---------------|---------------|---|--------------|---------------|--------------|---|----------------|--------------|--------------|
| C | 27.574693000 | 12.706328000 | 5.169880000 | C | 23.418425000 | 18.485752000 | 3.457264000 | H | 23.260607000 | 19.261322000 | 2.703258000 |
| C | 28.317303000 | 12.007757000 | 4.205518000 | C | 22.440168000 | 17.489258000 | 3.647453000 | H | 21.911701000 | 15.738145000 | 4.810419000 |
| C | 27.719321000 | 10.995889000 | 3.458148000 | C | 22.661948000 | 16.513847000 | 4.638719000 | H | 24.001888000 | 15.762207000 | 6.165985000 |
| C | 26.365116000 | 10.659894000 | 3.653260000 | C | 23.829519000 | 16.519266000 | 5.398176000 | H | 28.336650000 | 18.227537000 | 12.622133000 |
| C | 25.634753000 | 11.351814000 | 4.637610000 | C | 33.868402000 | 16.903517000 | 6.130170000 | H | 36.518319000 | 15.237732000 | 2.665227000 |
| C | 26.230598000 | 12.363594000 | 5.385989000 | C | 35.111037000 | 16.894786000 | 5.299740000 | H | 38.025834000 | 18.622194000 | 4.888594000 |
| O | 26.931555000 | 18.384129000 | 5.758523000 | C | 35.273589000 | 15.953360000 | 4.269720000 | H | 35.982137000 | 18.582362000 | 6.314059000 |
| O | 26.170872000 | 16.600509000 | 6.885981000 | C | 36.411218000 | 15.974768000 | 3.465053000 | H | 29.744092000 | 17.535168000 | 12.384541000 |
| O | 30.105748000 | 19.067967000 | 8.303371000 | C | 37.420946000 | 16.937184000 | 3.666016000 | H | 27.922245000 | 20.821784000 | 8.026682000 |
| O | 33.030738000 | 15.984965000 | 5.924660000 | C | 37.253524000 | 17.869750000 | 4.709717000 | H | 30.220707000 | 15.453178000 | 12.731924000 |
| O | 33.739090000 | 17.835948000 | 6.976645000 | C | 36.114983000 | 17.853124000 | 5.512664000 | H | 28.277801000 | 21.434884000 | 10.082352000 |
| O | 29.018847000 | 16.691082000 | 6.827642000 | C | 33.836768000 | 16.959027000 | 10.535646000 | H | 28.568164000 | 21.460749000 | 6.728070000 |
| O | 32.998611000 | 16.055251000 | 10.7621234000 | C | 26.050688000 | 17.523841000 | 10.664730000 | H | 31.572471000 | 18.263494000 | 11.198340000 |
| O | 33.722051000 | 17.930086000 | 9.746622000 | C | 28.183309000 | 13.821338000 | 10.638056000 | H | 26.795610000 | 18.780328000 | 8.303465000 |
| O | 31.097157000 | 18.009121000 | 10.409884000 | C | 31.573374000 | 20.879085000 | 10.504645000 | H | 31.467718000 | 23.993960000 | 2.673382000 |
| O | 29.749760000 | 14.773253000 | 8.371141000 | C | 31.605338000 | 20.824051000 | 6.099522000 | H | 35.140890000 | 23.624003000 | 4.919039000 |
| O | 28.026953000 | 20.737022000 | 7.017560000 | C | 32.203661000 | 19.212657000 | 5.289662000 | H | 34.092954000 | 21.848666000 | 6.319067000 |
| O | 29.228605000 | 18.402121000 | 12.303425000 | C | 31.462853000 | 22.541459000 | 4.263256000 | H | 31.977135000 | 13.770570000 | 8.675775000 |
| O | 27.950034000 | 20.637448000 | 9.629658000 | C | 32.051061000 | 23.530704000 | 3.473039000 | H | 28.305926000 | 10.461932000 | 2.706163000 |
| O | 26.951910000 | 18.331483000 | 11.002727000 | C | 33.385415000 | 23.932736000 | 3.684993000 | H | 24.586619000 | 11.095965000 | 4.812383000 |
| O | 26.092594000 | 16.693016000 | 9.723110000 | C | 34.107223000 | 23.321917000 | 4.729984000 | H | 25.666271000 | 12.901463000 | 6.150530000 |
| O | 29.344618000 | 14.162957000 | 10.964869000 | C | 33.528854000 | 22.330811000 | 5.518578000 | H | 32.681405000 | 13.673475000 | 6.631238000 |
| O | 27.457253000 | 14.318751000 | 9.743002000 | C | 28.201704000 | 13.798353000 | 5.970230000 | H | 32.840093000 | 14.026046000 | 9.985327000 |
| O | 31.575111000 | 16.539101000 | 8.367431000 | C | 27.574523000 | 12.706304000 | 5.169874000 | H | 31.647602000 | 18.217871000 | 5.475790000 |
| O | 30.385390000 | 20.576798000 | 10.782413000 | C | 28.317302000 | 12.008117000 | 4.205690000 | H | 29.643218000 | 13.824017000 | 8.341943000 |
| O | 32.331738000 | 20.313942000 | 9.680914000 | C | 27.719465000 | 10.995805000 | 3.458028000 | C | 26.061212000 | 17.496911000 | 5.997092000 |
| O | 28.977500000 | 16.772899000 | 9.786854000 | C | 26.356090000 | 10.660029000 | 3.653236000 | C | 24.806451000 | 17.506258000 | 5.189841000 |
| O | 30.394865000 | 20.512361000 | 5.873051000 | C | 25.634768000 | 11.3517197000 | 4.637625000 | C | 24.586177000 | 18.494785000 | 4.217563000 |
| O | 32.350174000 | 20.250972000 | 6.942435000 | C | 26.230600000 | 12.363559000 | 5.386042000 | C | 23.418425000 | 18.485752000 | 3.457264000 |
| O | 31.138591000 | 17.924251000 | 6.252243000 | O | 26.495955000 | 18.351288000 | 5.725926000 | C | 22.440168000 | 17.489258000 | 3.647453000 |
| O | 27.687954000 | 18.367279000 | 8.299222000 | O | 26.145618000 | 16.617016000 | 6.904739000 | C | 22.661948000 | 16.513847000 | 4.638719000 |
| O | 30.581736000 | 16.174936000 | 12.232364000 | O | 30.099498000 | 19.096208000 | 8.306309000 | C | 23.829519000 | 16.519266000 | 5.398176000 |
