

Supplementary Information

Reaction Mechanisms for the Electrochemical Reduction of CO₂ to CO and Formate on the Cu(100) Surface at 298K from Quantum Mechanics Free Energy Calculations with Explicit Water

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S1. Simulation Model

Here we simulate the water/Cu(100) interface using 48 explicit water molecules (5 layers, 1.21 nm thick) on a 4×4 Cu (100) surface slab (3 layers) with an area of 1.02 nm². To equilibrate the waters interacting at the interface, we carried out 2 ns of reactive molecular dynamics (RMD) simulations using the ReaxFF reactive force field for Cu and H₂O.¹ Starting from this well-equilibrated interface, we carried out 10 ps of ab initio AIMD simulation at 298 K. After that, we used metadynamics and thermodynamic integration to calculate free energy barriers for various reaction steps (the results were averaged over three independent calculations). The simulation box is 40 Å along the z axis with a vacuum of 24 Å. The lateral dimensions of the slab were fixed using the 3.61 Å lattice constant.

Electronic structure calculations were performed within the DFT framework, as implemented in the Vienna ab initio simulation program (VASP),²⁻⁵ a plane-wave pseudopotential package. The exchange and correlation energies were calculated using the Perdew, Burke, and Ernzerhof (PBE) functional within the generalized gradient approximation (GGA).^{6,7}

We used a plane-wave cutoff energy of 400 eV and the First order Methfessel-Paxton scheme with a smearing width of 0.2 eV. Dipole corrections were applied along the z axis. The PBE-D3 method was employed to correct van der Waals interaction of water-water and water-Cu.⁸ The Energy minimization criterion was that all forces on free atoms be < 0.01 eV/Å. The charges on various species were derived using a Bader analysis^{9,10}.

We used a 1.2 fs time step in the Molecular Dynamics (MD) simulations with the hydrogen mass set to 2 amu. These MD simulations used only the gamma point of the Brillouin zone with no consideration of symmetry. The velocities were rescaled every 20 MD steps to readjust the target temperature to equilibrium. We employed a Nose Hoover thermostat for the free energy calculations with a temperature damping parameter of 100 fs.

S2. Metadynamics

The metadynamics Hamiltonian $\tilde{H}(p, q, t)$ is written as¹¹:

$$\tilde{H}(p, q, t) = H(p, q) + \tilde{V}(t, \xi), \quad (\text{S1})$$

where $H(p, q)$ is the Hamiltonian for the original (unbiased) system, ξ is the collective variable (CV), and $\tilde{V}(t, \xi)$ is the time-dependent bias potential. The bias term is defined as a sum of Gaussian hills with **height h** and **width ω** :

$$\tilde{V}(t, \xi) = h \sum_{i=1}^{\lfloor t/t_G \rfloor} \exp\left[-\frac{|\xi^{(t)} - \xi^{(i \cdot t_G)}|^2}{2\omega}\right], \quad (\text{S2})$$

The biased potential is related to the free energy via:

$$A(\xi) = \lim_{t \rightarrow \infty} \tilde{V}(t, \xi) + \text{const} \quad (\text{S3})$$

In principle, for smaller perturbations, better accuracy should be achieved, but this also requires longer simulation times. Although many papers has been published discussing about how to choose the parameters,^{11,12} there is still no general rule. One must consider each specified case. In this work, we used an ideal double well model with a transition barrier of 0.9 eV to derive the optimal parameters for the best balance of accuracy and efficiency, as shown in the following:

- $h = 0.08$ eV
- $\omega = 0.18$ Å
- $t_G = 20$ time step

We carried out metadynamics simulations until the first barrier crossing.

S3. Constrained Molecular dynamics¹³

The correct (*unbiased*) average for a quantity $\alpha(\xi)$ of constrained (*biased*) molecular dynamics can be obtained from (S4)

$$\alpha(\xi) = \frac{\left\langle |\mathbf{Z}|^{-\frac{1}{2}} \alpha(\xi^*) \right\rangle_{\xi^*}}{\left\langle |\mathbf{Z}|^{-\frac{1}{2}} \right\rangle_{\xi^*}} \quad (\text{S4})$$

where \mathbf{Z} is a mass metric tensor defined as:

$$\mathbf{Z}_{\alpha,\beta} = \sum_{i=1}^{3N} m_i^{-1} \nabla_i \xi_\alpha \cdot \nabla_i \xi_\beta \quad (\text{S5})$$

the free energy gradient can be computed using the equation:¹³

$$\left(\frac{\partial A}{\partial \xi_k} \right)_{\xi^*} = \frac{1}{\left\langle |\mathbf{Z}|^{-\frac{1}{2}} \right\rangle_{\xi^*}} \left\langle |\mathbf{Z}|^{-\frac{1}{2}} \left[\lambda_k + \frac{k_B T}{2|\mathbf{Z}|} \sum_{j=1}^r (\mathbf{Z}^{-1})_{kj} \sum_{i=1}^{3N} m_i^{-1} \nabla_i \xi_j \cdot \nabla_i |\mathbf{Z}| \right] \right\rangle_{\xi^*} \quad (\text{S6})$$

The free-energy difference between states (1) and (2) can be computed by integrating the free-energy gradients over a connecting path:

$$\Delta A_{1 \rightarrow 2} = \int_{\xi^{(1)}}^{\xi^{(2)}} \left(\frac{\partial A}{\partial \xi} \right)_{\xi} \cdot d\xi \quad (\text{S7})$$

We first employed slow-growth to generate the reaction path. We applied an increment of 0.0008 Å/step (or 0.00067 Å/fs) to collective variables to drive the chemical reactions. We found that simulation times of 2.4 to 9.6 ps were necessary to complete the reaction, depending on the length of reaction pathways. From the reactive trajectories, we selected eleven (11) windows for thermodynamic integration calculations. Simulations of 2.4 ps were carried out at each window to produce the potential of mean force (PMF). Energy profiles were obtained by integrating the PMF.

S4. Collective variables and free energy barriers

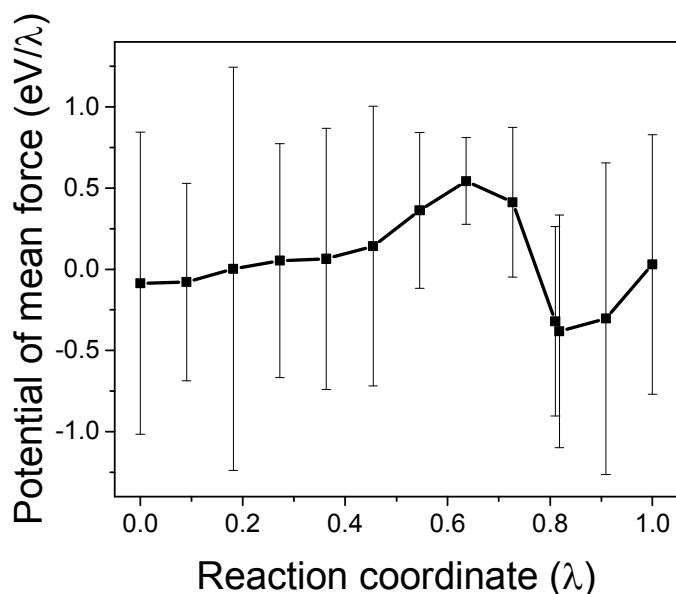


Figure S1. Potential of mean force (PMF, in eV/ λ) for formation of chemisorbed CO₂ (*CO₂^{δ-}) along the reaction coordinate (λ , the center of mass of CO₂) with error bars. The free energy barrier (ΔG^\ddagger) and free energy difference (ΔG) derived from integrating the PMFs are 0.29 eV and 0.22 eV with estimated errors of 0.34 eV and 0.36 eV according to the error propagation of error bars in each PMF point.

Due to the expensive cost of AIMD simulations, it is impractical to extend metadynamics simulation to at least several hundred picoseconds for sufficiently sampling in the phase space. In this work, we employed thermodynamic integration to explore the reaction phase space along the reactive pathways generated from metadynamics simulations, which can significantly enhance the samplings. The free energy differences and free energy barriers can be obtained by integrating the potential of mean force (PMF) generated from independent calculations at each selected window.

Figure S1 shows the PMFs for formation of chemisorbed CO₂ (*CO₂^{δ-}) along the reaction coordinate (λ , the center of mass of CO₂). The error bars associated with each PMF is from 0.2 eV/ λ to 1.5 eV/ λ , which lead to about 0.36 eV errors in the calculated free energy barriers according to the error propagation. However, these PMFs are not fully independent. Therefore, the real errors of the data should be lower than 0.36 eV, which can be obtained from independent simulations as shown in Figure S2.

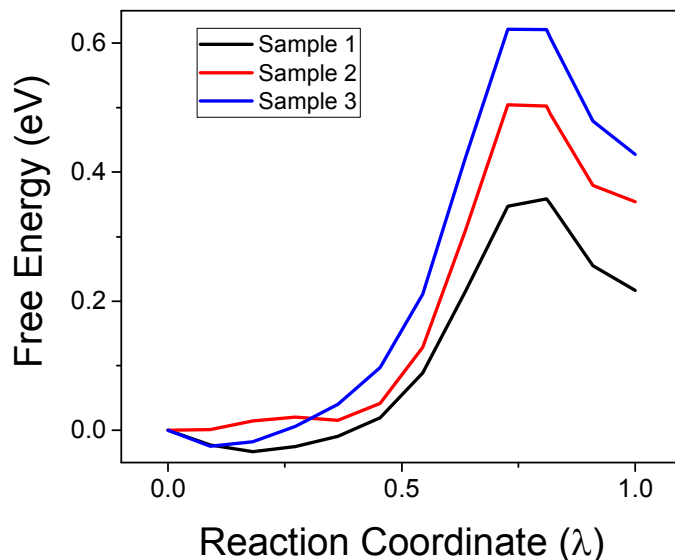


Figure S2. Free energy profiles for formation of chemisorbed CO₂ (*CO₂^{δ-}) along the reaction coordinate (λ , the center of mass of CO₂) from three independent simulations. The free energy barriers are: 0.29 eV, 0.39 eV and 0.61 eV leading to a mean of 0.43 eV, with a standard deviation of 0.17 eV.

We carried out three independent calculations by using reactive trajectories from three metadynamics simulations. The free energy barriers are 0.29 eV, 0.39 eV and 0.61 eV with a standard deviation of 0.17 eV, which is 0.19 eV lower than derived from analyzing a single PMF profile. Therefore, with consideration of the uncertainties three independent calculations from different metadynamics simulations are consistent.

The 0.17 eV error is 40% of derived free energy barrier (0.43 eV), which attributes to the following reasons:

1. The errors in calculating force are much larger than energy;
2. The small simulation size used in the simulation due to the expensive cost of AIMD calculation;
3. The limited simulation time accessed in the simulation due to the expensive cost of AIMD calculation.

Therefore, this 0.17 eV is the intrinsic nature in free energy calculations with small simulation size and limited simulation time, which cannot be fully eliminated under the current framework, but is possible to be reduced by extend the simulation to larger scale for future development of faster DFT calculations, or by employing less expensive methods (such as reactive force field).

S5. Collective variables and free energy barriers

In free energy calculations, the collective variables (CV) are the distance between hydrogen (H) and carbon (C) [R(C-H)], the distance between H and oxygen (O) [R(O-H)] or the distance between C and O [R(C-O)]. The distances are a natural choice for Langmuir-Hinshelwood (LH) model. The Eley-Rideal model is more complex, because the proton transfer procedure involves a hydrogen bond (HB) channel established by several water molecules. In our previous work with H_3O^+ (pH 0), we employed a CV defined by HB bond network. In the current work, the simulation is at pH 7. Therefore, H_2O must provide the H^+ instead of H_3O^+ . In this condition, we defined the CV using R(O-H) or R(C-H) (C (or O) for the reaction intermediates with H from the nearest water, which is from solvent (the second layer of water). The produced OH, is instead on surface, which is achieved by proton transfer. The steps following the proton transfer can be described using brute force simulation since the barrier for proton transfer is smaller (about 0.15 eV based on our previous calculation).¹⁴

The CVs for elementary reaction in CO formation and formate (HCOO^-) formation are shown in Table S1.

