# Electronic Supplementary Information (ESI)

# Adsorption and Dehydrogenation of Tetrahydroxybenzene on Cu(111)

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## 1. Experimental Section

The STM and lab-based XPS experiments were conducted employing a commercially available UHV system (SPECS) with a base pressure in the low $10^{-10}$ mbar regime. The system incorporates an Aarhus type STM, a non-monochromatic dual anode X-ray source and a hemispherical energy analyzer for XPS. In the experiments discussed in this paper, only the Al-anode was used (excitation energy 1486.6 eV).
THB/DHBQ molecules were sublimated from a quartz crucible placed in a home-build evaporator (Knudsen type) cell at a crucible temperature of 340 K.
THB was obtained according to a literature procedure[1] by reduction of 2,5-dihydroxybenzo-quinone (DHBQ) with metallic tin and hydrochloric acid followed by recrystallization from THF. DHBQ (purity >99%) was bought from Sigma Aaldrich. All molecules were thoroughly degassed in the crucible prior to use, but not purified further.
All STM images were collected at RT, all XP spectra were collected nominally at RT unless stated otherwise. Here, nominal RT refers to the sample not being actively heated or cooled – by placing the X-ray source close to the surface, the sample temperature typically stabilised at around 320 K during measurements.

## 2. DHBQ on Cu(111)

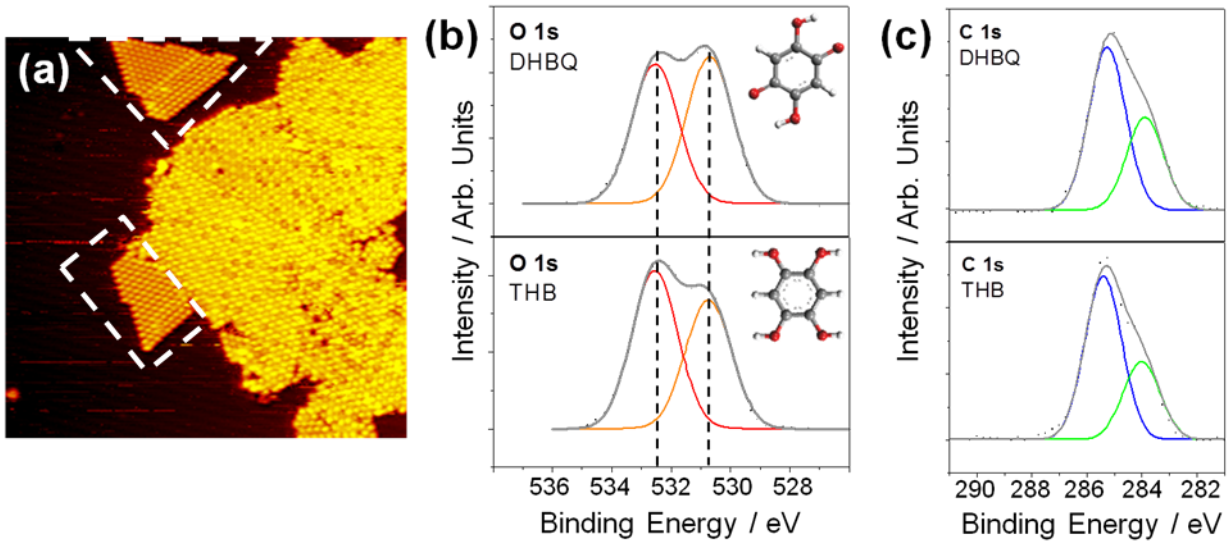


**Fig. S1** STM image ($I_T$ 0.33 nA, $U_T$ -1.63 V) (a) with the single layer islands highlighted by white dashed lines and XP spectrum of the O 1s region (b) and C 1s region (c) of DHB adsorbed on Cu(111) at RT. For comparison, corresponding spectra of THB annealed to 370 K are also shown in the bottom of (b) and (c).