| O | 31.943615000 | 13.875915000 | 9.701223000 | O | 33.005319000 | 16.017506000 | 5.880291000 | C | 33.868402000 | 16.903517000 | 6.130170000 |
| O | 31.854960000 | 13.828300000 | 7.097839000 | O | 33.749535000 | 17.817849000 | 6.996390000 | C | 35.111037000 | 16.894786000 | 5.299740000 |
| O | 29.355125000 | 14.198484000 | 5.649080000 | O | 28.994849000 | 16.723039000 | 6.802766000 | C | 35.273589000 | 15.953360000 | 4.269720000 |
| O | 27.518860000 | 14.270726000 | 6.930400000 | O | 32.999742000 | 16.051548000 | 10.751966000 | C | 36.411218000 | 15.974768000 | 3.465053000 |
| H | 38.310456000 | 16.957106000 | 3.033983000 | O | 33.720890000 | 17.934862000 | 9.752759000 | C | 37.420946000 | 16.937184000 | 3.666016000 |
| H | 33.842421000 | 24.702469000 | 3.061987000 | O | 31.095371000 | 18.012027000 | 10.403233000 | C | 37.253524000 | 17.869750000 | 4.709717000 |
| H | 25.895873000 | 9.871742000 | 3.061378000 | O | 29.727203000 | 14.793101000 | 8.358444000 | C | 36.114983000 | 17.853124000 | 5.512664000 |
| H | 21.528671000 | 17.479236000 | 3.047105000 | O | 27.987636000 | 20.757162000 | 7.039734000 | C | 33.836768000 | 16.959027000 | 10.535646000 |
| H | 34.801033000 | 16.893740000 | 11.087493000 | O | 29.228409000 | 18.401356000 | 12.300947000 | C | 26.050688000 | 17.523841000 | 10.664730000 |
| H | 27.739369000 | 12.975915000 | 11.208938000 | O | 27.946747000 | 20.653074000 | 9.648286000 | C | 28.183309000 | 13.821338000 | 10.638056000 |
| H | 25.113258000 | 17.543899000 | 11.263512000 | O | 26.948285000 | 18.334948000 | 11.002714000 | C | 31.573374000 | 20.879085000 | 10.504645000 |
| H | 31.999686000 | 21.7516108000 | 11.047434000 | O | 26.092545000 | 16.692551000 | 9.723809000 | C | 31.605338000 | 20.824051000 | 6.099522000 |
| H | 25.348026000 | 19.260712000 | 4.062103000 | O | 29.343167000 | 14.166889000 | 10.964390000 | C | 32.203661000 | 21.926570000 | 5.289662000 |
| H | 29.363154000 | 12.279966000 | 4.048983000 | O | 27.458955000 | 14.314549000 | 9.737248000 | C | 31.468253000 | 22.554145900 | 4.263256000 |
| H | 44.486877000 | 15.211001000 | 4.104793000 | O | 31.557306000 | 16.545001000 | 8.355536000 | C | 32.051061000 | 23.530704000 | 3.473090000 |
| H | 30.440854000 | 22.218873000 | 4.083647000 | O | 30.387297000 | 20.576675000 | 10.790652000 | C | 33.385415000 | 23.932736000 | 3.684993000 |
| Zr | 29.050680000 | 18.736118000 | 6.504362000 | O | 32.327562000 | 20.317059000 | 9.675617000 | C | 34.107723000 | 23.321917000 | 4.729984000 |
| Zr | 29.007074000 | 18.891954000 | 10.068135000 | O | 28.973031000 | 16.784121000 | 9.783270000 | C | 33.528854000 | 22.330811000 | 5.518780000 |
| Zr | 30.756451000 | 15.780121000 | 10.183927000 | O | 30.388103000 | 20.544789000 | 5.8889432000 | C | 28.201704000 | 13.798353000 | 5.970230000 |
| Zr | 30.910224000 | 15.619958000 | 6.595657000 | O | 32.357196000 | 20.236582000 | 6.924628000 | C | 27.574523000 | 12.706304000 | 5.169874000 |
| Zr | 27.747374000 | 16.004985000 | 8.316763000 | O | 31.136738000 | 17.942730000 | 6.261391000 | C | 28.317020000 | 12.008117000 | 4.205690000 |
| Zr | 32.103101000 | 18.520917000 | 8.329794000 | O | 27.672050000 | 18.385902000 | 8.303127000 | C | 27.719465000 | 10.995805000 | 3.458028000 |
| H | 28.401995000 | 18.587539000 | 3.920160000 | O | 30.584006000 | 16.179666000 | 12.220422000 | C | 26.365090000 | 10.660029000 | 3.653236000 |
| H | 31.448875000 | 16.452024000 | 4.051133000 | O | 31.929033000 | 13.881026000 | 9.679834000 | C | 25.634768000 | 11.351779000 | 4.637625000 |
| O | 30.822163000 | 15.853825000 | 4.438474000 | O | 31.875088000 | 13.875151000 | 7.095402000 | C | 26.230600000 | 12.363559000 | 5.386042000 |
| O | 29.202950000 | 18.297940000 | 4.377157000 | O | 29.394168000 | 14.100660000 | 5.741768000 | C | 26.943862000 | 18.346072000 | 5.712586000 |
| Cu | 28.977280000 | 16.295000000 | 4.188094000 | O | 27.469184000 | 14.346658000 | 6.859886000 | O | 26.144857000 | 16.615433000 | 6.902270000 |
| O | 27.288028000 | 16.050459000 | 3.585261000 | H | 38.310869000 | 15.9656653000 | 3.034501000 | O | 30.101437000 | 19.088003000 | 8.292775000 |
| H | 26.699017000 | 15.677176000 | 4.251590000 | H | 33.843883000 | 24.702990000 | 3.062399000 | O | 33.027566000 | 15.992360000 | 5.911948000 |
| H | 21.528033000 | 17.479776000 | 3.048008000 | H | 21.528033000 | 17.479776000 | 3.048008000 | O | 29.005623000 | 16.710476000 | 6.813448000 |
| H | 27.738840000 | 12.978103000 | 5.1211836000 | H | 27.738840000 | 12.978103000 | 5.1211836000 | O | 32.998905000 | 16.053702000 | 10.757259000 |
| H | 25.113436000 | 17.540660000 | 11.264477000 | H | 25.113436000 | 17.540660000 | 11.264477000 | O | 33.722347000 | 17.930711000 | 9.747236000 |
| H | 32.001917000 | 21.751684000 | 11.046271000 | H | 32.001917000 | 21.751684000 | 11.046271000 | O | 31.095705000</ | | |