Table S1. Free-energy barriers (ΔG^\ddagger , in eV), free energy differences (ΔG , in eV) and collective variables (CV) for various reduction steps of *CO formation and formate (HCOO^-) formation on Cu(100) at pH 7 and 298 K. (e^- is implicitly involved in the simulations.) For every reaction we carried out three independent R μ D calculations to obtain the average value with the uncertainties in parenthesis.

| ID | Reaction Equation | ΔG^\ddagger (eV) | ΔG (eV) | CV |
|----|---|--------------------------|-----------------|---------|
| 0a | $\text{CO}_2(aq) + \delta \cdot e^- \rightarrow \text{CO}_2^{\delta-}$ | 0.43(0.17) | 0.33(0.13) | COM |
| 0b | $\text{CO}_2(aq) + \text{H}^* + e^- \rightarrow \text{HCOO}^-$ | 0.80(0.08) | 0.30(0.09) | R(C-H) |
| 1 | $\text{CO}_2^{\delta-} + \text{H}_2\text{O} + (1-\delta) \cdot e^- \rightarrow \text{cis-}^* \text{COO}_a\text{H} + ^* \text{OH}^{(1-\delta)-}$ | 0.37(0.09) | 0.27(0.10) | R(O-H) |
| 1b | $\text{CO}_2^{\delta-} + \text{H}_2\text{O} + (1-\delta) \cdot e^- \rightarrow \text{trans-}^* \text{COO}_s\text{H} + ^* \text{OH}^{(1-\delta)-}$ | 0.40(0.12) | 0.25(0.10) | R(O-H) |
| 1c | $\text{CO}_2^{\delta-} + \text{H}^* \rightarrow \text{cis-}^* \text{COO}_a\text{H} + \delta \cdot e^-$ | 1.54(0.10) | 1.14(0.13) | R(O-H) |
| 1d | $\text{CO}_2^{\delta-} + \text{H}^* + (1-\delta) \cdot e^- \rightarrow \text{HCOO}^-$ | 0.99(0.02) | 0.52(0.08) | R(C-H) |
| 1e | $\text{CO}_2^{\delta-} + \text{H}_2\text{O} + (2-\delta) \cdot e^- \rightarrow \text{HCOO}^- + \text{OH}^-$ | 1.12(0.17) | 0.91(0.11) | R(C-H) |
| 2 | $^* \text{COOH} + e^- \rightarrow ^* \text{CO} + \text{OH}^-$ | 0.30(0.09) | -0.10(0.12) | R(C-O) |
| 2b | $^* \text{COOH} + \text{H}_2\text{O} + e^- \rightarrow$ $\text{HCOOH}(aq) + \text{OH}^-$ (or $\text{HCOO}^- + \text{H}_2\text{O}$) | 1.06(0.13) | 0.81(0.14) | R(C-H) |
| 2c | $^* \text{COOH} + \text{H}^* \rightarrow \text{HCOOH}(aq)$ | 0.80(0.10) | 0.58(0.09) | R(C-H) |
| 3 | $^* \text{CO} \rightarrow \text{CO}(aq)$ | | 0.90(0.08) | COM |
| 4 | $\text{H}_2\text{O} + e^- \rightarrow \text{H}^* + \text{OH}^-$ | 0.70(0.12) | 0.57(0.07) | R(Cu-H) |

S6. Constant potential corrections

We determined the electrochemical reaction energetics at constant potential using the correction method proposed by Chan and Norskov:^{15,16}

$$\Delta E_{\Phi_1-\Phi_2} = E_{\Phi_1} - E_{\Phi_2} = \frac{\Delta q \cdot \Delta \Phi}{2} \quad (\text{S8})$$

However for plane wave calculations the atomic charges are ambiguous. Instead we use the capacitance (C) defined as:

$$C = \frac{\Delta q}{\Delta \Phi} \quad (\text{S9})$$

to replace charge (q), in S8. We calculate C from the change in the work function as the number of total electrons is varied. For the Cu(100) bare surface, the calculated C is 0.79 e/V. The reaction intermediates have very small influence on C ranging from 0.79 e/V to 0.83 eV. Therefore, we use one C value (0.79 e/V) in our calculation.

Inserting S9 to S8 leads to the ΔE in S10:

$$\Delta E_{\Phi_1-\Phi_2} = \frac{C \cdot \Delta \Phi^2}{2} \quad (\text{S10})$$

For the cases reported here, these corrections of the free energy barriers were insignificant (< 0.01 eV).

Table S2. Tabulated Changes in work function of initial state (Φ_0 , in eV), transition state (Φ_{TS} , in eV), final state (Φ_1 , in eV) and resultant extrapolated energy differences ($\Delta E_{\Phi_{TS}-\Phi_0}$ and $\Delta E_{\Phi_1-\Phi_0}$) from equation S10. After applying these corrections, all calculated free energies are under a working condition of about -0.4 V (the average of Φ_0) compared with RHE.

| | Φ_0 (eV) | Φ_{TS} (eV) | Φ_1 (eV) | $\Delta E_{\Phi_{TS}-\Phi_0}$ (eV) | $\Delta E_{\Phi_1-\Phi_0}$ (eV) |
|----|---------------|------------------|---------------|---------------------------------------|---------------------------------|
| 0a | 3.69 | 3.72 | 3.80 | 0.00 | 0.01 |
| 0b | 3.61 | 3.60 | 3.82 | 0.00 | 0.03 |
| 1 | 3.71 | 3.65 | 3.72 | 0.00 | 0.00 |
| 1b | 3.62 | 3.71 | 3.76 | 0.01 | 0.01 |
| 1c | 3.72 | 3.81 | 3.90 | 0.01 | 0.02 |
| 1d | 3.69 | 3.79 | 4.03 | 0.01 | 0.07 |
| 1e | 3.67 | 3.73 | 3.93 | 0.00 | 0.04 |
| 2 | 3.66 | 3.60 | 3.48 | 0.00 | 0.02 |
| 2b | 3.75 | 3.67 | 3.68 | 0.00 | 0.00 |
| 2c | 3.58 | 3.45 | 3.50 | 0.01 | 0.00 |

Table S3. Free-energy barriers (ΔG^\ddagger , in eV) and free energy differences (ΔG , in eV) after corrections.

| ID | Reaction Equation | ΔG^\ddagger (eV) | ΔG (eV) |
|----|---|--------------------------|-----------------|
| 0a | $\text{CO}_2(aq) + \delta \cdot e^- \rightarrow \text{CO}_2^{\delta-}$ | 0.43 | 0.32 |
| 0b | $\text{CO}_2(aq) + \text{H}^* + e^- \rightarrow \text{HCOO}^-$ | 0.80 | 0.27 |
| 1 | $\text{CO}_2^{\delta-} + \text{H}_2\text{O} + (1-\delta) \cdot e^- \rightarrow \text{cis-}^* \text{COO}_a\text{H} + ^* \text{OH}^{(1-\delta)-}$ | 0.37 | 0.27 |
| 1b | $\text{CO}_2^{\delta-} + \text{H}_2\text{O} + (1-\delta) \cdot e^- \rightarrow \text{trans-}^* \text{COO}_s\text{H} + ^* \text{OH}^{(1-\delta)-}$ | 0.39 | 0.24 |
| 1c | $\text{CO}_2^{\delta-} + \text{H}^* \rightarrow \text{cis-}^* \text{COO}_a\text{H} + \delta \cdot e^-$ | 1.53 | 1.12 |
| 1d | $\text{CO}_2^{\delta-} + \text{H}^* + (1-\delta) \cdot e^- \rightarrow \text{HCOO}^-$ | 0.98 | 0.45 |
| 1e | $\text{CO}_2^{\delta-} + \text{H}_2\text{O} + (2-\delta) \cdot e^- \rightarrow \text{HCOO}^- + \text{OH}^-$ | 1.12 | 0.87 |
| 2 | $^* \text{COOH} + e^- \rightarrow ^* \text{CO} + \text{OH}^-$ | 0.30 | -0.12 |
| 2b | $^* \text{COOH} + \text{H}_2\text{O} + e^- \rightarrow \text{HCOOH}(aq) + \text{OH}^-$ (or $\text{HCOO}^- + \text{H}_2\text{O}$) | 1.06 | 0.81 |
| 2c | $^* \text{COOH} + \text{H}^* \rightarrow \text{HCOOH}(aq)$ | 0.79 | 0.58 |

Structure 1: CO₂ + 48 Cu + 1 H* + 48 H₂O

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CO2

| | | | |
|----|------------------|------------------|-----------------|
| Cu | 0.000000000000 | 0.000000000000 | 32.000000400000 |
| Cu | 2.5569545991297 | 0.000000000000 | 32.000000400000 |
| Cu | 5.1140115705318 | 0.000000000000 | 32.000000400000 |
| Cu | 7.6709658628516 | 0.000000000000 | 32.000000400000 |
| Cu | 0.000000000000 | 2.5560455953674 | 32.000000400000 |
| Cu | 2.5569545991297 | 2.5560455953674 | 32.000000400000 |
| Cu | 5.1140115705318 | 2.5560455953674 | 32.000000400000 |
| Cu | 7.6709658628516 | 2.5560455953674 | 32.000000400000 |
| Cu | 0.000000000000 | 5.1119888384809 | 32.000000400000 |
| Cu | 2.5569545991297 | 5.1119888384809 | 32.000000400000 |
| Cu | 5.1140115705318 | 5.1119888384809 | 32.000000400000 |
| Cu | 7.6709658628516 | 5.1119888384809 | 32.000000400000 |
| Cu | 0.000000000000 | 7.6689550928826 | 32.000000400000 |
| Cu | 2.5569545991297 | 7.6689550928826 | 32.000000400000 |
| Cu | 5.1140115705318 | 7.6689550928826 | 32.000000400000 |
| Cu | 7.6709658628516 | 7.6689550928826 | 32.000000400000 |
| Cu | 1.2779659495530 | 1.2780227976837 | 30.193200000000 |
| Cu | 3.8350227164151 | 1.2780227976837 | 30.193200000000 |
| Cu | 6.3919775200849 | 1.2780227976837 | 30.193200000000 |
| Cu | 8.9490342869470 | 1.2780227976837 | 30.193200000000 |
| Cu | 1.2779659495530 | 3.8339661430472 | 30.193200000000 |
| Cu | 3.8350227164151 | 3.8339661430472 | 30.193200000000 |
| Cu | 6.3919775200849 | 3.8339661430472 | 30.193200000000 |
| Cu | 8.9490342869470 | 3.8339661430472 | 30.193200000000 |
| Cu | 1.2779659495530 | 6.3910342384528 | 30.193200000000 |
| Cu | 3.8350227164151 | 6.3910342384528 | 30.193200000000 |
| Cu | 6.3919775200849 | 6.3910342384528 | 30.193200000000 |
| Cu | 8.9490342869470 | 6.3910342384528 | 30.193200000000 |
| Cu | 1.2779659495530 | 8.9469776860663 | 30.193200000000 |
| Cu | 3.8350227164151 | 8.9469776860663 | 30.193200000000 |
| Cu | 6.3919775200849 | 8.9469776860663 | 30.193200000000 |
| Cu | 8.9490342869470 | 8.9469776860663 | 30.193200000000 |
| Cu | 10.1977896738845 | 10.1321723065365 | 28.606055600000 |
| Cu | 2.4689326489542 | 0.0701875723687 | 28.318143600000 |
| Cu | 4.9785253963687 | 10.1854284030235 | 28.324613200000 |
| Cu | 7.5903000916762 | 10.2188103707690 | 28.583639200000 |
| Cu | 0.0140434099148 | 2.5348330140759 | 28.419744000000 |
| Cu | 2.6790661069236 | 2.5241156799260 | 28.370198000000 |

| | | | |
|----|-------------------|------------------|-------------------|
| Cu | 5. 1474598952353 | 2. 6207881505329 | 28. 5279936000000 |
| Cu | 7. 7453839595825 | 2. 5917957754512 | 28. 5137060000000 |
| Cu | 10. 2060559536357 | 5. 1861293959971 | 28. 4429268000000 |
| Cu | 2. 5778961207040 | 5. 2100330951390 | 28. 4055848000000 |
| Cu | 5. 1871232702525 | 5. 2080374818145 | 28. 3527280000000 |
| Cu | 7. 6242006543301 | 5. 0712356679604 | 28. 2475444000000 |
| Cu | 10. 1450581356951 | 7. 5931500075543 | 28. 4651704000000 |
| Cu | 2. 5744831661851 | 7. 7972442871692 | 28. 4419352000000 |
| Cu | 4. 9570395938418 | 7. 7825586303712 | 28. 3647072000000 |
| Cu | 7. 5914910258537 | 7. 5189128237845 | 28. 4258908000000 |
| 0 | 3. 9350924819493 | 7. 8173180079181 | 24. 3627208000000 |
| 0 | 2. 1766541864953 | 2. 8628942780661 | 14. 4646212000000 |
| 0 | 5. 9070406795007 | 8. 3569760433031 | 22. 1751320000000 |
| 0 | 6. 5691831053928 | 8. 8903117564521 | 25. 3243420000000 |
| 0 | 8. 0523849047719 | 1. 1828918481343 | 25. 5809584000000 |
| 0 | 4. 2667913258998 | 4. 1799748389570 | 21. 6368832000000 |
| 0 | 7. 4467110652256 | 8. 4844405913088 | 14. 3619272000000 |
| 0 | 8. 7351952799819 | 1. 7380977123493 | 14. 9633164000000 |
| 0 | 2. 8908503050011 | 0. 2882776280058 | 21. 3552584000000 |
| 0 | 0. 7703325318840 | 1. 2117999692129 | 18. 5024892000000 |
| 0 | 5. 8861129643767 | 7. 7981279317021 | 19. 6761340000000 |
| 0 | 4. 1788518053462 | 4. 0254041216899 | 17. 3104168000000 |
| 0 | 7. 5096706263516 | 1. 7288298742535 | 22. 9424164000000 |
| 0 | 0. 6910812571113 | 1. 4004985680033 | 22. 4747288000000 |
| 0 | 6. 3374814152746 | 3. 2251638943325 | 25. 6451088000000 |
| 0 | 8. 8611399697344 | 9. 9182918835565 | 18. 5314012000000 |
| 0 | 1. 2908065619700 | 5. 2038451294081 | 22. 4747656000000 |
| 0 | 1. 8694301904307 | 8. 4640898752995 | 15. 7093408000000 |
| 0 | 7. 8061889985686 | 5. 6369232823165 | 15. 1829168000000 |
| 0 | 4. 8094945591599 | 2. 4529140942695 | 15. 2819304000000 |
| 0 | 8. 7517600545350 | 7. 2591218423416 | 24. 5488128000000 |
| 0 | 2. 0421252595543 | 5. 3822515495646 | 25. 3481004000000 |
| 0 | 1. 9575502175385 | 8. 1025058453086 | 21. 8517068000000 |
| 0 | 3. 5350928214592 | 6. 3834657954204 | 20. 3586820000000 |
| 0 | 8. 9003251302206 | 6. 1384618005292 | 21. 9444848000000 |
| 0 | 7. 3280429884114 | 4. 0312538444081 | 21. 5982400000000 |
| 0 | 7. 6797893095756 | 3. 2660837323593 | 19. 1034464000000 |
| 0 | 0. 2630745473936 | 1. 3447000251714 | 12. 9529560000000 |
| 0 | 3. 8089047986712 | 3. 6104763669587 | 24. 2582100000000 |
| 0 | 6. 6047848272660 | 1. 0482041553590 | 18. 3001112000000 |
| 0 | 6. 6059064223820 | 5. 2540877137827 | 17. 4473888000000 |