Fig. S1 displays the result of a control experiment, where DHBQ was deposited on a Cu(111) substrate at room temperature. Apart from the tendency to from double layers on Cu(111), DHBQ adapts to the adsorption geometry observed for THB annealed to 370 K, as becomes apparent in Fig. S1a (highlighted regions). The O 1s spectrum of DHBQ adsorbed on Cu(111) at RT bears very close resemblance to the one of the annealed THB, as demonstrated in Fig. S1b and thereby offers additional support for the conclusion that DHBQ is formed from THB as a result of annealing to 370 K. The binding energies of the two O 1s components are 532.5 eV and 530.7 eV (THB annealed to 370 K has virtually identical BEs of 532.6 eV and 530.8 eV). The C 1s spectrum in (c) exhibits two components with an intensity ratio of ~2:1 in favour for the high BE component at 285.3 eV over the low BE feature at 283.9 eV (THB: 285.4 eV and 284.0 eV). The C 1s spectrum of THB on Cu(111) before annealing is virtually identical to the one after annealing and hence is not provided separately.

## 3. Synchrotron-based XP Spectrum of THB on Cu(111) at RT

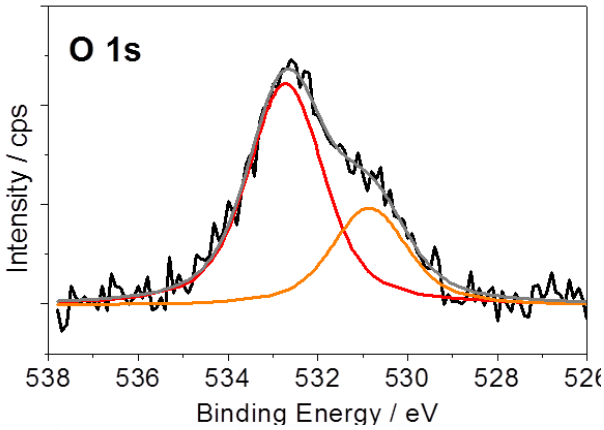


**Fig. S2** Synchrotron XP (photon energy of 610 eV) spectrum of the O 1s region of THB adsorbed on Cu(111) after deposition of THB at RT.

The thermal load provided by the laboratory X-ray source caused a temperature increase of the sample as noted in the experimental section. Therefore, we provide the spectrum collected at a synchrotron facility (Astrid, located in Aarhus) that is void of this problem. The dehydrogenation level deduced from the spectrum (intensity ratio as judged form the areas under the peaks) amounts to 30%.

## 4. Computational Details

Density functional theory calculations were performed with the GPAW[2] software, a grid based implementation of the projector augmented wave method, [3] using the ASE interface.[4] To ensure convergence of relative energies a grid spacing of 0.16 Å was used. The meta-GGA functional M06-L[5] was used to describe the exchange and correlation contributions to the total energy, as it has previously been shown to give good results for the adsorption of aromatic molecules on transition metal surfaces.[6] 4 layers of copper with 25 atoms in each layer were used to model the surface. The bottom layer was fixed in the geometry of the bulk using the lattice constant of 3.59 Å obtained with the M06-L functional (to be compared with the experimental value of 3.61 Å [7]). Periodic boundary conditions were used in the x- and y-directions, while the z-direction remained aperiodic with a minimum of 6 Å of vacuum between the slab and the cell boundary. Starting configurations with the centre of the molecule at the top, bridge and hollow sites were tried for both the THB and the DHBQ molecule. Initial tests showed that the energy difference between adsorption configurations at fcc and hcp hollow sites were within the accuracy of the calculations and therefore only the fcc site was calculated at high accuracy. The molecule was oriented parallel to the surface and the 8 different orientations shown in Fig. S3a-h were tried for the bridge site, whereas only two different orientations were tried at the top(i-j) and the hollow(k-l) site due to the higher symmetry of these sites. In addition a vertical configuration(m-n) was tried for both molecules. This was found to have a considerably higher energy than the flat configuration with the lowest energy, and as the experimentally observed corrugation is not consistent with an upright orientation of the molecule, no exhaustive search in vertical configurations was performed.