| | | | | | | | | | | | |
|-------------|--------------|--------------|--------------|----|--------------|--------------|--------------|----|--------------|--------------|--------------|
| H | 25.116589000 | 17.537348000 | 11.269682000 | O | 31.100716000 | 18.006597000 | 10.393610000 | C | 37.253512000 | 17.869764000 | 4.709700000 |
| H | 32.002700000 | 21.747476000 | 11.052364000 | O | 29.737250000 | 14.780533000 | 8.352606000 | C | 36.114975000 | 17.853136000 | 5.512654000 |
| H | 25.346017000 | 19.265723000 | 4.073508000 | O | 27.987898000 | 20.751539000 | 7.017840000 | C | 33.836795000 | 16.958991000 | 10.535645000 |
| H | 29.362670000 | 12.283661000 | 4.051590000 | O | 29.232300000 | 18.392587000 | 12.291379000 | C | 26.050726000 | 17.523769000 | 10.664674000 |
| H | 34.491232000 | 15.208765000 | 4.106915000 | O | 27.954656000 | 20.645930000 | 9.632729000 | C | 28.183323000 | 13.821410000 | 10.637981000 |
| H | 30.437701000 | 22.224908000 | 4.087639000 | O | 26.949626000 | 18.335656000 | 10.999690000 | C | 31.573389000 | 20.879028000 | 10.504674000 |
| Zr | 29.045025000 | 18.767224000 | 6.484117000 | O | 26.092295000 | 16.695306000 | 9.721185000 | C | 31.605286000 | 20.824378000 | 6.099579000 |
| Zr | 29.006367000 | 18.902989000 | 10.053903000 | O | 29.348901000 | 14.158723000 | 9.054293000 | C | 32.203630000 | 21.926628000 | 5.289717000 |
| Zr | 30.756826000 | 15.783581000 | 10.168070000 | O | 27.456836000 | 14.317326000 | 9.741343000 | C | 31.468222000 | 22.541516000 | 4.263310000 |
| Zr | 30.883577000 | 15.617316000 | 6.549860000 | O | 31.562317000 | 16.545203000 | 8.332372000 | C | 32.051064000 | 23.530702000 | 3.473038000 |
| Zr | 27.750149000 | 16.019286000 | 8.317179000 | O | 30.387613000 | 20.573185000 | 10.789024000 | C | 33.385412000 | 23.932742000 | 3.684998000 |
| Zr | 32.093083000 | 18.510581000 | 8.327580000 | O | 32.326773000 | 20.319408000 | 9.672359000 | C | 34.107731000 | 23.321899000 | 4.729966000 |
| H | 29.880910000 | 19.139575000 | 3.969494000 | O | 28.974646000 | 16.777475000 | 9.779359000 | C | 33.528879000 | 22.330759000 | 5.518255000 |
| H | 31.591246000 | 16.191687000 | 4.026152000 | O | 30.379481000 | 20.569836000 | 9.535640000 | C | 28.201314000 | 13.798751000 | 5.970324000 |
| O | 30.836802000 | 15.749159000 | 4.423129000 | O | 32.370536000 | 20.211536000 | 6.900195000 | C | 27.574674000 | 12.706050000 | 5.170120000 |
| O | 29.113322000 | 18.721175000 | 4.368683000 | O | 31.110861000 | 17.925780000 | 6.172797000 | C | 28.317350000 | 12.007993000 | 4.205421000 |
| Cu | 29.054193000 | 16.658538000 | 4.218060000 | O | 27.681386000 | 18.382895000 | 8.293377000 | C | 27.719397000 | 10.995770000 | 3.458207000 |
| O | 27.224244000 | 15.641497000 | 4.031307000 | O | 30.588810000 | 16.171039000 | 12.207446000 | C | 26.365115000 | 10.659918000 | 3.653273000 |
| H | 26.596564000 | 16.216426000 | 3.566954000 | O | 31.937697000 | 13.877917000 | 9.674412000 | C | 25.634731000 | 11.351883000 | 4.637534000 |
| C | 27.053003000 | 17.894219000 | 1.958514000 | O | 31.840057000 | 13.840329000 | 7.087260000 | C | 26.230583000 | 12.363614000 | 5.385982000 |
| H | 27.712437000 | 17.248959000 | 1.396367000 | O | 29.362827000 | 14.159252000 | 5.666081000 | O | 26.930250000 | 18.385248000 | 5.756165000 |
| H | 26.826904000 | 15.457406000 | 4.897128000 | O | 27.502058000 | 14.286819000 | 6.911607000 | O | 26.168884000 | 16.604645000 | 6.889123000 |
| H | 26.032829000 | 18.008870000 | 1.623266000 | H | 38.310516000 | 16.956811000 | 3.034069000 | O | 30.105952000 | 19.069396000 | 8.303021000 |
| H | 27.475272000 | 18.582709000 | 2.677336000 | H | 33.844200000 | 24.702312000 | 3.061820000 | O | 33.033382000 | 15.982270000 | 5.927828000 |
| 117 | | | | | | | | | | | |
| TSA2 | | | | | | | | | | | |
| H | 23.260405000 | 19.260492000 | 2.702848000 | H | 25.115883000 | 17.538420000 | 11.268240000 | O | 31.097505000 | 18.008449000 | 10.407995000 |
| H | 21.911213000 | 15.738194000 | 4.810076000 | H | 32.001341000 | 21.749969000 | 11.049024000 | O | 29.747675000 | 14.774940000 | 8.366172000 |
| H | 24.006263000 | 15.760697000 | 6.163552000 | H | 25.341769000 | 19.268942000 | 4.069950000 | O | 28.025388000 | 20.738894000 | 7.017955000 |
| H | 28.341877000 | 18.211452000 | 12.622446000 | H | 29.365974000 | 12.277184000 | 4.056188000 | O | 29.229503000 | 18.399908000 | 12.302325000 |
| H | 36.518461000 | 15.237678000 | 2.665339000 | H | 34.495767000 | 15.203692000 | 4.108244000 | O | 27.950294000 | 20.637917000 | 9.630472000 |
| H | 38.025542000 | 18.622458000 | 4.888406000 | H | 30.442023000 | 22.214163000 | 4.083012000 | O | 26.952072000 | 18.331119000 | 11.003103000 |
| H | 35.981223000 | 18.583461000 | 6.312840000 | Zr | 29.037590000 | 18.767805000 | 6.498876000 | O | 26.092650000 | 16.692936000 | 9.723156000 |