| | | | |
|---|-------------------|------------------|-------------------|
| O | 9. 3552140214099 | 8. 1885262172681 | 16. 5919212000000 |
| O | 4. 3051845074877 | 0. 0876866380216 | 19. 1336420000000 |
| O | 0. 6786733490744 | 8. 4903783512804 | 25. 5225092000000 |
| O | 10. 0570598098901 | 2. 9535343051979 | 20. 3492092000000 |
| O | 9. 6919036414759 | 7. 4955420516625 | 19. 6672676000000 |
| O | 2. 2873989971462 | 6. 2908299504641 | 17. 7702100000000 |
| O | 6. 8285786939913 | 3. 4502358869801 | 13. 6719908000000 |
| O | 3. 0616428452707 | 0. 6016051776962 | 16. 7210968000000 |
| O | 8. 8744973524733 | 9. 9026746269739 | 21. 8046328000000 |
| O | 1. 1933675899767 | 0. 8722534735442 | 25. 0350760000000 |
| O | 2. 9245738382809 | 3. 0743076129540 | 19. 5178624000000 |
| O | 8. 7536545040588 | 4. 6887157451884 | 25. 0187048000000 |
| O | 0. 2051808285648 | 2. 8023501080571 | 16. 5011428000000 |
| O | 6. 7510521005385 | 0. 5747725271951 | 15. 8901912000000 |
| O | 3. 8201962250923 | 1. 1059391087632 | 25. 1965180000000 |
| O | 10. 2015524940815 | 5. 1832915493913 | 17. 5489208000000 |
| O | 0. 5046103163991 | 3. 4964970607061 | 25. 6873500000000 |
| O | 5. 2071362824753 | 0. 7282125639200 | 22. 9528364000000 |
| O | 5. 7143765742553 | 6. 3211633343458 | 24. 4741620000000 |
| H | 1. 6308602514937 | 2. 8828902888121 | 15. 2820500000000 |
| H | 1. 6279291932260 | 2. 3758126833928 | 13. 8489960000000 |
| H | 5. 8947127466056 | 8. 2136630514560 | 21. 1867756000000 |
| H | 6. 7989063823151 | 8. 0504446423662 | 22. 3686900000000 |
| H | 7. 0432787121062 | 9. 7628188100058 | 25. 4083560000000 |
| H | 6. 2317142901788 | 8. 6076131954045 | 26. 2249568000000 |
| H | 0. 0402332234704 | 4. 1974129636076 | 17. 2739528000000 |
| H | 9. 6174652952845 | 5. 5617064412601 | 16. 8480844000000 |
| H | 7. 2731477237820 | 1. 8672255611671 | 25. 6193548000000 |
| H | 8. 5868353579211 | 1. 2660932897386 | 26. 4413544000000 |
| H | 3. 7544430565817 | 4. 9254981240229 | 21. 2778532000000 |
| H | 5. 2564329803653 | 4. 3550549642393 | 21. 5345068000000 |
| H | 7. 7582046293490 | 9. 0466325847845 | 13. 5968080000000 |
| H | 8. 2910313416706 | 2. 4163795544064 | 14. 4473540000000 |
| H | 3. 7307773689545 | 0. 6142078996664 | 21. 8929412000000 |
| H | 2. 0012825068698 | 0. 7927260790770 | 21. 6472216000000 |
| H | 0. 5662545830247 | 1. 8015012014649 | 19. 3478204000000 |
| H | 10. 1756280711820 | 0. 6116344715704 | 18. 4875064000000 |
| H | 5. 0830476909958 | 7. 2391757295974 | 19. 9154180000000 |
| H | 5. 3259617528232 | 8. 5574538425330 | 19. 1611056000000 |
| H | 3. 8844142185973 | 3. 7356412101287 | 18. 2297036000000 |
| H | 4. 9963203767802 | 4. 6904194347520 | 17. 3967660000000 |

| | | | |
|---|-------------------|-------------------|-------------------|
| H | 6. 5660290985198 | 1. 3539785995176 | 23. 0123012000000 |
| H | 8. 0464958912257 | 1. 5419455995308 | 23. 7547320000000 |
| H | 10. 1818864839767 | 0. 7706022457516 | 22. 3008408000000 |
| H | 0. 3048071513687 | 2. 1088052034306 | 21. 9149908000000 |
| H | 6. 1354685023031 | 3. 6059224585388 | 26. 5393356000000 |
| H | 5. 5487575665954 | 3. 4551010444116 | 25. 1647276000000 |
| H | 0. 2932883787323 | 5. 3592537854565 | 22. 2537716000000 |
| H | 1. 3756321654916 | 4. 4169195907975 | 23. 0872840000000 |
| H | 2. 2453100844829 | 9. 3743779985128 | 16. 0425872000000 |
| H | 2. 2932084446306 | 7. 8003601515354 | 16. 2952708000000 |
| H | 7. 5092134794410 | 6. 5198432717587 | 14. 7608884000000 |
| H | 3. 9877826007877 | 2. 4334088835417 | 14. 6726788000000 |
| H | 4. 6205512411405 | 3. 1551845029715 | 16. 0567640000000 |
| H | 9. 5742307540547 | 7. 7655644752372 | 24. 8683980000000 |
| H | 7. 9862410648523 | 7. 7532516320278 | 25. 0246976000000 |
| H | 2. 3359409424188 | 5. 7564501625261 | 26. 2121200000000 |
| H | 1. 4098105957420 | 4. 5515939910723 | 25. 5363324000000 |
| H | 2. 3034857617082 | 9. 0304076564291 | 21. 6833724000000 |
| H | 3. 0734111567128 | 6. 9795733994115 | 21. 0431328000000 |
| H | 3. 0143126972562 | 6. 4385982817274 | 19. 5592592000000 |
| H | 9. 0835384645474 | 6. 8769636800830 | 22. 5923696000000 |
| H | 9. 1074577817805 | 6. 3976879529510 | 21. 0355056000000 |
| H | 7. 5492597533471 | 3. 2822573312127 | 22. 2327216000000 |
| H | 7. 8044227956278 | 4. 8481120491355 | 21. 8488508000000 |
| H | 7. 6150011608074 | 4. 1009419255082 | 18. 6351932000000 |
| H | 7. 4829187368629 | 3. 6272151015833 | 20. 0513644000000 |
| H | 0. 8670335235402 | 0. 5456502946085 | 13. 0012840000000 |
| H | 9. 8615253947584 | 1. 2944506922966 | 13. 6687060000000 |
| H | 4. 1031119711047 | 4. 0018096265596 | 23. 4022916000000 |
| H | 3. 2625414242965 | 4. 3747804214753 | 24. 6685488000000 |
| H | 5. 8190621940762 | 0. 8063227733343 | 18. 8540836000000 |
| H | 6. 8542854863258 | 1. 9749001321845 | 18. 5573500000000 |
| H | 7. 0936627446614 | 5. 3474487157660 | 16. 6044452000000 |
| H | 6. 3772023683032 | 6. 1427957691909 | 17. 8740356000000 |
| H | 0. 0308844157442 | 8. 3755516992461 | 16. 3039480000000 |
| H | 3. 7234290647445 | 10. 1943825381076 | 18. 3306752000000 |
| H | 3. 7148191577854 | 10. 1499660567004 | 19. 8677596000000 |
| H | 4. 7936587651836 | 0. 7234296154915 | 23. 8685788000000 |
| H | 5. 4513002882716 | 10. 0045561217751 | 22. 9175048000000 |
| H | 0. 5717910718727 | 9. 5047277348763 | 25. 3940620000000 |
| H | 0. 8985858646699 | 8. 3580612225935 | 26. 5273272000000 |

| | | | |
|---|------------------|------------------|-------------------|
| H | 9. 2227424601065 | 3. 2087192307190 | 19. 9216948000000 |
| H | 0. 3671451154203 | 3. 7831293839005 | 20. 3011372000000 |
| H | 9. 7630308940707 | 3. 7624091363774 | 25. 3698272000000 |
| H | 0. 8869426294406 | 2. 7263539174717 | 25. 2287256000000 |
| H | 9. 3772204805188 | 8. 2701189595624 | 19. 1620684000000 |
| H | 9. 8264474998372 | 6. 7517206156602 | 19. 0625208000000 |
| H | 2. 9047482869725 | 5. 5125849259274 | 17. 5172896000000 |
| H | 1. 3983260835564 | 5. 9957388934541 | 17. 4615496000000 |
| H | 6. 0114629540654 | 3. 2801613083845 | 14. 1810832000000 |
| H | 6. 8016714563691 | 2. 9813781059867 | 12. 8284648000000 |
| H | 2. 4842293777480 | 1. 1688000593585 | 17. 2526672000000 |
| H | 3. 3791532604431 | 1. 1840771301785 | 16. 0549920000000 |
| H | 8. 9627709891246 | 9. 6308558753322 | 20. 8650916000000 |
| H | 8. 2253450577416 | 0. 4243000923309 | 21. 7900128000000 |
| H | 2. 2073957310462 | 0. 8331548103354 | 25. 1000440000000 |
| H | 0. 9784607819170 | 1. 0903432224313 | 24. 0424248000000 |
| H | 2. 6523336487354 | 2. 1232877917210 | 19. 5937292000000 |
| H | 3. 5058280557425 | 3. 1856113433568 | 20. 2934912000000 |
| H | 8. 7892445671518 | 5. 7037039868081 | 24. 9101132000000 |
| H | 7. 7983321056369 | 4. 3988209311223 | 25. 2306564000000 |
| H | 9. 8869919548573 | 2. 4068469910507 | 15. 7440528000000 |
| H | 0. 3664046806031 | 2. 0639077380055 | 17. 1809084000000 |
| H | 6. 5159254903112 | 0. 8173116834943 | 16. 8459124000000 |
| H | 6. 0782336068295 | 1. 1474833875632 | 15. 4290472000000 |
| H | 3. 7869066234324 | 2. 0804107863712 | 24. 9835104000000 |
| H | 3. 9461289492545 | 0. 8719584822832 | 26. 1298880000000 |
| H | 3. 6078403377015 | 9. 0054727659988 | 27. 8660184000000 |
| H | 8. 9678135138612 | 9. 2925953779615 | 17. 7344252000000 |
| H | 7. 9115751679057 | 1. 2207133065454 | 15. 3758992000000 |
| H | 7. 9658750165813 | 0. 2095990108202 | 18. 4971344000000 |
| H | 8. 7858840771441 | 8. 0500781783525 | 15. 7616380000000 |
| H | 7. 0863251788017 | 9. 0998086195185 | 15. 0512992000000 |
| H | 7. 5304916738631 | 5. 0012522888493 | 14. 5151692000000 |
| H | 1. 1165327508199 | 8. 0416760910391 | 21. 3656708000000 |
| C | 4. 8573366708062 | 7. 0999759486537 | 24. 3987408000000 |