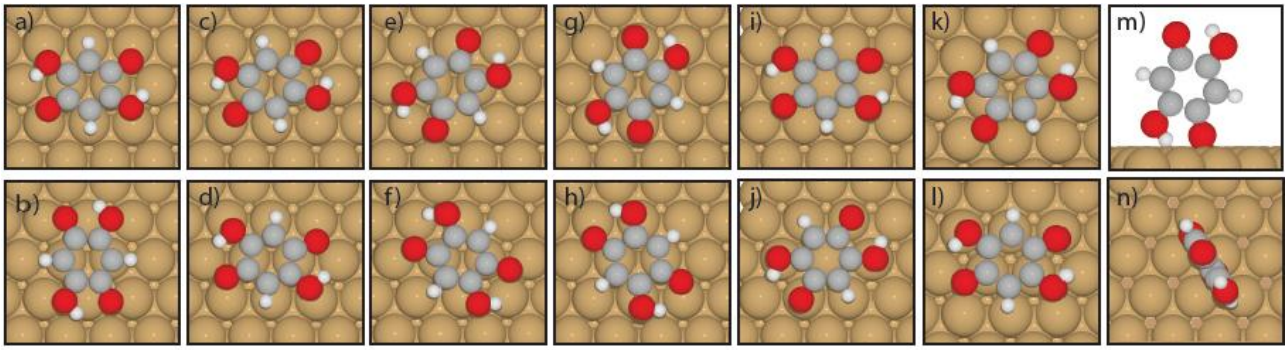


**Figure S3**: Calculated adsorption configurations for DHBQ at the bridge site a-h), top site i-j), hollow site k-l) as well as the calculated vertical configuration seen in side m) and top n) view.

All structures were relaxed down to a maximum force of 0.05 eV/Å with 2x2 k-points. The structure with the lowest energy was selected for both THB and DHBQ and relaxed with 4x4 k-points to get a more accurate value of the adsorption energy. This configuration was also used to make simulated STM images based on the Tersoff-Hamann model[8], and for calculations of the core level shifts.

**Adsorption energies**

The adsorption energies, Eads, of the molecules are calculated as:

$$E_{ads} = E_{tot} - E_{Cu} - E_{THB} + n \cdot E_{H_2} \tag{1}$$

where $E_{tot}$ is the total energy of the molecule on the surface and $E_{Cu}$ and $E_{THB}$ are the energies of the surface and the molecule respectively. $E_{H_2}$ is the energy of a hydrogen molecule with n = 0 for THB and n = 1 for DHBQ.

The energy calculated by DFT concerns the electronic energy at 0 K only. To be able to compare the stability of THB and DHBQ, we need to consider the free energy of adsorption, F:

$$F = E_{ads} - T \cdot S \tag{2}$$

The entropies of THB and DHBQ are expected to be of a similar size and are therefore not included here, but the reaction also produces molecular hydrogen which has a high entropy in the gas phase, in particular at the low pressure in the STM chamber. The entropy of a hydrogen molecule at room temperature as a function of the pressure (p) is given by:

$$S_{H_2}(p) = S^{\oplus}_{H_2} - R \cdot ln\left(\frac{p}{p_0}\right) \tag{3}$$

where $S^{\oplus}_{H_2}$ is the standard molar entropy of hydrogen [9] and $p_0$ is the standard pressure. The exact pressure at the surface during the experiment is unknown, but a conservative estimate is $10^{-9}$ mbar. The corresponding contribution to the free energy is -1.11 eV per $H_2$ molecule at 298 K. The magnitude of the entropy term, and therefore also the pressure, is crucial to the energetic balance of the reaction. The maximum pressure at which the reaction would occur (neglecting zero point energy effects, see below) is found to be $6 \cdot 10^{-7}$ mbar.

The reaction also changes the zero point energy (ZPE), but a full calculation of all vibrational modes is beyond the scope of this article. The dominating change is expected to be due to the high frequency stretching modes in $H_2$(g) (4400 $cm^{-1}$ [7]) and in the hydroxyl groups (~ 3600 $cm^{-1}$). When the hydrogens from two hydroxyl groups of the THB molecule react to form a desorbing hydrogen molecule, these frequencies give rise to a change in zero point energy, ΔZPE:

$$\Delta ZPE\left(2 \cdot OH \rightarrow H_2\right) = \frac{1}{2} \cdot \hbar \cdot \omega_{H_2} - 2 \cdot \left(\frac{1}{2} \cdot \hbar \cdot \omega_{OH}\right) = -0.17\ eV \tag{4}$$