| H | 29.749352000 | 17.518674000 | 12.381703000 | Zr | 29.010513000 | 18.895516000 | 4.059010000 | O | 29.346403000 | 14.160558000 | 10.961107000 |
| H | 27.917488000 | 20.825207000 | 8.029283000 | Zr | 30.758276000 | 15.708665000 | 10.154392000 | O | 27.456488000 | 14.319513000 | 9.743796000 |
| H | 30.229081000 | 15.436045000 | 12.716809000 | Zr | 30.875834000 | 15.615752000 | 6.539603000 | O | 31.575192000 | 16.539964000 | 8.363802000 |
| H | 28.285218000 | 21.428875000 | 10.087837000 | Zr | 27.748149000 | 16.013381000 | 8.305153000 | O | 30.385628000 | 20.576307000 | 10.783233000 |
| H | 28.605582000 | 21.444480000 | 6.744893000 | Zr | 32.097869000 | 18.515764000 | 8.319617000 | O | 32.331248000 | 20.314481000 | 9.680112000 |
| H | 31.576792000 | 18.250474000 | 11.196169000 | H | 28.210463000 | 18.879045000 | 3.990001000 | O | 28.977221000 | 16.773103000 | 9.784526000 |
| H | 26.802918000 | 18.781762000 | 8.296760000 | H | 31.875695000 | 15.893771000 | 4.063508000 | O | 30.393072000 | 20.518204000 | 5.878663000 |
| H | 31.468711000 | 23.991280000 | 2.671091000 | O | 31.000708000 | 15.634193000 | 4.369395000 | O | 32.351816000 | 20.248868000 | 6.939465000 |
| H | 35.141018000 | 23.623895000 | 4.918918000 | O | 29.106626000 | 18.784256000 | 4.341848000 | O | 31.137616000 | 17.924829000 | 6.249704000 |
| H | 34.094089000 | 21.848178000 | 6.317989000 | Cu | 29.662997000 | 16.963403000 | 3.946124000 | O | 27.687047000 | 18.368569000 | 8.299930000 |
| H | 31.972277000 | 13.763242000 | 8.659805000 | O | 27.289681000 | 15.421667000 | 3.251395000 | O | 30.582077000 | 16.173328000 | 12.228057000 |
| H | 28.306954000 | 10.458694000 | 2.709532000 | H | 28.726103000 | 14.649098000 | 3.500568000 | O | 31.944092000 | 13.876896000 | 9.692054000 |
| H | 24.586247000 | 11.096835000 | 4.811347000 | C | 25.693111000 | 14.739988000 | 3.973673200 | O | 31.845905000 | 13.826143000 | 7.088846000 |
| H | 25.669318000 | 12.906358000 | 6.149314000 | H | 25.288823000 | 14.544589000 | 3.921274000 | O | 29.345384000 | 14.207498000 | 5.633174000 |
| H | 32.655937000 | 13.668475000 | 6.604330000 | H | 28.138770000 | 16.272408000 | 3.305877000 | O | 27.520396000 | 14.257337000 | 6.937760000 |
| H | 32.849794000 | 14.029731000 | 9.956778000 | H | 25.214367000 | 15.553613000 | 2.412849000 | H | 38.310448000 | 16.957090000 | 3.033968000 |
| H | 31.629137000 | 18.275589000 | 5.438866000 | H | 25.879491000 | 13.858923000 | 2.337678000 | H | 33.844224000 | 24.702427000 | 3.061936000 |
| H | 29.639846000 | 13.820820000 | 8.340127000 | C | 25.895680000 | 9.874758000 | 3.058954500 | H | 25.895068000 | 9.874758000 | 3.058954500 |
| C | 26.061234000 | 17.496841000 | 5.997016000 | C | 21.528648000 | 17.479611000 | 3.047118000 | H | 34.799713000 | 16.894833000 | 11.089911000 |
| C | 24.806443000 | 17.506181000 | 5.189853000 | A2 | 27.738560000 | 12.978002000 | 12.112696000 | H | 37.738560000 | 12.978002000 | 12.112696000 |
| C | 24.586160000 | 18.494800000 | 4.217585000 | C | 23.418442000 | 18.485733000 | 4.375261000 | H | 34.799713000 | 16.894833000 | 11.089911000 |
| C | 23.418442000 | 18.485733000 | 4.357240000 | H | 23.262285000 | 19.258034000 | 2.700188000 | H | 25.113054000 | 17.544145000 | 11.263178000 |
| C | 22.440154000 | 17.489278000 | 3.647474000 | H | 21.913703000 | 15.735122000 | 4.807160000 | H | 31.999750000 | 21.751515000 | 11.047528000 |
| C | 22.661943000 | 16.513855000 | 4.638725000 | H | 24.008407000 | 15.755649000 | 6.157856000 | H | 25.345185000 | 19.264782000 | 4.066291000 |
| C | 23.829534000 | 16.519245000 | 5.398157000 | H | 28.340566000 | 12.243131000 | 12.640235000 | H | 29.362778000 | 12.281817000 | 4.048467000 |
| C | 33.868625000 | 16.903376000 | 6.130048000 | H | 36.517666000 | 15.238499000 | 2.664512000 | H | 34.490139000 | 15.210359000 | 4.105293000 |
| C | 35.111056000 | 16.894790000 | 5.299770000 | H | 38.025467000 | 18.622531000 | 4.888409000 | H | 30.440765000 | 22.218952000 | 4.083986000 |
| C | 35.273620000 | 15.953318000 | 4.269766000 | H | 35.983231000 | 18.583232000 | 6.312373000 | Zr | 29.050748000 | 18.737206000 | 6.505760000 |
| C | 36.411224000 | 15.974759000 | 3.465059000 | H | 29.745018000 | 15.725658700 | 12.398700000 | Zr | 29.007486000 | 18.892187000 | 10.067743000 |
| C | 37.420943000 | 16.937190000 | 3.666011000 | H | 27.932338000 | 20.808666000 | 8.028432000 | Zr | 30.757054000 | 15.779981000 | 10.178780000 |
| C | 37.253512000 | 17.869763000 | 4.709710100 | H | 30.224844000 | 15.441518000 | 12.743711000 | Zr | 30.907106000 | 15.622961000 | 6.587487000 |
| C | 36.114980000 | 17.853129000 | 5.512661000 | H | 28.272323000 | 21.424694000 | 10.085120000 | Zr | 27.743225000 | 16.006470000 | 8.314479000 |
| C | 33.836796000 | 16.959013000 | 10.535634000 | H | | | | | | | |

| | | | | | | | | | | | |