Structure 2: CO₂ (chemisorbed) + 48 Cu + 1 H* + 48 H₂O

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CO2 chemisorbed

| | | | |
|----|------------------|------------------|-------------------|
| Cu | 0. 0000000000000 | 0. 0000000000000 | 32. 0000004000000 |
|----|------------------|------------------|-------------------|

| | | | |
|----|------------------|-------------------|-------------------|
| Cu | 2. 5569545991297 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 1. 2779659495530 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 0. 0021388748295 | 10. 1306639144803 | 28. 5276752000000 |
| Cu | 2. 5147555416739 | 0. 1259131086979 | 28. 3511068000000 |
| Cu | 5. 0994601855153 | 0. 0593206464633 | 28. 3607424000000 |
| Cu | 7. 6785380360967 | 10. 1984679370101 | 28. 2190816000000 |
| Cu | 0. 0251211943009 | 2. 3595401065356 | 28. 1989440000000 |
| Cu | 2. 5463803922352 | 2. 4921888319848 | 28. 3925440000000 |
| Cu | 5. 0998061649333 | 2. 5086265425981 | 28. 3777080000000 |
| Cu | 7. 6539824971788 | 2. 4293714398911 | 28. 3536536000000 |
| Cu | 0. 1821187384915 | 5. 0276785978353 | 28. 3177540000000 |
| Cu | 2. 5328755361529 | 4. 8417669251488 | 28. 2904572000000 |

| | | | |
|----|-------------------|------------------|-------------------|
| Cu | 5. 3853450342364 | 5. 0862446392704 | 28. 3379704000000 |
| Cu | 7. 8297964945645 | 5. 0967234241614 | 28. 5677716000000 |
| Cu | 10. 2008717849458 | 7. 5202538325845 | 28. 4969568000000 |
| Cu | 2. 6132630306519 | 7. 7534973387870 | 28. 4447640000000 |
| Cu | 5. 1418950775966 | 7. 7010129230787 | 28. 3060464000000 |
| Cu | 7. 6587204618484 | 7. 6993216057656 | 28. 5939140000000 |
| 0 | 3. 3618309719825 | 6. 6848838781664 | 26. 5705976000000 |
| 0 | 0. 7064981531578 | 0. 6874561213993 | 14. 4674892000000 |
| 0 | 5. 3720825580597 | 6. 4746851710738 | 21. 4574104000000 |
| 0 | 5. 2529927197558 | 9. 8846181965502 | 24. 9205484000000 |
| 0 | 7. 6918039894534 | 9. 9189097803296 | 26. 1770076000000 |
| 0 | 3. 6552352226275 | 2. 8531035334508 | 21. 7228004000000 |
| 0 | 4. 1070795358465 | 7. 1849118570727 | 14. 7666936000000 |
| 0 | 7. 0914266110597 | 1. 4873312139931 | 14. 2385340000000 |
| 0 | 2. 6025312256837 | 8. 8548596351293 | 22. 6459696000000 |
| 0 | 9. 3139610637459 | 9. 6170025335653 | 18. 0707596000000 |
| 0 | 3. 4033974894738 | 6. 3729869082794 | 19. 3775388000000 |
| 0 | 2. 7929128690163 | 2. 2481051893780 | 17. 5710064000000 |
| 0 | 6. 2053805827298 | 1. 4215914145403 | 23. 2092124000000 |
| 0 | 8. 9242570266640 | 1. 3266085229964 | 22. 3474860000000 |
| 0 | 5. 1330285752016 | 3. 1222044799910 | 25. 5172884000000 |
| 0 | 7. 7527626379831 | 7. 6004750955776 | 18. 1311948000000 |
| 0 | 9. 4192000665496 | 4. 0939419924971 | 22. 7442164000000 |
| 0 | 1. 1020643067753 | 6. 0098998032324 | 15. 9539788000000 |
| 0 | 5. 5647012554241 | 5. 2943185912837 | 15. 9120472000000 |
| 0 | 3. 0993991915538 | 1. 3475479945277 | 15. 0572628000000 |
| 0 | 8. 7519366748291 | 7. 4497206552029 | 25. 6782524000000 |
| 0 | 0. 8185902688199 | 4. 6645122490353 | 24. 6823308000000 |
| 0 | 0. 6950108796822 | 7. 3258161455800 | 21. 6630112000000 |
| 0 | 1. 3362085113599 | 4. 7016986326728 | 21. 1139440000000 |
| 0 | 8. 1480476513641 | 6. 3848102807205 | 23. 1997164000000 |
| 0 | 6. 2236324032419 | 3. 9358296418478 | 21. 4644808000000 |
| 0 | 7. 0029857629545 | 2. 9001951817078 | 19. 3401788000000 |
| 0 | 8. 9064563191323 | 0. 5760542309929 | 12. 4080672000000 |
| 0 | 2. 7598244324511 | 2. 5335047865264 | 24. 1782992000000 |
| 0 | 5. 6006056965043 | 9. 1759738293603 | 17. 6913916000000 |
| 0 | 5. 1659626863332 | 2. 9313311258695 | 17. 5490304000000 |
| 0 | 8. 0032691225161 | 5. 8100944000276 | 16. 3697696000000 |
| 0 | 2. 8507795885645 | 8. 9328772060402 | 18. 3241080000000 |
| 0 | 1. 1644800982987 | 7. 3393505695849 | 24. 9843076000000 |
| 0 | 0. 0515732281426 | 0. 6850389313092 | 20. 0336020000000 |

| | | | |
|---|------------------|------------------|-------------------|
| O | 7. 4192459447405 | 8. 1250026866480 | 20. 6321080000000 |
| O | 1. 1713665511779 | 4. 3356919832669 | 18. 3657156000000 |
| O | 4. 7437944687805 | 3. 4113181040280 | 14. 2085916000000 |
| O | 1. 0331971189627 | 8. 6929120913370 | 16. 4172344000000 |
| O | 6. 4642208452155 | 0. 6620255229505 | 20. 4869876000000 |
| O | 9. 5734521725267 | 1. 0903418931812 | 24. 9206808000000 |
| O | 2. 9087576801452 | 0. 4755222317420 | 20. 3586244000000 |
| O | 7. 8743390691246 | 5. 0755741356223 | 26. 2756900000000 |
| O | 8. 9300161573072 | 1. 1177564484541 | 16. 2711420000000 |
| O | 5. 2157112130936 | 9. 7078084102033 | 14. 8699536000000 |
| O | 2. 1066284840959 | 0. 1460380566988 | 25. 0568008000000 |
| O | 8. 9487812709611 | 3. 4489239171811 | 17. 6052084000000 |
| O | 9. 4201643704019 | 3. 0895656652733 | 26. 4453448000000 |
| O | 5. 0212683256971 | 7. 5586150687658 | 23. 8685216000000 |
| O | 5. 3661987602837 | 5. 9165272469987 | 25. 8416856000000 |
| H | 0. 0453842566795 | 0. 9682091716244 | 15. 1685720000000 |
| H | 0. 2533799647894 | 0. 7293220787114 | 13. 5878536000000 |
| H | 4. 6498851413789 | 6. 4650060834627 | 20. 7806348000000 |
| H | 6. 1024911309605 | 7. 1230762695156 | 21. 1492776000000 |
| H | 4. 4318473371967 | 9. 9887695391861 | 25. 4878700000000 |
| H | 5. 2152213397823 | 9. 0044362577101 | 24. 3425012000000 |
| H | 8. 8142566393602 | 2. 6185117586980 | 17. 0085184000000 |
| H | 8. 6844917559394 | 4. 1996624636916 | 17. 0527948000000 |
| H | 6. 8098169552474 | 9. 8925657825967 | 25. 5681768000000 |
| H | 8. 3787798218598 | 0. 2435123718356 | 25. 6626068000000 |
| H | 3. 0452716678321 | 3. 5850262387592 | 21. 4524416000000 |
| H | 4. 5335803197793 | 3. 3045894477959 | 21. 6861632000000 |
| H | 4. 4582463951772 | 8. 1303086438460 | 14. 6472584000000 |
| H | 6. 4943471334322 | 2. 2846609972419 | 14. 0718748000000 |
| H | 3. 4522478810734 | 8. 5381906575643 | 22. 9320800000000 |
| H | 2. 3308147608202 | 9. 2813185317907 | 23. 5047764000000 |
| H | 9. 6759574981671 | 9. 9389412718270 | 19. 0028496000000 |
| H | 8. 8178512254033 | 8. 7421111121726 | 18. 0579544000000 |
| H | 2. 6378883177113 | 5. 7604522276754 | 19. 4185176000000 |
| H | 2. 9787192592531 | 7. 1875447946710 | 18. 9446976000000 |
| H | 2. 7320232527382 | 1. 4953748127932 | 18. 1673368000000 |
| H | 3. 8075930836208 | 2. 4712356589531 | 17. 4901328000000 |
| H | 5. 8350605973561 | 0. 7570673104966 | 23. 8391600000000 |
| H | 5. 8424095151861 | 2. 2469036495831 | 23. 7038560000000 |
| H | 8. 0042586870590 | 1. 0426333706512 | 22. 6001964000000 |
| H | 8. 8448717781882 | 2. 3288051868889 | 22. 4925396000000 |

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|---|-------------------|------------------|-------------------|
| H | 5. 3386054954856 | 4. 0869159857349 | 25. 2941372000000 |
| H | 4. 2652005160130 | 2. 9210633849864 | 25. 0802668000000 |
| H | 8. 8649938102335 | 4. 8934959178288 | 22. 7942496000000 |
| H | 10. 0625734925276 | 4. 2045437766237 | 22. 0021220000000 |
| H | 1. 0863541003620 | 6. 9291798940312 | 16. 2506844000000 |
| H | 1. 1873832607883 | 5. 4752463942842 | 16. 7686304000000 |
| H | 5. 0103686956551 | 6. 1108608434993 | 15. 6410212000000 |
| H | 2. 1509036225998 | 1. 2372993819143 | 14. 6705728000000 |
| H | 2. 9455291663055 | 1. 7323498306349 | 15. 9737760000000 |
| H | 9. 7522196253107 | 7. 5449176582547 | 25. 7053616000000 |
| H | 8. 3586007231531 | 8. 2775346410891 | 25. 9853744000000 |
| H | 0. 1629681691986 | 4. 4358357392533 | 23. 9435072000000 |
| H | 0. 2655832305516 | 4. 3019034695062 | 25. 4342712000000 |
| H | 1. 3885096973794 | 7. 8724534594753 | 22. 0518456000000 |
| H | 1. 2083032033921 | 5. 6858392751416 | 21. 3771032000000 |
| H | 1. 1654040055000 | 4. 5786772563328 | 20. 1021824000000 |
| H | 8. 3518983562782 | 6. 9491827555276 | 23. 9763276000000 |
| H | 8. 3895306490484 | 6. 9225116600325 | 22. 3958964000000 |
| H | 6. 9522259904106 | 3. 8509595824313 | 22. 1130176000000 |
| H | 5. 8891062028059 | 4. 9530374243004 | 21. 5101748000000 |
| H | 7. 8239102423084 | 3. 2359040302332 | 18. 8485984000000 |
| H | 6. 7114415991125 | 3. 4798592468353 | 20. 0820020000000 |
| H | 8. 6173787032074 | 0. 0312189711648 | 11. 7020376000000 |
| H | 8. 0776648221165 | 0. 7787076035540 | 12. 9943892000000 |
| H | 3. 2131405132741 | 2. 5893549656102 | 23. 2769116000000 |
| H | 2. 1985716707021 | 3. 3253152168192 | 24. 4071448000000 |
| H | 4. 6431981150042 | 8. 8900400781919 | 17. 8663604000000 |
| H | 5. 7158616369596 | 9. 9418472169354 | 18. 3516716000000 |
| H | 5. 8567241451471 | 2. 8503794910991 | 18. 2623464000000 |
| H | 5. 1489301287893 | 3. 9399627915020 | 17. 3511136000000 |
| H | 8. 6406368448753 | 6. 1470749318505 | 15. 7155848000000 |
| H | 2. 3005405901801 | 9. 0796127100150 | 17. 4701520000000 |
| H | 2. 7028680181940 | 9. 6399870051729 | 19. 0254420000000 |
| H | 5. 1383240136541 | 6. 9632689205531 | 24. 7278172000000 |
| H | 5. 1764427025556 | 7. 0965315550252 | 22. 9896388000000 |
| H | 1. 8058106809795 | 7. 2943295861552 | 25. 7163092000000 |
| H | 0. 9917239739837 | 6. 3235864549362 | 24. 8108596000000 |
| H | 9. 8033796826437 | 0. 7904579694924 | 20. 8832288000000 |
| H | 1. 0202989285345 | 0. 6969449217534 | 20. 2793568000000 |
| H | 8. 6401523918740 | 3. 7096379094085 | 26. 2555260000000 |
| H | 9. 4905030190085 | 2. 3338356825766 | 25. 7035840000000 |

| | | | |
|---|------------------|-------------------|-------------------|
| H | 6. 9190586014037 | 8. 9353765028835 | 20. 4679844000000 |
| H | 7. 6019160208148 | 7. 6872691933159 | 19. 7653364000000 |
| H | 1. 7703303535990 | 3. 6795706822867 | 17. 9582088000000 |
| H | 0. 3068126661151 | 4. 0198746459836 | 18. 0244296000000 |
| H | 4. 1225788615149 | 2. 7166330096090 | 14. 5888484000000 |
| H | 4. 1955376675821 | 3. 8606461342927 | 13. 4955316000000 |
| H | 0. 2572094650280 | 9. 0847497502067 | 16. 9246440000000 |
| H | 0. 9381273338443 | 9. 0864267525192 | 15. 4912992000000 |
| H | 6. 9448470052000 | 1. 4874581062478 | 20. 2410168000000 |
| H | 6. 2584329419166 | 0. 8140400923723 | 21. 4126732000000 |
| H | 0. 2866142383780 | 0. 7610034243934 | 25. 1352772000000 |
| H | 9. 5156867002808 | 1. 0922070355008 | 23. 9035868000000 |
| H | 2. 8634913407784 | 10. 1654063185265 | 21. 1612072000000 |
| H | 3. 2552924242588 | 1. 3362207391051 | 20. 6985796000000 |
| H | 8. 2918224001389 | 6. 0092232149572 | 26. 1359668000000 |
| H | 6. 8981195343094 | 5. 2857115949626 | 26. 0448216000000 |
| H | 8. 1746738510198 | 1. 1414514553381 | 15. 6636992000000 |
| H | 8. 8095756390820 | 0. 4160664107737 | 17. 0048560000000 |
| H | 5. 3807151689594 | 9. 5973744183330 | 15. 8116308000000 |
| H | 4. 3707390676536 | 10. 2201532200691 | 14. 9712944000000 |
| H | 2. 4473486672251 | 1. 0955314898748 | 24. 9014964000000 |
| H | 2. 3728219597517 | 10. 1030869862013 | 25. 9503192000000 |
| H | 3. 9636299034092 | 9. 0184929747346 | 28. 0652856000000 |
| H | 7. 9001860736323 | 6. 9405239184545 | 17. 3773844000000 |
| H | 6. 4251123872311 | 0. 7360039119607 | 14. 4550384000000 |
| H | 6. 9805214410450 | 8. 1015075785214 | 17. 8792068000000 |
| H | 7. 0679854060876 | 5. 7944266319430 | 16. 0017420000000 |
| H | 3. 2415485631810 | 7. 1833712562653 | 15. 1395012000000 |
| H | 5. 3364959721468 | 4. 6950096419232 | 15. 1908132000000 |
| H | 0. 4534911670670 | 7. 7054992442461 | 20. 8061680000000 |
| C | 4. 6070154995175 | 6. 2638560927077 | 26. 7908656000000 |