Some changes will also occur in the C-O and C-C vibrational modes, however the extent of these changes depends on how strongly the carbonyls bind to the surface. Some bond lengths found in the THB and DHBQ molecules on the surface and in the gas phase are given in table S1 (cf. Fig. S5 for numbering of the atoms). The relatively short Cu-O distance for the carbonyl oxygen (Cu(6)-O(9)) of DHBQ indicates a partial bond to the surface. This leads to an elongation of the carbonyl group (C(8)-O(9)) from 1.23 Å, typical of a double bond, when the molecule is in the gas phase, to 1.31 Å, which is intermediate between a single and a double bond, when the molecule is at the surface. This in turn influences the character of the bonding in the carbon ring, which is aromatic in the THB molecule when all C-O bonds are single bonds, but non-aromatic in DHBQ when two of the C-O bonds are double bonds. The interaction between DHBQ and the surface results in the C-C bond lengths becoming more similar, indicating that aromaticity is partially regained, however the remaining differences in C-C bond length and the buckling of the ring reveal that the pi-system is not fully restored.

The change in ZPE due to the changed character of the C-O and C-C bonds is therefore not easily estimated, but as the frequencies associated with these bonds are relatively small (< 2000 $cm^{-1}$), their contributions to ΔZPE are also expected to be small, and we consider the result in (4) a reasonable estimate of ΔZPE.

**Table S1**: Bond lengths in THB and DHBQ in Å. The numbering of the atoms is shown in figure S5.

| | C(2)-O(5) | C(3)-O(4) | C(1)-C(2) | C(2)-C(3) | C(3)-C(1) | O(5)-Cu(6) | O(4)-Cu(7) | C(1)-Cu plane | C(2)-Cu plane | C(3)-Cu plane |
|---|---|---|---|---|---|---|---|---|---|---|
| THB (gas) | 1.37 | 1.36 | 1.38 | 1.39 | 1.38 | - | - | - | - | - |
| THB (surf) | 1.37 | 1.36 | 1.39 | 1.39 | 1.39 | 3.23 | 3.03 | 2.86 | 2.88 | 2.86 |

| | C(8)-O(9) | C(3)-O(10) | C(1)-C(8) | C(8)-C(3) | C(3)-C(1) | O(9)-Cu(6) | O(10)-Cu(7) | C(1)-Cu plane | C(8)-Cu plane | C(3)-Cu plane |
|---|---|---|---|---|---|---|---|---|---|---|
| DHBQ(gas) | 1.23 | 1.32 | 1.43 | 1.50 | 1.35 | - | - | - | - | - |
| DHBQ(surf) | 1.31 | 1.35 | 1.42 | 1.43 | 1.39 | 2.27 | 2.79 | 2.30 | 2.21 | 2.34 |