|---|--------------|--------------|--------------|-------------|--------------|--------------|--------------|---|--------------|--------------|--------------|
| H | 30.223037000 | 15.447363000 | 12.736106000 | Zr | 30.908302000 | 15.573259000 | 6.562558000 | O | 30.586140000 | 16.171278000 | 12.203751000 |
| H | 28.284107000 | 21.433271000 | 10.078560000 | Zr | 27.754663000 | 16.013134000 | 8.306372000 | O | 31.936464000 | 13.875416000 | 9.692157000 |
| H | 28.597579000 | 21.447686000 | 6.739507000 | Zr | 32.101505000 | 18.508834000 | 8.328772000 | O | 31.868575000 | 13.804752000 | 7.112244000 |
| H | 31.572827000 | 18.260511000 | 11.205477000 | H | 28.248958000 | 18.745102000 | 3.897784000 | O | 29.392090000 | 14.097052000 | 5.722634000 |
| H | 26.802994000 | 18.779055000 | 8.291409000 | O | 30.934206000 | 15.594852000 | 4.405443000 | O | 27.488257000 | 14.333988000 | 6.878147000 |
| H | 31.468570000 | 23.991759000 | 2.671501000 | O | 29.123024000 | 18.666242000 | 4.293908000 | H | 38.310222000 | 16.957965000 | 3.033513000 |
| H | 35.141199000 | 23.623194000 | 4.918611000 | Cu | 29.948510000 | 17.014701000 | 4.051924000 | H | 33.844589000 | 24.701965000 | 3.061570000 |
| H | 34.094259000 | 21.848398000 | 6.318011000 | | | | | H | 25.896730000 | 9.870049000 | 3.062882000 |
| H | 31.988114000 | 13.746396000 | 8.706891000 | | | | | H | 21.527736000 | 17.480940000 | 3.048527000 |
| H | 28.306139000 | 10.461557000 | 2.706897000 | 114 | | | | H | 34.792111000 | 16.900787000 | 11.103213000 |
| H | 24.586143000 | 11.097390000 | 4.811343000 | TSA3 | | | | H | 27.730565000 | 12.987299000 | 11.218451000 |
| H | 25.667244000 | 12.905217000 | 6.147914000 | H | 23.260612000 | 19.260495000 | 2.702909000 | H | 25.114643000 | 17.535138000 | 11.265954000 |
| H | 32.685267000 | 13.627306000 | 6.642667000 | H | 21.912385000 | 15.737250000 | 4.809559000 | H | 31.998212000 | 21.753902000 | 11.045060000 |
| H | 32.845294000 | 14.016085000 | 10.015967000 | H | 24.005167000 | 15.760933000 | 6.163353000 | H | 25.339633000 | 19.271249000 | 4.070416000 |
| H | 31.701644000 | 18.293823000 | 5.511248000 | H | 28.342222000 | 18.208652000 | 12.629729000 | H | 29.367120000 | 12.271330000 | 4.059553000 |
| H | 29.640217000 | 13.816102000 | 8.357389000 | H | 36.515430000 | 15.240725000 | 2.662148000 | H | 34.481510000 | 15.220433000 | 4.100573000 |
| C | 26.061470000 | 17.496677000 | 5.997014000 | H | 38.025643000 | 18.622478000 | 4.888472000 | H | 30.442180000 | 22.213978000 | 4.082307000 |
| C | 24.806468000 | 17.506254000 | 5.189812000 | H | 35.982377000 | 18.585152000 | 6.311654000 | Zr | 29.038491000 | 18.793718000 | 6.522579000 |
| C | 24.586191000 | 18.494717000 | 4.217544000 | H | 29.749104000 | 17.511868000 | 12.383116000 | Zr | 29.011010000 | 18.895152000 | 10.069000000 |
| C | 23.418421000 | 18.485754000 | 3.457271000 | H | 27.909009000 | 20.837179000 | 8.046758000 | Zr | 30.761582000 | 15.781486000 | 10.150076000 |
| C | 22.440168000 | 17.489259000 | 3.647452000 | H | 30.225893000 | 15.433730000 | 12.709289000 | Zr | 30.918794000 | 15.568070000 | 6.522310000 |
| C | 22.661953000 | 16.513842000 | 4.638712000 | H | 28.291180000 | 21.430159000 | 10.039691000 | Zr | 27.765753000 | 16.018894000 | 8.292792000 |
| C | 23.829488000 | 16.519306000 | 5.398227000 | H | 28.566670000 | 21.470788000 | 6.748635000 | Zr | 32.106326000 | 18.510919000 | 8.329010000 |
| C | 33.868311000 | 16.903813000 | 6.130146000 | H | 31.573382000 | 18.250020000 | 11.205707000 | H | 28.168027000 | 18.801808000 | 4.006553000 |
| C | 35.110984000 | 16.894773000 | 5.299659000 | H | 26.801960000 | 18.776006000 | 8.298977000 | O | 31.014977000 | 15.665987000 | 4.413153000 |
| C | 35.273587000 | 15.953360000 | 4.269718000 | H | 31.468723000 | 23.991086000 | 2.671015000 | O | 29.078788000 | 18.833853000 | 4.320605000 |
| C | 36.411222000 | 15.974763000 | 3.465059000 | H | 35.141146000 | 23.623355000 | 4.918694000 | Cu | 29.936055000 | 17.147539000 | 4.130689000 |
| C | 37.420944000 | 16.937187000 | 3.666013000 | H | 34.094285000 | 21.847749000 | 6.317259000 | C | 28.763429000 | 15.593787000 | 3.089210000 |
| C | 37.253520000 | 17.869755000 | 4.709710000 | H | 31.979583000 | 13.744750000 | 8.678391000 | H | 28.770138000 | 14.525701000 | 2.869848000 |
| C | 36.115004000 | 17.853079000 | 5.512698000 | H | 28.306689000 | 10.459130000 | 2.708995000 | H | 27.891152000 | 15.803621000 | 3.707852000 |
| C | 33.836799000 | 16.959024000 | 5.1053756000 | H | 24.586517000 | 11.096328000 | 4.811897000 | H | 28.730651000 | 16.141161000 | 2.150239000 |
| C | 26.050663000 | 17.523755000 | 10.664681000 | H | 25.668313000 | 12.905903000 | 6.148111000 | H | 29.940909000 | 15.402937000 | 3.720918000 |
| C | 28.183389000 | 13.821184000 | 10.638034000 | H | 32.691790000 | 13.629956000 | 6.642264000 | | | | |
| C | 31.573351000 | 20.879123000 | 10.504641000 | H | 32.847856000 | 14.014449900 | 9.982657000 | 111 | | | |