Structure 3: *COOH (chemisorbed) + 48 Cu + 1 H* +1 *OH+ 48 H₂O

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*COOH + *OH

| | | | |
|----|------------------|------------------|-------------------|
| Cu | 0. 0000000000000 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 2. 5560455953674 | 32. 0000004000000 |

| | | | |
|----|------------------|-------------------|-------------------|
| Cu | 2. 5569545991297 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 1. 2779659495530 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 0. 0888384738744 | 0. 0474370487699 | 28. 3538000000000 |
| Cu | 2. 6051072025033 | 0. 0140325860236 | 28. 4252472000000 |
| Cu | 5. 0262234095817 | 0. 0798827132305 | 28. 4250520000000 |
| Cu | 7. 7893607764894 | 10. 1253987550338 | 28. 4324360000000 |
| Cu | 0. 1371133921708 | 2. 5572708571631 | 28. 4175844000000 |
| Cu | 2. 6296174358101 | 2. 5185630957189 | 28. 3886288000000 |
| Cu | 5. 0332081439332 | 2. 5873950375370 | 28. 5168260000000 |
| Cu | 7. 5214799480647 | 2. 2490613291636 | 28. 3561376000000 |
| Cu | 0. 0114057642838 | 5. 1447164062020 | 28. 5402120000000 |
| Cu | 2. 4803481288882 | 5. 1326835235030 | 28. 4684932000000 |
| Cu | 5. 0568409006198 | 5. 1165079818995 | 28. 3161736000000 |
| Cu | 7. 5420826491211 | 5. 0858270502548 | 28. 4894528000000 |
| Cu | 0. 0767900448958 | 7. 5590940077837 | 28. 4227524000000 |
| Cu | 2. 5316770339952 | 7. 7652310379747 | 28. 3534952000000 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Cu | 5. 1028596403939 | 7. 6561711839057 | 28. 4484132000000 |
| Cu | 7. 5628218806307 | 7. 5764062626796 | 28. 4539828000000 |
| 0 | 3. 1495148676227 | 6. 2330073688067 | 26. 6899892000000 |
| 0 | 1. 0975521542710 | 1. 2526221584860 | 14. 2955936000000 |
| 0 | 4. 8064281976789 | 6. 5161571591212 | 20. 7164752000000 |
| 0 | 5. 4884303330603 | 9. 4412785400089 | 24. 4322504000000 |
| 0 | 7. 9727174933596 | 9. 4752397540260 | 25. 8065548000000 |
| 0 | 3. 2291920969553 | 2. 3012299968601 | 21. 2908680000000 |
| 0 | 4. 7487768587558 | 7. 9210318227878 | 15. 3300784000000 |
| 0 | 7. 7065657438648 | 1. 7924281496264 | 14. 5065616000000 |
| 0 | 1. 9985547613667 | 8. 9293034661569 | 22. 6425752000000 |
| 0 | 9. 3321107165256 | 10. 1777858287384 | 17. 5849372000000 |
| 0 | 3. 2894858881996 | 6. 2185608747677 | 18. 3619188000000 |
| 0 | 3. 3375432782009 | 2. 7282101640409 | 16. 9957568000000 |
| 0 | 6. 3260255386897 | 1. 2211593210621 | 22. 7408044000000 |
| 0 | 8. 8984932699382 | 1. 4231680073491 | 22. 0956836000000 |
| 0 | 5. 1736405044908 | 3. 4447470045253 | 23. 8750212000000 |
| 0 | 7. 6477543563048 | 8. 2433263910627 | 16. 9408844000000 |
| 0 | 9. 5855866105773 | 3. 8497816623873 | 22. 5636844000000 |
| 0 | 2. 2382568292298 | 6. 8483166032642 | 15. 1263452000000 |
| 0 | 6. 0476023093412 | 5. 7272787476877 | 14. 9469932000000 |
| 0 | 3. 7217167580949 | 2. 0899147197258 | 14. 1042228000000 |
| 0 | 9. 2700237230599 | 7. 4663035608216 | 26. 3669896000000 |
| 0 | 0. 3956383562392 | 4. 0564652188488 | 24. 9515264000000 |
| 0 | 9. 8920814215250 | 7. 2946435959169 | 21. 5239352000000 |
| 0 | 1. 1470834595464 | 5. 1354798566074 | 21. 1346012000000 |
| 0 | 7. 7758339323566 | 5. 7308944100726 | 22. 1705288000000 |
| 0 | 5. 6118763621150 | 3. 9907730678978 | 21. 2475288000000 |
| 0 | 7. 2447178903645 | 3. 3320439828203 | 18. 6097628000000 |
| 0 | 8. 9806962615191 | 9. 9780694852869 | 12. 9298100000000 |
| 0 | 2. 6388709278941 | 2. 8140706169944 | 24. 2555444000000 |
| 0 | 4. 7032544353030 | 0. 5135076991592 | 17. 5571072000000 |
| 0 | 5. 3066176886859 | 4. 9108218742253 | 17. 2656384000000 |
| 0 | 8. 4407028765118 | 6. 3060557940322 | 15. 2927496000000 |
| 0 | 2. 7266666568243 | 8. 9703792354394 | 17. 8876404000000 |
| 0 | 1. 4729200846914 | 7. 2955969749525 | 25. 1128324000000 |
| 0 | 10. 0231696787764 | 9. 8373188785354 | 20. 1250420000000 |
| 0 | 6. 6461951784637 | 8. 3232517425448 | 19. 7288700000000 |
| 0 | 1. 7045527425579 | 4. 0762547868372 | 18. 6179016000000 |
| 0 | 6. 0707292385960 | 3. 4051671527985 | 13. 3628528000000 |
| 0 | 0. 9741235111167 | 9. 2424127120892 | 15. 9014248000000 |

| | | | |
|---|------------------|-------------------|-------------------|
| O | 6. 2025818618451 | 0. 8512642062611 | 19. 9349624000000 |
| O | 9. 7163582399014 | 0. 9022548516636 | 24. 6819056000000 |
| O | 2. 2851413868440 | 10. 1810623278606 | 20. 3781864000000 |
| O | 7. 8583114166239 | 4. 8892679824211 | 26. 3836788000000 |
| O | 9. 5065660569299 | 2. 1604678358582 | 16. 2149024000000 |
| O | 5. 5408572089127 | 0. 2820129747720 | 15. 2660532000000 |
| O | 2. 1376399191831 | 0. 1555209265526 | 25. 0640348000000 |
| O | 9. 4322154584006 | 4. 3857036871328 | 17. 6242084000000 |
| O | 8. 9608374724599 | 2. 6712090589142 | 26. 8065044000000 |
| O | 4. 0864258020588 | 7. 4185290870391 | 22. 9509876000000 |
| O | 4. 9967286386297 | 5. 7096439962797 | 25. 4361312000000 |
| H | 0. 6099531232552 | 1. 5982938383832 | 15. 0241892000000 |
| H | 0. 3194275686368 | 0. 8971369322226 | 13. 7787224000000 |
| H | 4. 0561633924690 | 6. 4987948017234 | 20. 0122472000000 |
| H | 5. 3836388637870 | 7. 2383869730679 | 20. 4317516000000 |
| H | 4. 6570448597044 | 9. 5942332982158 | 24. 9076112000000 |
| H | 5. 1366806369861 | 8. 9131597243046 | 23. 6949420000000 |
| H | 9. 4138204598852 | 3. 4828209181958 | 17. 1357136000000 |
| H | 8. 9649003528439 | 5. 0658103850080 | 17. 0845332000000 |
| H | 7. 1640106998382 | 9. 6211366034695 | 25. 2940020000000 |
| H | 8. 6350072903251 | 10. 1170860342237 | 25. 2707888000000 |
| H | 2. 5898278596099 | 2. 9174272726007 | 20. 8598632000000 |
| H | 4. 0968289112394 | 2. 8238528748594 | 21. 1994036000000 |
| H | 4. 9454699930143 | 8. 8440710327268 | 15. 0997076000000 |
| H | 7. 1169261020993 | 2. 5467018877688 | 14. 1145580000000 |
| H | 2. 8059413514276 | 8. 4249533795893 | 22. 8039976000000 |
| H | 1. 7687185783617 | 9. 4104661148593 | 23. 4516244000000 |
| H | 9. 5326760998837 | 10. 0894902919440 | 18. 5639568000000 |
| H | 8. 6392738925537 | 9. 5227364145482 | 17. 2904788000000 |
| H | 2. 4661831199406 | 5. 6321042396367 | 18. 3168432000000 |
| H | 3. 0467987635074 | 7. 2412619364252 | 18. 2457928000000 |
| H | 3. 6955919882608 | 1. 8073117624317 | 17. 3177052000000 |
| H | 4. 0950146413975 | 3. 2964145599909 | 16. 8236828000000 |
| H | 6. 0648870647109 | 0. 5672130821630 | 23. 4126956000000 |
| H | 5. 9612074749033 | 2. 0985043335463 | 23. 0734600000000 |
| H | 7. 9523337523782 | 1. 3644782434094 | 22. 3949912000000 |
| H | 9. 2373212534836 | 2. 3219993243850 | 22. 2604592000000 |
| H | 5. 5389515096886 | 4. 1977245193693 | 24. 4167588000000 |
| H | 4. 2284937667642 | 3. 3669436473724 | 24. 1904408000000 |
| H | 8. 7594807238235 | 4. 4911493103171 | 22. 4322968000000 |
| H | 0. 0286244532319 | 4. 1943671404940 | 21. 8869212000000 |

| | | | |
|---|-------------------|-------------------|-------------------|
| H | 1. 5528375462595 | 7. 5388211040273 | 15. 2005008000000 |
| H | 2. 0185483422891 | 6. 1840728687309 | 14. 4288184000000 |
| H | 5. 5322199958629 | 6. 6839264091307 | 14. 8996688000000 |
| H | 2. 9024536549294 | 1. 7873800669381 | 13. 6938756000000 |
| H | 3. 4924467418230 | 2. 3266178548073 | 15. 0619384000000 |
| H | 0. 5531519548617 | 7. 5193970798026 | 25. 4635696000000 |
| H | 8. 6762136128680 | 8. 2595519329181 | 25. 9921156000000 |
| H | 10. 1608963841513 | 3. 9594056297275 | 24. 0592296000000 |
| H | 10. 0376734059718 | 3. 6650212224938 | 25. 6455348000000 |
| H | 0. 2475785966353 | 7. 6897427231582 | 22. 2106672000000 |
| H | 0. 5501809090230 | 5. 9598248066141 | 21. 1086144000000 |
| H | 1. 3855294472405 | 4. 9389626090252 | 20. 1707396000000 |
| H | 8. 2265471393494 | 6. 5735029490108 | 21. 7894680000000 |
| H | 7. 0433640052882 | 5. 4415057335254 | 21. 5523984000000 |
| H | 5. 6490334061842 | 3. 9678738727934 | 22. 2404692000000 |
| H | 5. 3426865799300 | 4. 9032310384421 | 21. 1386204000000 |
| H | 8. 1589547471163 | 3. 6612364386026 | 18. 3759056000000 |
| H | 7. 0337859082167 | 3. 7167073724223 | 19. 5046988000000 |
| H | 8. 7476192444092 | 10. 0622909729292 | 12. 0032652000000 |
| H | 8. 4725801294389 | 0. 4713929675879 | 13. 4256212000000 |
| H | 2. 6045447174903 | 2. 7173045876340 | 23. 2696792000000 |
| H | 1. 8424361255764 | 3. 3955794766908 | 24. 4596680000000 |
| H | 4. 0828236480355 | 9. 9511239507815 | 17. 6333496000000 |
| H | 5. 0261130602492 | 0. 8222188656774 | 18. 4547064000000 |
| H | 5. 7986859188050 | 4. 3027737192887 | 17. 9343788000000 |
| H | 4. 5259109900320 | 5. 3910541501430 | 17. 7693040000000 |
| H | 8. 9822948439261 | 6. 4444310309450 | 14. 4892476000000 |
| H | 2. 1528247645942 | 9. 0543418260721 | 17. 0754460000000 |
| H | 2. 3043226371376 | 9. 4132972129649 | 18. 6546668000000 |
| H | 3. 9602362779207 | 6. 7109296126382 | 23. 6080216000000 |
| H | 4. 3893070047430 | 7. 0288146494987 | 22. 0765688000000 |
| H | 2. 5820677141005 | 6. 6915653024157 | 25. 9267504000000 |
| H | 1. 2349317552579 | 6. 3974819191933 | 24. 6768216000000 |
| H | 9. 4717275760843 | 0. 2706061688465 | 20. 7075532000000 |
| H | 0. 7053425021311 | 0. 0216357940572 | 20. 2150356000000 |
| H | 8. 3863344046645 | 3. 9224609650990 | 26. 3449704000000 |
| H | 9. 1891713091301 | 1. 8834871972739 | 26. 1698684000000 |
| H | 6. 3263187467865 | 9. 2970201446266 | 19. 8992972000000 |
| H | 6. 7809497130299 | 8. 1945112167414 | 18. 7823216000000 |
| H | 2. 2544691813547 | 3. 5454902522841 | 17. 9425984000000 |
| H | 0. 7675616284399 | 4. 0388245369406 | 18. 3103052000000 |