**Core level shifts**

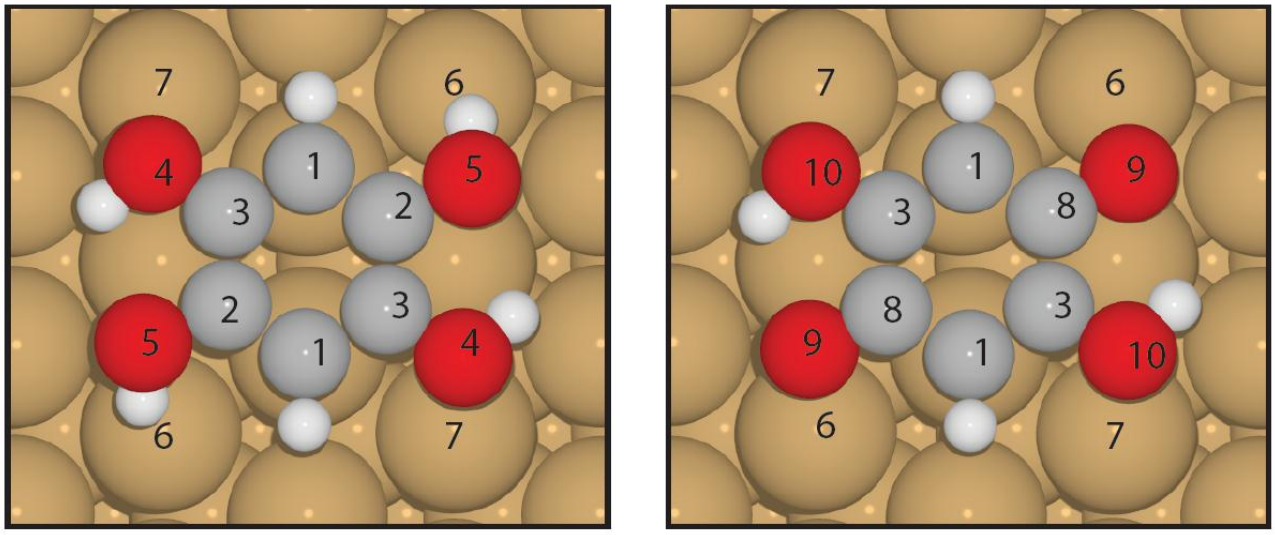


**Figure S4**: Numbering of atoms in THB(left) and DHBQ (right).

Core level shifts were calculated as the difference in total energy when one electron is removed from the 1s level of a selected atom ($E_{atom}$), compared to the energy when the core electron is removed on a reference atom ($E_{ref}$). The carbon bound to hydrogen (C(1) in Fig. S4) and the oxygen in the alcohol group (O(4) in Fig. S4) are used as reference atoms for the C1s and O1s shifts respectively. The sign convention is that a positive shift represents a shift towards higher binding energies, giving that:

$$\Delta_{CL} = E_{atom} - E_{ref} \quad (5)$$

The core level shifts calculated for the single (isolated) molecule on the surface in the optimised adsorption geometry are given in table S2. The core level shift calculations for an isolated DHBQ molecule on the surface predict a BE that is 2.95 eV higher for the hydroxyl oxygen compared to the carbonyl oxygen. This confirms the assignment of the experimental peaks, though the magnitude of the shift is overestimated. As the intermolecular hydrogen bonding affects the adsorption geometry and electronic structure, only a qualitative agreement with experiment is expected. In fact, a reduction in the difference of the core level binding energies of up to 1 eV for different oxygen species (C=O and C-O-H) in formic acid due to hydrogen bonding interactions have been reported in literature.[10] Similarly, hydrogen bonding between hydroxyl and carbonyl groups in the DHBQ overlayer is thought to reduce the difference in O1s binding energy between these two species in an analogous fashion. Taking this into account, the calculations agree reasonably well with the experimental value. The C1s shifts show almost perfect agreement with experiment, predicting peak separations of 1.26 eV between C3 and C1 carbons (cf. Fig. 4b for labelling) and 1.34 eV between C2 and C1 carbons. This renders the experimental observation of a single peak, comprising both C2 and C3 species, plausible.

**Table S2**: Calculated values of the core level shifts in eV as well as the experimental values at RT. The numbering of the atoms is shown in figure S4.

| | C(2) | C(3) | O(5) |
|---|---|---|---|
| Exp | 1.4 | 1.4 | 1.9 (THB) /1.8 (DHBQ) |
| Calc. THB | 1.50 | 1.50 | - |
| Calc (DHBQ) | 1.26 | 1.34 | 2.95 |

**Structural model**

The structural model is based on the optimised hydrogen bonding pattern in the gas phase. To calculate this, one molecule is placed in a unit cell with $|a| = |b| = 7.5$ Å and $< (a, b) = 60^{o}$, corresponding to the experimentally observed unit cell, and periodic boundary conditions. The molecule is rotated in steps of 4º, thereby probing all possible structures under the assumption that all molecules have the same orientation. The orientation is kept fixed by fixing the two carbon atoms on either side of the ring that are bound to hydrogen (C1 in Fig. S4), and the rest of the molecule is relaxed freely. The energy as a function of the orientation shows a clear minimum when the molecules form parallel rows inter-linked via double hydrogen bonds. As the experiment does not exclude a structure where the molecules have different orientations, all possible combinations of orientations (in steps of 10º) for two molecules in a unit cell were also tried. However, the lowest energy was still found when both molecules have the same orientation.
The optimised gas phase structure is transferred to a 22.5x22.5 $Å^2$ slab of copper with an orientation with respect to the Cu<110> direction of 17º(Fig. S5). This slab is the smallest possible able to accommodate an integer multiple of the experimentally observed unit cells for the overlayer. Since the molecular overlayer and the substrate are not directly commensurate, the molecules occupy inequivalent adsorption sites within the computational unit cell. Due to the large size of the cell the structure is only relaxed on two layers of copper with 2x2 k-points meaning that the calculated total energy gain from adsorption and hydrogen bonding is not sufficiently accurate to be included in this discussion.