| C | 31.605542000 | 20.823806000 | 6.099570000 | H | 31.761178000 | 18.335382000 | 5.517490000 | Cu^{II}(O⁻)(OH) | | | |
| C | 32.203612000 | 21.926568000 | 5.289625000 | H | 29.632882000 | 13.826933000 | 8.342510000 | H | 23.262280000 | 19.258212000 | 2.700033000 |
| C | 31.468266000 | 22.514437000 | 4.263233000 | C | 26.061367000 | 17.496750000 | 5.996918000 | H | 21.913861000 | 15.735291000 | 4.807428000 |
| C | 32.051060000 | 23.530707000 | 3.473042000 | C | 24.806451000 | 17.506215000 | 5.189837000 | H | 24.007974000 | 15.756038000 | 6.157612000 |
| C | 33.385415000 | 23.932735000 | 3.684992000 | C | 24.586182000 | 18.494779000 | 4.217556000 | H | 28.340435000 | 18.222238000 | 12.647452000 |
| C | 34.107724000 | 23.321915000 | 4.729982000 | C | 23.418419000 | 18.485758000 | 3.457274000 | H | 28.770138000 | 14.525701000 | 2.869848000 |
| C | 33.528830000 | 22.330860000 | 5.518628000 | C | 22.440168000 | 17.489259000 | 3.647451000 | H | 35.167600000 | 15.238399000 | 2.664616000 |
| C | 28.201270000 | 13.799126000 | 5.970356000 | C | 22.661956000 | 15.613839000 | 4.638708000 | H | 38.025385000 | 18.622623000 | 4.888359000 |
| C | 27.574729000 | 12.706325000 | 5.169858000 | C | 23.829497000 | 16.519293000 | 5.398214000 | H | 35.982899000 | 18.582878000 | 6.313695000 |
| C | 28.317320000 | 12.007746000 | 4.205528000 | C | 33.868454000 | 16.903655000 | 6.130211000 | H | 29.745226000 | 17.524537000 | 12.402636000 |
| C | 27.719332000 | 10.995867000 | 3.458170000 | C | 35.111011000 | 16.894745000 | 5.299700000 | H | 27.928101000 | 20.813016000 | 8.038806000 |
| C | 26.365104000 | 10.659926000 | 3.653225000 | C | 35.273595000 | 15.953349000 | 4.269730000 | H | 30.225532000 | 15.442476000 | 12.746252000 |
| C | 25.634748000 | 11.351827000 | 4.637596000 | C | 36.411230000 | 15.974762000 | 3.465060000 | H | 28.277735000 | 21.425568000 | 10.089543000 |
| C | 26.230631000 | 12.363515000 | 5.386074000 | C | 37.420940000 | 16.937192000 | 3.666008000 | H | 28.636031000 | 21.445700000 | 6.772892000 |
| O | 26.952629000 | 18.350697000 | 5.710515000 | C | 37.253517000 | 17.869759000 | 4.709706000 | H | 31.572060000 | 18.254983000 | 11.210830000 |
| O | 26.149834000 | 16.640601000 | 6.1919852000 | C | 36.114999000 | 17.853104000 | 5.512699000 | H | 26.807132000 | 18.765852000 | 8.277437000 |
| O | 30.104762000 | 19.079738000 | 8.297031000 | C | 33.863852000 | 16.948997000 | 10.535769000 | H | 31.468181000 | 23.992707000 | 2.672394000 |
| O | 33.039201000 | 15.975144000 | 5.944623000 | C | 26.050678000 | 17.523703000 | 10.664678000 | H | 35.141060000 | 23.623389000 | 4.918829000 |
| O | 33.727203000 | 17.851041000 | 6.961787000 | C | 28.183455000 | 13.821192000 | 10.638027000 | H | 34.093490000 | 21.849332000 | 6.318739000 |
| O | 29.038054000 | 18.672050000 | 6.829488000 | C | 31.573342000 | 20.879104000 | 10.504629000 | H | 31.985580000 | 13.755659000 | 8.690617000 |
| O | 32.997510000 | 16.056302000 | 10.759949000 | C | 31.605395000 | 20.823923000 | 6.099492000 | H | 28.305715000 | 10.462140000 | 2.706146000 |
| O | 33.723313000 | 17.929580000 | 9.744982000 | C | 32.203616000 | 21.926579000 | 5.289643000 | H | 24.585154000 | 11.100383000 | 4.808988000 |
| O | 31.096355000 | 18.012430000 | 10.404282000 | C | 31.468260000 | 22.514494000 | 4.623424000 | H | 25.665152000 | 12.910055000 | 6.142755000 |
| O | 29.745995000 | 14.775195000 | 8.369241000 | C | 32.051058000 | 23.530710000 | 3.473045000 | H | 32.688682000 | 13.653112000 | 6.620075000 |
| O | 27.993340000 | 20.744763000 | 7.016107000 | C | 33.854516000 | 13.932733000 | 3.684990000 | H | 32.850529000 | 14.027285000 | 9.990648000 |
| O | 29.226641000 | 18.400705000 | 12.299311000 | C | 34.107726000 | 23.321911000 | 4.729978000 | H | 31.572683000 | 18.273294000 | 5.472416000 |
| O | 27.955663000 | 20.648667000 | 9.624430000 | C | 33.528836000 | 22.330848000 | 5.518616000 | H | 29.648154000 | 13.819078000 | 8.337211000 |
| O | 26.946783000 | 18.340608000 | 10.998721000 | C | 28.201250000 | 13.799221000 | 5.970430000 | C | 26.061235000 | 17.496996000 | 5.997018000 |
| O | 26.097417000 | 16.694266000 | 9.720309000 | C | 27.574728000 | 12.706373000 | 5.169841000 | C | 24.806427000 | 17.506202000 | 5.189877000 |
| O | 29.341943000 | 14.167618000 | 10.969052000 | C | 28.317305000 | 12.007744000 | 4.205543000 | C | 24.586328000 | 18.494700000 | 4.217604000 |
| O | 27.462599000 | 14.315430000 | 9.735303000 | C | 27.719330000 | 10.995864000 | 3.458173000 | C | 23.418386000 | 18.485812000 | 3.457289000 |
| O | 31.565641000 | 16.544896000 | 8.352642000 | C | 26.365104000 | 10.659925000 | 3.653226000 | C | 22.440162000 | 17.489271000 | 3.647493000 |
| O | 30.385452000 | | | | | | | | | | |

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|----|--------------|---------------|--------------|---|--------------|---------------|--------------|---|---------------|--------------|--------------|