| | | | |
|---|------------------|------------------|-------------------|
| H | 5. 1845331801726 | 3. 0012487582281 | 13. 3702792000000 |
| H | 5. 9145827853651 | 4. 2405548987173 | 13. 8519308000000 |
| H | 0. 1135563152860 | 9. 6273274322005 | 16. 3762152000000 |
| H | 1. 1799156074856 | 9. 9533611808650 | 15. 2319456000000 |
| H | 6. 8022600202327 | 1. 4684904237901 | 19. 4695504000000 |
| H | 6. 2115849969633 | 1. 0980530772189 | 20. 8497276000000 |
| H | 0. 4300879042658 | 0. 5451832165911 | 24. 6792332000000 |
| H | 9. 4393951193766 | 0. 8295394547005 | 23. 7179272000000 |
| H | 2. 3403425410506 | 9. 7151432119770 | 21. 2994920000000 |
| H | 2. 8771864190651 | 0. 7505052120017 | 20. 4369876000000 |
| H | 8. 8891838361629 | 6. 6138753405171 | 26. 0173136000000 |
| H | 6. 9912793248638 | 4. 8250413807748 | 25. 8943736000000 |
| H | 8. 7576751469318 | 2. 2356530816634 | 15. 5358296000000 |
| H | 9. 2643777030393 | 1. 4055999229437 | 16. 8210220000000 |
| H | 5. 1777231229852 | 0. 4074249562012 | 16. 2230824000000 |
| H | 4. 9134123358030 | 0. 9069716443396 | 14. 7212044000000 |
| H | 2. 3825959038777 | 1. 1473331823076 | 24. 7766100000000 |
| H | 2. 0536611112810 | 0. 1400929347269 | 26. 0559272000000 |
| H | 3. 6315367063295 | 8. 9925148275153 | 27. 9318892000000 |
| H | 8. 1341380106124 | 7. 5380023882467 | 16. 3988376000000 |
| H | 6. 9610315398843 | 1. 1846062739483 | 14. 9063544000000 |
| H | 6. 8682300011482 | 8. 3391463011378 | 16. 3747552000000 |
| H | 7. 4624783383003 | 6. 0619783886755 | 15. 0291472000000 |
| H | 3. 7810023716559 | 7. 7700831074058 | 15. 2253676000000 |
| H | 5. 6729510870973 | 5. 3797765882222 | 15. 8603336000000 |
| H | 9. 7433963831266 | 8. 0835340728508 | 20. 9846052000000 |
| C | 4. 4721971484698 | 5. 7904547305448 | 26. 5667856000000 |

Structure 4: *CO (chemisorbed) + 48 Cu + 1 H* +1 *OH+ 48 H₂O

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*CO + *OH

| | | | |
|----|------------------|------------------|-------------------|
| Cu | 0. 0000000000000 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 5. 1119888384809 | 32. 0000004000000 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Cu | 5. 1140115705318 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 1. 2779659495530 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 0. 0233027313889 | 0. 0241375449006 | 28. 4459452000000 |
| Cu | 2. 5664672433997 | 0. 1135190789855 | 28. 4978384000000 |
| Cu | 5. 1103995985883 | 0. 1366399520981 | 28. 4242508000000 |
| Cu | 7. 6527535185604 | 10. 1877382306097 | 28. 2505024000000 |
| Cu | 10. 2061284630673 | 2. 6712611041661 | 28. 3526012000000 |
| Cu | 2. 3799366792762 | 2. 6130599929946 | 28. 5532532000000 |
| Cu | 5. 0179443460803 | 2. 5660314329899 | 28. 3142136000000 |
| Cu | 7. 6048063756216 | 2. 4180971499704 | 28. 4774468000000 |
| Cu | 0. 0404389907152 | 5. 1537024432873 | 28. 6184732000000 |
| Cu | 2. 6971759766724 | 5. 0627367498933 | 28. 3281984000000 |
| Cu | 5. 1196817262730 | 5. 2584845661968 | 28. 5132980000000 |
| Cu | 7. 7441550832341 | 5. 0037409516921 | 28. 2949416000000 |
| Cu | 0. 0575821021316 | 7. 6044843182272 | 28. 3297460000000 |
| Cu | 2. 6096788761490 | 7. 7308895561934 | 28. 3616472000000 |
| Cu | 5. 2669518591886 | 7. 7367771114131 | 28. 2803300000000 |
| Cu | 7. 6779136777322 | 7. 6097753469246 | 28. 4411024000000 |
| 0 | 2. 1600693670217 | 5. 1078720488273 | 26. 3586200000000 |
| 0 | 1. 2474115591065 | 1. 9566012670018 | 14. 6282176000000 |
| 0 | 4. 9694946483499 | 7. 3423306459461 | 19. 0952624000000 |

| | | | |
|---|-------------------|-------------------|-------------------|
| 0 | 5. 4873967924164 | 10. 1336855043430 | 24. 4577892000000 |
| 0 | 7. 7396856795907 | 10. 1918076785116 | 26. 1016664000000 |
| 0 | 4. 3024334444240 | 4. 2175744148599 | 21. 8572976000000 |
| 0 | 2. 5202875306418 | 8. 6124665940855 | 15. 3542440000000 |
| 0 | 7. 1635834157683 | 0. 8402948258518 | 15. 4301108000000 |
| 0 | 1. 7865734889946 | 6. 3210469738415 | 22. 0858612000000 |
| 0 | 10. 1318495558096 | 0. 7376459447719 | 18. 1846548000000 |
| 0 | 1. 3019961274687 | 8. 4213554064551 | 17. 8848584000000 |
| 0 | 2. 0775994507346 | 2. 8232623810874 | 21. 0002648000000 |
| 0 | 6. 0344118312461 | 1. 4720266379221 | 22. 1733796000000 |
| 0 | 8. 6759825849326 | 2. 1137152486138 | 22. 6948140000000 |
| 0 | 6. 2153374878901 | 3. 0917429768545 | 25. 5090716000000 |
| 0 | 8. 4361451115864 | 7. 8705170489030 | 18. 2275272000000 |
| 0 | 8. 6918961041106 | 4. 6017083539421 | 21. 6563544000000 |
| 0 | 8. 2445216036151 | 8. 5080388696893 | 14. 3449508000000 |
| 0 | 4. 0317489861544 | 6. 5333255482617 | 14. 6236560000000 |
| 0 | 3. 0909472917483 | 2. 3587645402567 | 16. 7332108000000 |
| 0 | 8. 3109920939222 | 7. 4433674534659 | 25. 4215120000000 |
| 0 | 0. 1708785493416 | 5. 6315041343643 | 24. 0030468000000 |
| 0 | 1. 8795454095546 | 9. 0333620680394 | 22. 0783900000000 |
| 0 | 0. 7045975674339 | 4. 7881059186467 | 20. 2576084000000 |
| 0 | 7. 7566979876741 | 6. 7571517268628 | 22. 8191408000000 |
| 0 | 6. 1195636760753 | 5. 1478144790676 | 20. 3278920000000 |
| 0 | 6. 3528348016497 | 3. 6608033075864 | 18. 0677920000000 |
| 0 | 1. 0152039392867 | 9. 8528467686148 | 13. 3830800000000 |
| 0 | 3. 5682631762963 | 3. 7732922177835 | 24. 3828324000000 |
| 0 | 6. 1460495612878 | 9. 5967529428098 | 17. 6729904000000 |
| 0 | 4. 1557012517208 | 4. 7268190046100 | 16. 9421512000000 |
| 0 | 6. 9989489614211 | 6. 1913025575007 | 15. 1975200000000 |
| 0 | 3. 1136586979835 | 8. 9559327414004 | 19. 8603892000000 |
| 0 | 0. 4974727906641 | 7. 1822641954740 | 26. 2023780000000 |
| 0 | 10. 0884555756461 | 0. 9101118442067 | 20. 9170296000000 |
| 0 | 8. 4995442291825 | 8. 4951408497081 | 20. 9744040000000 |
| 0 | 0. 7030252684175 | 5. 8073003164233 | 17. 4646796000000 |
| 0 | 2. 1197199648287 | 4. 5994950503595 | 14. 4590180000000 |
| 0 | 2. 5875685107177 | 1. 3155674653345 | 18. 9873200000000 |
| 0 | 5. 8969334374369 | 1. 3666417512401 | 19. 3534560000000 |
| 0 | 9. 6413877828877 | 1. 1025602573871 | 24. 9529348000000 |
| 0 | 1. 4364696240684 | 9. 4534367812126 | 24. 8425704000000 |
| 0 | 7. 9622353294672 | 4. 9489296326471 | 26. 1709420000000 |
| 0 | 9. 3321888508074 | 2. 3987669912492 | 16. 0446480000000 |

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| O | 4. 2868426893735 | 0. 0455465484494 | 15. 7768580000000 |
| O | 3. 2186834451322 | 1. 4099537281061 | 25. 3340136000000 |
| O | 8. 5363580551238 | 4. 8518643175255 | 16. 8705684000000 |
| O | 10. 1591062500299 | 3. 3697497964771 | 26. 2942908000000 |
| O | 5. 1113159378095 | 8. 0462381794593 | 22. 9682592000000 |
| O | 5. 0072941525740 | 6. 5687465855833 | 25. 5350940000000 |
| H | 0. 3219261270646 | 2. 0133759906201 | 14. 9956060000000 |
| H | 1. 2974572824938 | 1. 2169094019035 | 13. 9545572000000 |
| H | 4. 4735820888419 | 6. 7016378480415 | 18. 5783700000000 |
| H | 4. 3371997226480 | 8. 0079808292819 | 19. 5085728000000 |
| H | 4. 6353600397530 | 0. 2558636610464 | 24. 7231480000000 |
| H | 5. 3850026342685 | 9. 2782338536757 | 23. 8497952000000 |
| H | 8. 8322799886870 | 3. 9552886355738 | 16. 4585252000000 |
| H | 7. 9622838054483 | 5. 3503280758735 | 16. 1850724000000 |
| H | 6. 9979766805086 | 0. 2201760579649 | 25. 4894924000000 |
| H | 8. 5589733275568 | 0. 4367741837963 | 25. 8015668000000 |
| H | 3. 6283273713853 | 3. 7897450613973 | 21. 3243336000000 |
| H | 4. 9732082766757 | 4. 7033155119831 | 21. 2930496000000 |
| H | 3. 1531460663267 | 9. 3474808282593 | 15. 3025908000000 |
| H | 6. 9498763371063 | 0. 3116855168791 | 16. 2081476000000 |
| H | 2. 7580621157704 | 6. 0227947557136 | 22. 0902620000000 |
| H | 1. 2947984669723 | 5. 8909473635443 | 22. 8756780000000 |
| H | 9. 9227326616638 | 0. 6349780451914 | 19. 1192880000000 |
| H | 0. 1835061333436 | 10. 1023172481726 | 17. 9063948000000 |
| H | 0. 9419357664623 | 7. 4932409153267 | 17. 7408484000000 |
| H | 1. 9270933926742 | 8. 3777104013267 | 18. 6688504000000 |
| H | 1. 5228994348471 | 3. 4228474054582 | 20. 4916144000000 |
| H | 2. 4355707424027 | 2. 1823666169252 | 20. 3206600000000 |
| H | 5. 6596014768786 | 0. 9879190868598 | 22. 8929736000000 |
| H | 5. 5679742023097 | 2. 3142037840941 | 22. 2313148000000 |
| H | 7. 6595906772985 | 1. 8541167016780 | 22. 7169804000000 |
| H | 8. 5706541981469 | 3. 1008031451926 | 22. 5139396000000 |
| H | 6. 1573656347795 | 2. 5043016741868 | 26. 3485660000000 |
| H | 5. 2731084110610 | 3. 3749568779214 | 25. 3782652000000 |
| H | 8. 8670222334604 | 5. 3912633536508 | 22. 2441160000000 |
| H | 9. 5430181538729 | 4. 5857124655953 | 21. 0822608000000 |
| H | 7. 8530293755418 | 9. 3797938744649 | 14. 4827568000000 |
| H | 8. 8165282606528 | 8. 5712717035485 | 13. 5688144000000 |
| H | 3. 4184628835222 | 7. 2438880232732 | 14. 7465116000000 |
| H | 2. 4475004359086 | 2. 1214756149033 | 15. 9948868000000 |
| H | 3. 3899405980226 | 3. 3105871262697 | 16. 7454604000000 |