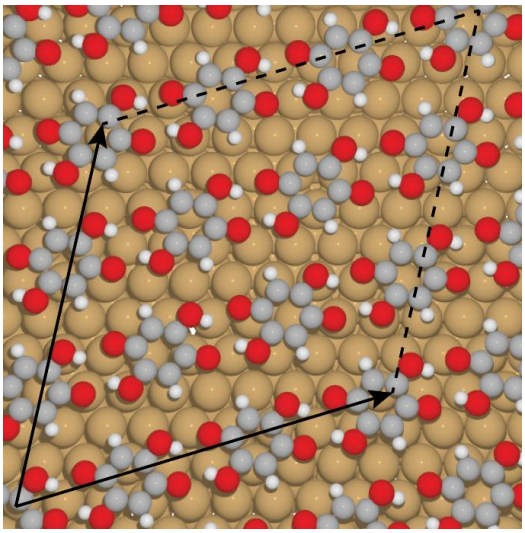

**Figure S5:** DHBQ overlayer structure. The computational unit cell is marked.

**Adsorption structures for 4,5-dihydroxybenzo-1,2-dione**

The molecule 4,5-dihydroxybenzo-1,2-dione has the same stoichiometry as DHBQ (2,5-dihydroxybenzo-1,4-dione) and is expected to provide a very similar XPS signal. It might therefore be considered an alternative dehydrogenation product. However, oxidation of hydroxybenzenes generally leads to para-quinone derivatives while ortho-quionones are synthesized by more complicated multi- step approaches. The reason is stabilization of the p-semiquinone intermediate in contrast to the o-semiquinone owing to charge separation. From organic synthesis considerations DHBQ is thus the anticipated dehydrogenation product. We nevertheless performed calculations for adsorbed 4,5-dihydroxybenzo-1,2-dione as reported in Fig. S6. For an isolated molecule, an upright configuration is most stable (Fig. S6a-b) with a binding energy of -1.51 eV (comp. -1.31 eV for DHBQ), but an upright geometry does not allow for hydrogen bonding. The second best geometry (Fig. S6c-d) with a binding energy of -1.38 eV has a tilt of ~21˚ which leads to a slight asymmetry in the simulated STM-images (Fig. S6e). Hydrogen-bonded structures were made for DHBQ and for 4,5-dihydroxybenzo-1,2-dione in a commensurate 3x3 cell (approximating the experimentally observed unit cell size), in both cases such that each molecule makes two hydrogen bonds to one of its neighbours (Fig. S4f-g). In these calculations the DHBQ structure is more stable by 0.23 eV. From the higher stability of the hydrogen-bonded phase for DHBQ and the good agreement in the STM data for DHBQ and annealed THB we conclude the dehydrogenation product is DHBQ.

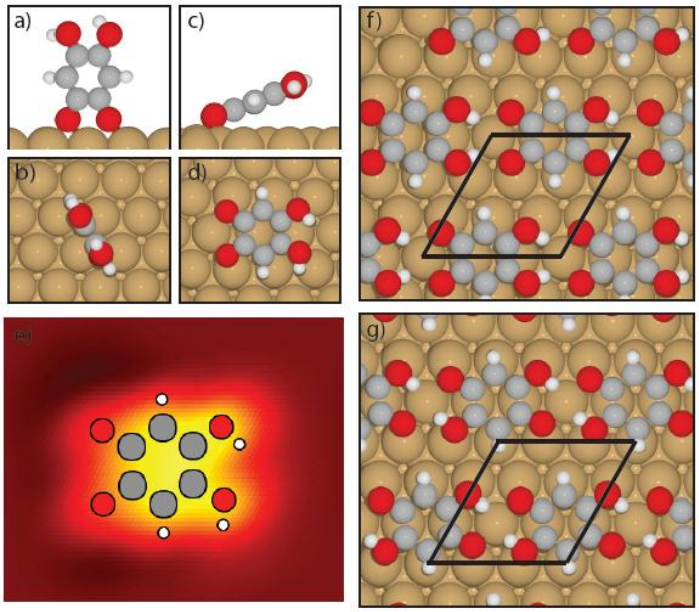


**Figure S6:** Most stable adsorption configuration for 4,5-dihydroxybenzo-1,2-dione in side (a) and top (b) view. The most stable non-vertical adsorption geometry (c-d) gives rise to an asymmetry in the simulated STM image (e). Hydrogen bonded structures of 4,5-dihydroxybenzo-1,2-dione (f) and DHBQ (g) are calculated in the commensurate unit cell marked in black.