| O | 26.945459000 | 18.370414000 | 5.741697000 | C | 36.411218000 | 15.974768000 | 3.465053000 | H | 29.7511448000 | 17.516954000 | 12.397951000 |
| O | 26.158977000 | 16.625926000 | 6.909749000 | C | 37.420944000 | 16.937188000 | 3.666013000 | H | 27.927187000 | 20.812224000 | 8.044448000 |
| O | 30.103819000 | 19.074848000 | 8.308762000 | C | 37.253524000 | 17.869750000 | 4.709717000 | H | 30.234799000 | 15.431702000 | 12.736417000 |
| O | 33.018404000 | 15.998604000 | 5.905270000 | C | 36.114994000 | 17.853109000 | 5.512680000 | H | 28.276736000 | 21.422763000 | 10.104952000 |
| O | 33.74435000 | 17.825757000 | 6.987701000 | C | 33.86774000 | 16.959039000 | 10.535665000 | H | 28.648604000 | 21.435935000 | 6.784570000 |
| O | 29.008722000 | 16.695572000 | 6.801523000 | C | 26.050678000 | 17.523767000 | 10.664674000 | H | 31.576736000 | 18.248158000 | 11.207450000 |
| O | 32.998793000 | 16.054381000 | 10.758437000 | C | 28.183338000 | 13.821294000 | 10.638023000 | H | 26.802443000 | 18.774434000 | 8.295075000 |
| O | 33.721332000 | 17.932187000 | 9.749023000 | C | 31.573342000 | 20.879084000 | 10.504629900 | H | 31.468184000 | 23.992511000 | 2.672213000 |
| O | 31.095427000 | 18.007968000 | 10.409452000 | C | 31.605304000 | 20.824051000 | 6.099572000 | H | 35.140966000 | 23.623862000 | 4.919032000 |
| O | 29.747839000 | 14.778458000 | 8.366118000 | C | 32.203669000 | 21.926550000 | 5.289640000 | H | 34.093600000 | 21.849191000 | 6.318892000 |
| O | 28.020119000 | 20.744881000 | 7.026752000 | C | 31.468258000 | 22.541449000 | 4.263246000 | H | 31.975892000 | 13.775555000 | 8.648791000 |
| O | 29.228184000 | 18.397705000 | 12.306422000 | C | 32.051064000 | 23.530698000 | 3.473034000 | H | 28.307257000 | 10.456934000 | 2.710933000 |
| O | 27.951941000 | 20.640347000 | 9.634789000 | C | 33.385413000 | 23.932740000 | 3.684997000 | H | 24.586330000 | 11.097245000 | 4.811612000 |
| O | 26.951767000 | 18.332039000 | 11.003817000 | C | 34.107717000 | 23.321930000 | 4.729996000 | H | 25.668648000 | 12.906206000 | 6.148034000 |
| O | 26.094880000 | 16.691365000 | 9.725560000 | C | 33.528855000 | 22.330809000 | 5.518577000 | H | 32.683386000 | 13.729948000 | 6.588858000 |
| O | 29.344285000 | 14.164129000 | 10.965013000 | C | 28.201510000 | 13.798820000 | 5.970239000 | H | 32.854301000 | 14.034253000 | 9.942705000 |
| O | 27.458710000 | 14.317725000 | 9.740867000 | C | 27.574685000 | 12.706294000 | 5.169935000 | H | 31.553446000 | 18.281247000 | 5.465835000 |
| O | 31.568035000 | 16.540692000 | 8.363011000 | C | 28.317298000 | 12.007751000 | 4.205522000 | H | 29.648904000 | 13.819527000 | 8.330336000 |
| O | 30.387080000 | 20.574587000 | 10.787417000 | C | 27.719334000 | 10.995864000 | 3.458173000 | C | 26.061244000 | 17.496966000 | 5.997055000 |
| O | 32.329840000 | 20.314825000 | 9.678488000 | C | 26.365105000 | 10.659923000 | 3.653228000 | C | 24.806431000 | 17.506204000 | 5.189869000 |
| O | 28.976568000 | 16.774866000 | 9.777140000 | C | 25.634743000 | 11.351841000 | 4.637582000 | C | 24.586330000 | 18.494699000 | 4.217602000 |
| O | 30.390818000 | 20.522194000 | 5.881926000 | C | 26.230610000 | 12.363563000 | 3.586024000 | C | 23.418386000 | 18.485811000 | 3.457289000 |
| O | 32.352275000 | 20.246098000 | 6.936917000 | O | 26.938033000 | 18.378821000 | 5.746171000 | C | 22.440162000 | 17.489271000 | 3.647493000 |
| O | 31.138031000 | 17.932227000 | 6.261588000 | O | 26.154954000 | 16.632506000 | 6.915878000 | C | 22.661695000 | 16.513839000 | 4.638696000 |
| O | 27.688199000 | 18.372919000 | 8.300655000 | O | 30.104424000 | 19.0711143000 | 8.303234000 | C | 23.829526000 | 16.519249000 | 5.398180000 |
| O | 30.580608000 | 16.174568000 | 12.229454000 | O | 33.027135000 | 15.989001000 | 5.918022000 | C | 33.868442000 | 16.903604000 | 6.130150000 |
| O | 31.940414000 | 13.874637000 | 9.701100000 | O | 33.740015000 | 17.833754000 | 6.978805000 | C | 35.111037000 | 16.894783000 | 5.299741000 |
| O | 31.875129000 | 13.841048000 | 7.100532000 | O | 29.015498000 | 16.693040000 | 6.820299000 | C | 35.273596000 | 15.953348000 | 4.269732000 |
| O | 29.376040000 | 14.160143000 | 5.686583000 | O | 32.998419000 | 16.055491000 | 10.761092000 | C | 36.411218000 | 15.974768000 | 3.465053000 |
| O | 27.509375000 | 14.291835000 | 6.914977000 | O | 33.721785000 | 17.930893000 | 9.747207000 | C | 37.420944000 | 16.937188000 | 3.666013000 |
| H | 38.310546000 | 16.957068000 | 3.034098000 | O | 31.095066000 | 10.0806842000 | 10.408087000 | C | 37.253524000 | 17.869750000 | 4.709717000 |
| H | 33.844162000 | 24.702512000 | 3.062022000 | O | 29.751518000 | 14.774186000 | 8.368704000 | C | 36.114994000 | 17.853109000 | 5.512680000 |