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|---|-------------------|------------------|-------------------|
| H | 9. 3271011227298 | 7. 3913720995259 | 25. 7087992000000 |
| H | 7. 9859706629661 | 8. 3656139191253 | 25. 5290376000000 |
| H | 0. 2120152260129 | 4. 6871135898786 | 24. 2604520000000 |
| H | 0. 3784101561808 | 6. 1850704197681 | 24. 8441848000000 |
| H | 1. 5720403755235 | 8. 0890438143064 | 22. 1317368000000 |
| H | 1. 1563305086202 | 5. 3971769826214 | 20. 9452324000000 |
| H | 0. 7249191282538 | 5. 2510541606695 | 19. 3418712000000 |
| H | 8. 0371122094287 | 6. 9747720459823 | 23. 7798112000000 |
| H | 8. 1254767641121 | 7. 5575616892265 | 22. 3314476000000 |
| H | 6. 9921119049530 | 5. 1796288520046 | 20. 7728708000000 |
| H | 6. 0044240166127 | 6. 0220518071858 | 19. 8902600000000 |
| H | 7. 2122756979443 | 4. 0395397757173 | 17. 6340216000000 |
| H | 6. 3264444366194 | 4. 2135453557095 | 18. 8954100000000 |
| H | 1. 4272661420156 | 9. 7429747427654 | 12. 5419604000000 |
| H | 1. 4943867627278 | 9. 2543023425328 | 13. 9958228000000 |
| H | 3. 8116037040336 | 4. 0586706491811 | 23. 4423000000000 |
| H | 2. 9947490594238 | 4. 4064487814069 | 24. 8252280000000 |
| H | 5. 6832036548344 | 8. 8459244162960 | 18. 0438576000000 |
| H | 5. 9696575338487 | 0. 1736018969772 | 18. 3723900000000 |
| H | 5. 0926626052681 | 4. 5071324174134 | 17. 2129244000000 |
| H | 4. 1223420041894 | 5. 3042538151544 | 16. 0784356000000 |
| H | 7. 4116524993349 | 7. 0681341727157 | 14. 9364032000000 |
| H | 3. 0361942846922 | 9. 8452959125830 | 19. 4909424000000 |
| H | 2. 8094514624487 | 9. 0335472427963 | 20. 7739976000000 |
| H | 4. 8713572745104 | 7. 4941441918604 | 23. 7394188000000 |
| H | 6. 0547903564574 | 7. 7156389681244 | 22. 7625776000000 |
| H | 0. 8130566435320 | 8. 1149067257713 | 26. 1267176000000 |
| H | 1. 6647610186877 | 5. 9414404604282 | 26. 2649032000000 |
| H | 9. 4386070267384 | 1. 2425377518597 | 21. 4985296000000 |
| H | 0. 6243048772271 | 1. 4608520417551 | 21. 2069044000000 |
| H | 9. 3700505351930 | 3. 9279169230526 | 26. 0628172000000 |
| H | 9. 9983773848031 | 2. 4753455978564 | 25. 7818188000000 |
| H | 8. 7346284996288 | 9. 4294540428178 | 20. 9361760000000 |
| H | 8. 2340295195324 | 8. 2367629633178 | 20. 0612552000000 |
| H | 1. 4428052507150 | 5. 4409148307533 | 16. 9098592000000 |
| H | 10. 0696364634310 | 5. 4618693330351 | 17. 1205772000000 |
| H | 1. 7705788697047 | 3. 6937484633156 | 14. 4272740000000 |
| H | 1. 3502350467243 | 5. 1107456829345 | 14. 2407196000000 |
| H | 1. 6476490996220 | 1. 2949910835668 | 18. 5806624000000 |
| H | 3. 0509268921529 | 1. 8668832281544 | 18. 3368448000000 |
| H | 6. 0846275273774 | 2. 3553700446301 | 19. 1783236000000 |

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|---|------------------|-------------------|-------------------|
| H | 6. 1235819667382 | 1. 2202066577765 | 20. 2809592000000 |
| H | 0. 1456413808580 | 0. 4193387176457 | 24. 8511680000000 |
| H | 9. 2937505681485 | 1. 5272987977343 | 24. 1134560000000 |
| H | 1. 8464324281889 | 9. 4592548064296 | 23. 9149540000000 |
| H | 2. 0259400089800 | 10. 1112842667572 | 25. 2452820000000 |
| H | 7. 8082553639664 | 5. 9295488872345 | 26. 0413160000000 |
| H | 7. 1414491191564 | 4. 3282359129887 | 25. 9098004000000 |
| H | 8. 4222282096645 | 1. 8587735758518 | 15. 8464408000000 |
| H | 9. 5710754176717 | 1. 9544918494231 | 16. 9223000000000 |
| H | 4. 7570303547566 | 9. 8841480510326 | 16. 5984960000000 |
| H | 3. 9733469854139 | 0. 8912967187547 | 16. 1389096000000 |
| H | 3. 4596806603053 | 2. 3559179001505 | 24. 8282068000000 |
| H | 3. 4672797305611 | 1. 4753420942958 | 26. 2900040000000 |
| H | 3. 9683803450190 | 9. 0255956689996 | 27. 6542456000000 |
| H | 8. 3825698458774 | 7. 0181616306012 | 17. 8582096000000 |
| H | 6. 2073391555451 | 1. 0238353209498 | 15. 1059740000000 |
| H | 7. 5888774136733 | 8. 2724515888994 | 17. 9618152000000 |
| H | 6. 0568599944953 | 6. 2958125931500 | 14. 8771128000000 |
| H | 1. 9979573000129 | 8. 5629736044889 | 16. 2347576000000 |
| H | 3. 4754972275211 | 5. 8795745046199 | 14. 1951756000000 |
| H | 1. 0957613042595 | 9. 5035325345817 | 21. 7144864000000 |
| H | 1. 4386766107195 | 4. 4559680492544 | 26. 2752744000000 |
| C | 4. 9126164706446 | 6. 8816805750090 | 26. 6634904000000 |

Structure 5: *CO₂ + 48 Cu + 1 H* + 48 H₂O

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FORCE: 3. 341015 ... ENERGY: -912. 45512082

| | | | |
|----|------------------|------------------|-------------------|
| Cu | 0. 0000000000000 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 7. 6689550928826 | 32. 0000004000000 |

| | | | |
|----|-------------------|-------------------|-------------------|
| Cu | 2. 5569545991297 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 1. 2779659495530 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 10. 2257777008917 | 0. 0489111870749 | 28. 5154768000000 |
| Cu | 2. 5344262561988 | 0. 0969858668686 | 28. 5752984000000 |
| Cu | 5. 2611686950948 | 0. 0535646869985 | 28. 3197344000000 |
| Cu | 7. 6833536236980 | 10. 2131483790578 | 28. 3848728000000 |
| Cu | 10. 1899901544241 | 2. 5906285916577 | 28. 3149056000000 |
| Cu | 2. 5543366916092 | 2. 5927278864860 | 28. 4243588000000 |
| Cu | 5. 1006953003339 | 2. 5219963440970 | 28. 4825204000000 |
| Cu | 7. 6226091285533 | 2. 3826568896481 | 28. 4313460000000 |
| Cu | 10. 2072188658326 | 5. 1004967560521 | 28. 4538212000000 |
| Cu | 2. 6425578637493 | 5. 1481161165788 | 28. 4772984000000 |
| Cu | 5. 1951795896888 | 5. 0830927829028 | 28. 4049240000000 |
| Cu | 7. 6992512910257 | 5. 0622762158761 | 28. 5108176000000 |
| Cu | 10. 1881883615225 | 7. 5976069829706 | 28. 2519404000000 |
| Cu | 2. 4591950106790 | 7. 6179951224813 | 28. 3081840000000 |
| Cu | 5. 0529608790000 | 7. 6417592503680 | 28. 3547912000000 |
| Cu | 7. 5567255657897 | 7. 6389768232641 | 28. 3388552000000 |
| 0 | 2. 9667474305062 | 8. 2964030387930 | 24. 1610168000000 |
| 0 | 1. 2991392149527 | 2. 5666824587642 | 14. 1055120000000 |
| 0 | 5. 3109659023764 | 8. 4769248070284 | 22. 0388640000000 |
| 0 | 6. 4588423635211 | 8. 9647261394785 | 25. 4171192000000 |
| 0 | 7. 9666334509189 | 0. 8488444599208 | 25. 6441700000000 |
| 0 | 3. 7718288547138 | 4. 6433175614946 | 21. 7337496000000 |

| | | | |
|---|------------------|------------------|-------------------|
| 0 | 4. 6692510912967 | 8. 2148716465011 | 14. 5639720000000 |
| 0 | 7. 4830253022054 | 1. 8273516384294 | 13. 7052536000000 |
| 0 | 2. 2711573958007 | 1. 2803607440209 | 21. 3341868000000 |
| 0 | 9. 9838252838966 | 1. 2059857272459 | 17. 8642544000000 |
| 0 | 4. 3767314761722 | 7. 6899132761646 | 19. 4912544000000 |
| 0 | 3. 6026732481020 | 4. 7030838134745 | 17. 0016152000000 |
| 0 | 6. 8741480593751 | 1. 8959599594892 | 23. 1204800000000 |
| 0 | 0. 1851974746427 | 2. 7586837326779 | 22. 4584016000000 |
| 0 | 5. 7030641824837 | 3. 2433612252615 | 25. 6060740000000 |
| 0 | 8. 1923362895083 | 9. 4838595315977 | 17. 9873480000000 |
| 0 | 0. 0508217481653 | 5. 3723021129433 | 22. 4140148000000 |
| 0 | 1. 8277525054469 | 8. 2958243037715 | 15. 3541756000000 |
| 0 | 6. 4731813337427 | 6. 5858681442221 | 15. 3335684000000 |
| 0 | 3. 8081154787929 | 2. 8106790866179 | 15. 0961112000000 |
| 0 | 7. 9358351465167 | 7. 0819473302311 | 24. 9323104000000 |
| 0 | 1. 2045080658743 | 5. 8181071193266 | 24. 9346252000000 |
| 0 | 1. 3287005636763 | 8. 7632211367103 | 21. 0991276000000 |
| 0 | 1. 8931737055298 | 6. 2944390688487 | 20. 4382028000000 |
| 0 | 7. 8229914486072 | 6. 7220790553042 | 22. 4500092000000 |
| 0 | 6. 4124024758772 | 4. 3739684541950 | 21. 6106748000000 |
| 0 | 6. 9164600229136 | 3. 3746757926609 | 18. 9706304000000 |
| 0 | 9. 8824414511021 | 1. 1281955603436 | 12. 0038152000000 |
| 0 | 3. 5010983749431 | 3. 9469378777623 | 24. 2657116000000 |
| 0 | 6. 0304100060536 | 0. 7835740902356 | 17. 9837824000000 |
| 0 | 5. 8585520168994 | 5. 8829949717476 | 17. 6869236000000 |
| 0 | 8. 9322749948494 | 8. 0726670446953 | 15. 7357908000000 |
| 0 | 3. 5379475863053 | 0. 4191637678892 | 19. 0081548000000 |
| 0 | 0. 0389986200018 | 7. 8439784694129 | 26. 1832304000000 |
| 0 | 0. 5356918064379 | 3. 3711378402789 | 19. 3059940000000 |
| 0 | 8. 7295395443111 | 8. 7564574012079 | 20. 5295840000000 |
| 0 | 1. 4219703967532 | 6. 3087239056317 | 17. 5427232000000 |
| 0 | 5. 5930929421306 | 4. 0908086433802 | 13. 8701216000000 |
| 0 | 2. 1851116088808 | 0. 5763013692521 | 16. 8225700000000 |
| 0 | 8. 6129185038643 | 1. 8564201897640 | 20. 9881208000000 |
| 0 | 0. 0225973751826 | 1. 8064531691497 | 24. 8102616000000 |
| 0 | 3. 1214071847127 | 3. 5703879237130 | 19. 3057792000000 |
| 0 | 7. 8401496959839 | 4. 6599968888669 | 25. 7782148000000 |
| 0 | 9. 1854766007547 | 2. 8006096084922 | 15. 5442864000000 |
| 0 | 5. 7749112113552 | 0. 5702801732774 | 15. 3723652000000 |
| 0 | 2. 7950388578254 | 1. 3775639943976 | 25. 0789396000000 |
| 0 | 9. 1071065865924 | 5. 3772244281270 | 16. 5835460000000 |