**Coordinates**
Coordinates of optimised structures:

**THB on Cu, 4x4:**
E = -952.3449

| | | | | |
|---|---|---|---|---|
| 0 | Cu | 0.0000 | 0.0000 | 7.0000 |
| 1 | Cu | 2.5385 | 0.0000 | 7.0000 |
| 2 | Cu | 5.0770 | 0.0000 | 7.0000 |
| 3 | Cu | 7.6155 | 0.0000 | 7.0000 |
| 4 | Cu | 10.1541 | 0.0000 | 7.0000 |
| 5 | Cu | 1.2693 | 2.1984 | 7.0000 |
| 6 | Cu | 3.8078 | 2.1984 | 7.0000 |
| 7 | Cu | 6.3463 | 2.1984 | 7.0000 |
| 8 | Cu | 8.8848 | 2.1984 | 7.0000 |
| 9 | Cu | 11.4233 | 2.1984 | 7.0000 |
| 10 | Cu | 2.5385 | 4.3968 | 7.0000 |
| 11 | Cu | 5.0770 | 4.3968 | 7.0000 |
| 12 | Cu | 7.6155 | 4.3968 | 7.0000 |
| 13 | Cu | 10.1541 | 4.3968 | 7.0000 |
| 14 | Cu | 12.6926 | 4.3968 | 7.0000 |
| 15 | Cu | 3.8078 | 6.5953 | 7.0000 |
| 16 | Cu | 6.3463 | 6.5953 | 7.0000 |
| 17 | Cu | 8.8848 | 6.5953 | 7.0000 |
| 18 | Cu | 11.4233 | 6.5953 | 7.0000 |
| 19 | Cu | 13.9618 | 6.5953 | 7.0000 |
| 20 | Cu | 5.0770 | 8.7937 | 7.0000 |
| 21 | Cu | 7.6155 | 8.7937 | 7.0000 |
| 22 | Cu | 10.1541 | 8.7937 | 7.0000 |
| 23 | Cu | 12.6926 | 8.7937 | 7.0000 |
| 24 | Cu | 15.2311 | 8.7937 | 7.0000 |
| 25 | Cu | 1.2811 | 0.7371 | 9.0509 |
| 26 | Cu | 3.8140 | 0.7235 | 9.0520 |
| 27 | Cu | 6.3440 | 0.7371 | 9.0532 |
| 28 | Cu | 8.8761 | 0.7221 | 9.0516 |
| 29 | Cu | 11.4150 | 0.7359 | 9.0518 |