| H | 25.895898000 | 9.871775000 | 3.061155000 | O | 28.027748000 | 20.741966000 | 7.019303000 | C | 33.836774000 | 16.959039000 | 10.535665000 |
| H | 21.528520000 | 17.4749767000 | 3.047224000 | O | 29.226760000 | 18.400096000 | 12.303484000 | C | 26.050678000 | 17.523767000 | 10.664674000 |
| H | 34.800580000 | 16.893430000 | 11.088074000 | O | 27.952744000 | 20.640932000 | 9.630057000 | C | 28.183338000 | 13.821294000 | 10.638023000 |
| H | 27.738892000 | 12.976846000 | 11.209662000 | O | 26.951000000 | 18.333970000 | 11.001430000 | C | 31.573342000 | 20.879084000 | 10.504629000 |
| H | 25.119970000 | 17.545961000 | 11.261309000 | O | 26.093843000 | 16.690538000 | 9.726704000 | C | 31.605304000 | 20.824051000 | 6.099572000 |
| H | 23.545641000 | 19.264082000 | 4.065014000 | O | 27.457487000 | 14.318784000 | 9.743271000 | C | 31.468258000 | 22.541449000 | 4.262346000 |
| H | 29.363320000 | 12.279775000 | 4.049634000 | O | 31.573181000 | 16.653928000 | 8.364257000 | C | 32.051064000 | 23.530698000 | 3.473034000 |
| H | 34.489259000 | 15.211765000 | 4.104381000 | O | 30.386085000 | 20.576137000 | 10.784210000 | C | 33.885413000 | 23.932740000 | 3.684997000 |
| H | 30.440481000 | 22.219722000 | 4.084324000 | O | 32.331070000 | 20.314171000 | 9.679968000 | C | 34.107717000 | 23.321930000 | 4.729996000 |
| Zr | 29.052816000 | 18.749227000 | 6.519674000 | O | 28.975382000 | 16.773468000 | 9.780094000 | C | 33.528855000 | 22.330809000 | 5.518577000 |
| Zr | 29.003720000 | 18.890688000 | 10.074439000 | O | 30.394417000 | 20.513402000 | 5.872051000 | C | 28.201510000 | 13.798820000 | 5.970239000 |
| Zr | 30.752692000 | 15.779326000 | 10.197857000 | O | 32.350085000 | 20.250519000 | 6.941455000 | C | 27.574685000 | 12.706294000 | 5.169935000 |
| Zr | 30.906451000 | 15.616381000 | 6.587370000 | O | 31.136524000 | 17.926248000 | 6.252617000 | C | 28.317298000 | 12.007751000 | 4.205522000 |
| Zr | 27.736049000 | 16.003469000 | 8.307461000 | O | 27.689067000 | 18.372849000 | 8.299488000 | C | 27.719334000 | 10.995864000 | 3.458173000 |
| Zr | 32.103077000 | 18.518340000 | 8.331711000 | O | 30.579792000 | 16.174911000 | 12.230000000 | C | 26.365105000 | 10.659923000 | 3.653228000 |
| H | 28.494367000 | 18.733674000 | 3.893929000 | O | 31.943844000 | 13.876866000 | 9.701829000 | C | 25.634743000 | 11.351841000 | 4.637582000 |
| H | 31.328853000 | 16.538441000 | 4.060853000 | O | 31.865378000 | 13.830283000 | 7.097227000 | C | 26.230610000 | 12.363563000 | 5.386024000 |
| O | 30.734952000 | 15.884212000 | 4.439109000 | O | 29.361903000 | 14.189372000 | 5.658671000 | O | 26.928688000 | 18.387218000 | 5.765213000 |
| O | 29.240510000 | 18.349717000 | 4.370747000 | O | 27.522562000 | 14.271360000 | 6.932625000 | O | 26.164029000 | 16.607525000 | 6.893562000 |
| Cu | 28.866260000 | 16.374734000 | 4.263904000 | H | 38.310580000 | 16.957022000 | 3.034125000 | O | 30.102578000 | 19.076327000 | 8.311579000 |
| O | 27.210404000 | 15.913291000 | 3.906164000 | H | 33.844167000 | 24.702594000 | 3.062099000 | O | 32.999646000 | 16.020993000 | 5.875459000 |
| H | 25.895898000 | 9.871775000 | 17.481458000 | H | 25.896213000 | 9.871023000 | 3.061813000 | O | 33.755081000 | 17.808877000 | 7.003953000 |
| H | 21.527529000 | 17.481458000 | 3.048992000 | H | 21.527529000 | 17.481458000 | 3.048992000 | O | 29.008362000 | 16.706970000 | 6.836431000 |
| H | 34.801098000 | 16.893720000 | 11.087432000 | H | 34.801098000 | 16.893720000 | 11.087432000 | O | 33.003787000 | 16.046166000 | 10.745800000 |
| H | 27.739585000 | 12.976096000 | 11.209400000 | H | 27.739585000 | 12.976096000 | 11.209400000 | O | 33.719645000 | 17.935736000 | 9.754194000 |
| H | 25.113141000 | 17.545363000 | 11.263429000 | H | 25.113141000 | 17.545363000 | 11.263429000 | O | 31.099202000 | 18.003956000 | 10.405827000 |
| H | 32.000001000 | 17.252210000 | 11.046369000 | H | 32.000001000 | 17.252210000 | 11.046369000 | O | 29.747207000 | 14.779337000 | 8.358357000 |
| H | 25.345271000 | 19.265493000 | 4.066764000 | H | 25.345271000 | 19.265493000 | 4.066764000 | O | 28.018032000 | 20.746442000 | 7.034220000 |
| H | 29.034980000 | 18.907830000 | 18.890783000 | H | 29.034980000 | 18.907830000 | 10.069123000 | O | 29.233777000 | 18.389469000 | 12.306653000 |
| H | 27.933451000 | 20.810146000 | 8.030553000 | H | 30.751635000 | 15.779487000 | 10.180365000 | O | 27.454849000 | 14.317796000 | 9.744659000 |
| H | 30.222135000 | 15.443278000 | 12.745634000 | H | 30.909427000 | 15.616187000 | 6.519594000 | O | 31.561782000 | 16.540162000 | 8.351576000 |
| H | 28.279564000 | 21.425980000 | 10.084282000 | H | 27.735094000 | 16.002636000 | 8.308123000 | O | 30.389555000 | 20.571492000 | 10.792727000 |
| H | 28.654117000 | 21.434821000 | 6.769093000 | H | 32.101388000 | 18.518838000 | 8.330798000 | O | 32.32815 | | |

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