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| O | 0. 0010063368233 | 3. 7945000955747 | 26. 4127980000000 |
| O | 4. 4946479707390 | 0. 5717899968338 | 22. 7913896000000 |
| O | 4. 8197730012075 | 6. 8636886643377 | 24. 3452720000000 |
| H | 0. 4585600774642 | 2. 7454626026846 | 14. 6584784000000 |
| H | 1. 0039270352059 | 2. 2322879317878 | 13. 1926448000000 |
| H | 5. 1717636454073 | 8. 0110350368958 | 21. 1619728000000 |
| H | 5. 9959313110763 | 7. 9857833759537 | 22. 5621708000000 |
| H | 6. 8829818353694 | 9. 8725894038514 | 25. 6084088000000 |
| H | 5. 8668537843413 | 8. 8311305789940 | 26. 2205740000000 |
| H | 9. 1013241383887 | 4. 5388190800957 | 15. 9982176000000 |
| H | 8. 5028136988881 | 6. 0249034575422 | 16. 1407160000000 |
| H | 7. 7487135640495 | 1. 5667239452053 | 26. 2213252000000 |
| H | 8. 8309175477155 | 1. 1914855519549 | 25. 2388020000000 |
| H | 3. 2389091789600 | 5. 4344790110132 | 21. 3450348000000 |
| H | 4. 7500652562455 | 4. 6757223259536 | 21. 6539084000000 |
| H | 4. 8552129319371 | 9. 1355267953512 | 14. 9324756000000 |
| H | 6. 7495886168046 | 2. 4137205430571 | 13. 5413412000000 |
| H | 3. 0586791628721 | 1. 2208366200500 | 21. 9595580000000 |
| H | 1. 5546934399924 | 1. 8467264804023 | 21. 8203824000000 |
| H | 10. 1606001079545 | 2. 0018483251900 | 18. 3824180000000 |
| H | 9. 3578828593916 | 0. 5844649073067 | 18. 2396112000000 |
| H | 3. 4651297083013 | 7. 4211893253884 | 19. 5437912000000 |
| H | 4. 2482749328916 | 8. 6458609340815 | 19. 3400288000000 |
| H | 3. 4567908168485 | 4. 4063350794026 | 17. 9094292000000 |
| H | 4. 4830558705109 | 5. 1926510034905 | 17. 1369016000000 |
| H | 5. 9686139707446 | 1. 3761887318463 | 23. 0738460000000 |
| H | 7. 2817789029016 | 1. 8310157673161 | 24. 0289300000000 |
| H | 9. 7758460412570 | 2. 4239812286900 | 21. 8101268000000 |
| H | 0. 1205172207270 | 3. 8202544175356 | 22. 3788016000000 |
| H | 5. 3950470825508 | 2. 9759373832837 | 26. 4854100000000 |
| H | 4. 9126545150854 | 3. 6409716125965 | 25. 1898600000000 |
| H | 9. 3593385706053 | 5. 8197260436370 | 22. 3757880000000 |
| H | 0. 6217580473582 | 5. 6636724968145 | 21. 5906600000000 |
| H | 2. 2036838413103 | 9. 0648159074629 | 15. 8080772000000 |
| H | 1. 7442798317866 | 7. 6090746276485 | 16. 0534412000000 |
| H | 5. 6889213661267 | 7. 1860786318663 | 14. 9402408000000 |
| H | 3. 0000694517568 | 2. 8723601744192 | 14. 5504492000000 |
| H | 3. 7678897210327 | 3. 4767540164695 | 15. 8512764000000 |
| H | 8. 6364806942491 | 7. 4869151165906 | 25. 5738472000000 |
| H | 7. 2325108406123 | 7. 8135743285285 | 25. 1727048000000 |
| H | 0. 7931609350019 | 5. 5157986435473 | 24. 0817664000000 |

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| H | 0. 8039056259904 | 5. 1544991753170 | 25. 5401028000000 |
| H | 1. 7137598040608 | 9. 6409967239605 | 21. 2519444000000 |
| H | 1. 8005650480182 | 7. 2916798795563 | 20. 6902972000000 |
| H | 1. 4653634564866 | 6. 2616261223745 | 19. 5304336000000 |
| H | 8. 0339819291963 | 6. 8664490054407 | 23. 4394376000000 |
| H | 8. 0997229275766 | 7. 5347403063750 | 21. 9009488000000 |
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| H | 6. 6548798447945 | 3. 7355669766259 | 19. 8724832000000 |
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| H | 3. 3600946318824 | 3. 9858736567150 | 23. 2359600000000 |
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| H | 5. 1876466881246 | 0. 6144115816740 | 18. 4744800000000 |
| H | 6. 3869416428984 | 1. 6582953676218 | 18. 3249976000000 |
| H | 6. 1370513351297 | 6. 3272179660717 | 16. 7887284000000 |
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| H | 0. 4506029599302 | 7. 0698818297809 | 25. 5739608000000 |
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| H | 9. 2268469643814 | 4. 0879980975253 | 26. 2676156000000 |
| H | 0. 1037613035395 | 3. 0319001396217 | 25. 7615208000000 |
| H | 8. 6890938037758 | 9. 6763193967784 | 20. 9835616000000 |
| H | 8. 2852341665865 | 8. 9139201575829 | 19. 6363460000000 |
| H | 2. 1992913447087 | 5. 7634506067873 | 17. 1638292000000 |
| H | 0. 5405620062205 | 6. 0764980937173 | 17. 0434088000000 |
| H | 4. 8908674251316 | 3. 4991639453056 | 14. 1937392000000 |
| H | 5. 3822838885256 | 4. 3698772270424 | 12. 9670764000000 |
| H | 1. 2739394772899 | 0. 6686371104472 | 17. 2613688000000 |
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| H | 8. 4426612447871 | 2. 4738117455492 | 20. 2631608000000 |
| H | 7. 9476423205597 | 1. 8724361191116 | 21. 7465812000000 |
| H | 0. 8807110113865 | 1. 4524810384428 | 25. 1557296000000 |
| H | 0. 2521406569008 | 2. 1875745163695 | 23. 8657848000000 |

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| H | 3. 4579851259361 | 2. 6577182956608 | 19. 2621696000000 |
| H | 3. 2829262902479 | 3. 8146664548272 | 20. 2302884000000 |
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| H | 9. 4589525187389 | 2. 2709733004812 | 16. 3409340000000 |
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| H | 4. 0077615570997 | 8. 8795634405511 | 27. 9032388000000 |
| H | 8. 3221461717301 | 8. 9595756022864 | 17. 1230716000000 |
| H | 6. 9967703035607 | 1. 0707953734519 | 14. 1766088000000 |
| H | 7. 2541320486222 | 9. 8416857716983 | 18. 0902368000000 |
| H | 8. 1353818183812 | 7. 7608976828131 | 15. 2402588000000 |
| H | 3. 7073144827419 | 8. 0536565194860 | 14. 7558164000000 |
| H | 6. 3738710252462 | 5. 7607643969371 | 14. 7687996000000 |
| H | 0. 3328814942579 | 8. 8072567368533 | 20. 9800440000000 |
| C | 3. 8449086461937 | 7. 5442305382291 | 24. 2971296000000 |

Structure 6: *HCOO⁻ + 48 Cu + 48 H₂O

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FORCE: 2. 587094 ... ENERGY: -913. 22340993

| | | | |
|----|------------------|------------------|-------------------|
| Cu | 0. 0000000000000 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 0. 0000000000000 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 2. 5560455953674 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 5. 1119888384809 | 32. 0000004000000 |
| Cu | 0. 0000000000000 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 2. 5569545991297 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 5. 1140115705318 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 7. 6709658628516 | 7. 6689550928826 | 32. 0000004000000 |
| Cu | 1. 2779659495530 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 1. 2780227976837 | 30. 1932000000000 |

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|----|-------------------|-------------------|-------------------|
| Cu | 6. 3919775200849 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 1. 2780227976837 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 3. 8339661430472 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 6. 3910342384528 | 30. 1932000000000 |
| Cu | 1. 2779659495530 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 3. 8350227164151 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 6. 3919775200849 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 8. 9490342869470 | 8. 9469776860663 | 30. 1932000000000 |
| Cu | 0. 0513633700978 | 0. 1039360041279 | 28. 5549360000000 |
| Cu | 2. 6127375673797 | 0. 0586351624377 | 28. 3713316000000 |
| Cu | 5. 2457646850686 | 0. 0326521072183 | 28. 4949808000000 |
| Cu | 7. 7518416966118 | 10. 1935368283261 | 28. 4580888000000 |
| Cu | 0. 1777595819107 | 2. 6997710637298 | 28. 3890420000000 |
| Cu | 2. 5774886770146 | 2. 5413974643208 | 28. 5854204000000 |
| Cu | 5. 0320809239672 | 2. 3507896534592 | 28. 3430052000000 |
| Cu | 7. 6499311733051 | 2. 6152312718256 | 28. 4559496000000 |
| Cu | 10. 2014289519187 | 5. 2284931063278 | 28. 5194476000000 |
| Cu | 2. 5631977736941 | 5. 2479626318042 | 28. 4155988000000 |
| Cu | 5. 0312866951288 | 4. 9245269534866 | 28. 4615148000000 |
| Cu | 7. 5871942539743 | 5. 2163780146257 | 28. 4504512000000 |
| Cu | 0. 0208653304225 | 7. 8643740731738 | 28. 2863348000000 |
| Cu | 2. 3754482534124 | 7. 7881364703294 | 28. 4006472000000 |
| Cu | 5. 0142712166753 | 7. 3745110738968 | 28. 2236296000000 |
| Cu | 7. 6619345012127 | 7. 6872401543149 | 28. 6326352000000 |
| 0 | 4. 1482598818088 | 7. 3537973703739 | 24. 0846636000000 |
| 0 | 1. 8350125506448 | 2. 2414210043786 | 14. 8766236000000 |
| 0 | 6. 0095149150604 | 8. 8220665251558 | 22. 8359916000000 |
| 0 | 6. 7821017846065 | 10. 1072088883551 | 25. 0940300000000 |
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| 0 | 3. 6558828985525 | 4. 4322963553712 | 22. 0966704000000 |
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| 0 | 7. 9319668859472 | 2. 4270093625530 | 14. 4047644000000 |
| 0 | 1. 8242557917960 | 0. 8446055837627 | 21. 3291936000000 |
| 0 | 9. 9519648032498 | 0. 6944284469095 | 18. 1937016000000 |
| 0 | 4. 4880744640670 | 7. 6140362068336 | 20. 5192220000000 |

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| 0 | 3. 8678392170440 | 4. 5061025553750 | 17. 6670728000000 |
| 0 | 6. 5490023703661 | 2. 5975723894168 | 23. 0436572000000 |
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| 0 | 5. 6486871199562 | 3. 3818596734289 | 25. 6443304000000 |
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| 0 | 5. 3832506468580 | 7. 3672173766247 | 15. 4839580000000 |
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| 0 | 1. 0679666698268 | 5. 3793618622067 | 25. 4840008000000 |
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| 0 | 1. 5825331754962 | 6. 3216967726157 | 20. 9235404000000 |
| 0 | 7. 8869369948259 | 6. 3351643251182 | 22. 5725036000000 |
| 0 | 6. 0476799322730 | 4. 8150776291530 | 21. 5987604000000 |
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| 0 | 10. 1704290733418 | 7. 0033189177974 | 14. 9408460000000 |
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| 0 | 0. 0513307459670 | 7. 7174987934438 | 26. 3044448000000 |
| 0 | 9. 1185851671178 | 2. 8184923161594 | 20. 3433724000000 |
| 0 | 8. 3810988964334 | 8. 6214828971719 | 20. 9703444000000 |
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| H | 1. 5714987535910 | 1. 5888949157825 | 14. 1909956000000 |

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| H | 6. 5874912766761 | 8. 4813863836949 | 22. 1277680000000 |
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| H | 6. 3915352023246 | 9. 9628473227189 | 25. 9955832000000 |
| H | 9. 5416279977307 | 4. 4338167106780 | 16. 7552588000000 |
| H | 9. 6778899921318 | 5. 8886613602090 | 16. 2598036000000 |
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| H | 9. 9633888738640 | 0. 2108471766168 | 24. 7515372000000 |
| H | 3. 1506428034788 | 5. 2653058684513 | 21. 9744808000000 |
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| H | 7. 7813122295733 | 6. 7118104964211 | 23. 4519168000000 |

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| H | 6. 3434649263030 | 3. 8970656429015 | 21. 9709460000000 |
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| H | 9. 1064109460363 | 9. 6274267169542 | 13. 9422040000000 |
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| H | 3. 6263436401494 | 0. 6304251592715 | 26. 0873120000000 |
| H | 3. 2678777707499 | 6. 8332582452024 | 25. 9049408000000 |
| H | 8. 8474803791385 | 7. 8191068717349 | 17. 7085208000000 |
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| C | 4. 2235065700988 | 7. 1288825359823 | 25. 3613856000000 |

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