| | | | | |
|---|---|---|---|---|
| 30 | Cu | 2.5323 | 2.9405 | 9.0508 |
| 31 | Cu | 5.0696 | 2.9262 | 9.0587 |
| 32 | Cu | 7.6234 | 2.9273 | 9.0591 |
| 33 | Cu | 10.1574 | 2.9420 | 9.0517 |
| 34 | Cu | 12.6914 | 2.9259 | 9.0598 |
| 35 | Cu | 3.8091 | 5.1255 | 9.0502 |
| 36 | Cu | 6.3450 | 5.1343 | 9.0542 |
| 37 | Cu | 8.8803 | 5.1265 | 9.0528 |
| 38 | Cu | 11.4224 | 5.1339 | 9.0557 |
| 39 | Cu | 13.9525 | 5.1289 | 9.0577 |
| 40 | Cu | 5.0642 | 7.3270 | 9.0509 |
| 41 | Cu | 7.6262 | 7.3268 | 9.0494 |
| 42 | Cu | 10.1560 | 7.3235 | 9.0570 |
| 43 | Cu | 12.6918 | 7.3276 | 9.0604 |
| 44 | Cu | 15.2271 | 7.3271 | 9.0562 |
| 45 | Cu | 6.3460 | 9.5188 | 9.0541 |
| 46 | Cu | 8.8800 | 9.5287 | 9.0589 |
| 47 | Cu | 11.4174 | 9.5180 | 9.0551 |
| 48 | Cu | 13.9593 | 9.5229 | 9.0570 |
| 49 | Cu | 16.5040 | 9.5284 | 9.0628 |
| 50 | Cu | 0.0099 | 1.4616 | 11.0986 |
| 51 | Cu | 2.5349 | 1.4627 | 11.1085 |
| 52 | Cu | 5.0740 | 1.4680 | 11.1145 |
| 53 | Cu | 7.6038 | 1.4635 | 11.1058 |
| 54 | Cu | 10.1630 | 1.4612 | 11.0962 |
| 55 | Cu | 1.2809 | 3.6615 | 11.1138 |
| 56 | Cu | 3.8044 | 3.6606 | 11.1086 |
| 57 | Cu | 6.3444 | 3.6624 | 11.1212 |
| 58 | Cu | 8.8829 | 3.6757 | 11.1135 |
| 59 | Cu | 11.4174 | 3.6657 | 11.1059 |
| 60 | Cu | 2.5333 | 5.8646 | 11.1159 |
| 61 | Cu | 5.0662 | 5.8541 | 11.0981 |
| 62 | Cu | 7.6118 | 5.8606 | 11.1004 |
| 63 | Cu | 10.1648 | 5.8686 | 11.1226 |
| 64 | Cu | 12.6947 | 5.8556 | 11.1184 |
| 65 | Cu | 3.8146 | 8.0525 | 11.1171 |
| 66 | Cu | 6.3465 | 8.0701 | 11.0993 |
| 67 | Cu | 8.8801 | 8.0606 | 11.1062 |
| 68 | Cu | 11.4172 | 8.0672 | 11.1149 |
| 69 | Cu | 13.9736 | 8.0673 | 11.1165 |
| 70 | Cu | 5.0728 | 10.2549 | 11.1140 |
| 71 | Cu | 7.6248 | 10.2562 | 11.1122 |
| 72 | Cu | 10.1600 | 10.2719 | 11.1112 |
| 73 | Cu | 12.6908 | 10.2529 | 11.1127 |
| 74 | Cu | 15.2293 | 10.2681 | 11.1159 |
| 75 | Cu | 0.0021 | 0.0011 | 13.1678 |
| 76 | Cu | 2.5325 | 0.0012 | 13.1681 |
| 77 | Cu | 5.0623 | -0.0012 | 13.1676 |
| 78 | Cu | 7.6311 | -0.0038 | 13.1607 |
| 79 | Cu | 10.1646 | 0.0005 | 13.1705 |
| 80 | Cu | 1.2761 | 2.1905 | 13.1695 |
| 81 | Cu | 3.8142 | 2.2026 | 13.1693 |
| 82 | Cu | 6.3413 | 2.1784 | 13.1771 |
| 83 | Cu | 8.8893 | 2.1908 | 13.1211 |
| 84 | Cu | 11.4623 | 2.1997 | 13.1299 |
| 85 | Cu | 2.5324 | 4.3849 | 13.1688 |
| 86 | Cu | 5.0567 | 4.4059 | 13.1631 |
| 87 | Cu | 7.6004 | 4.3975 | 13.1605 |
| 88 | Cu | 10.1707 | 4.3865 | 13.1587 |
| 89 | Cu | 12.7010 | 4.4042 | 13.1648 |
| 90 | Cu | 3.8160 | 6.6073 | 13.1704 |
| 91 | Cu | 6.3316 | 6.5931 | 13.1273 |
| 92 | Cu | 8.8747 | 6.6166 | 13.1334 |
| 93 | Cu | 11.4557 | 6.6161 | 13.1772 |

| | | | |
|---|---|---|---|
| 94 Cu | 13.9782 | 6.5919 | 13.1714 |
| 95 Cu | 5.0821 | 8.7988 | 13.1719 |
| 96 Cu | 7.6110 | 8.8004 | 13.1688 |
| 97 Cu | 10.1568 | 8.7978 | 13.1570 |
| 98 Cu | 12.6972 | 8.8112 | 13.1693 |
| 99 Cu | 15.2274 | 8.7917 | 13.1745 |
| 100 O | 7.6610 | 6.8722 | 16.1100 |
| 101 O | 10.3405 | 6.7364 | 15.9818 |
| 102 O | 7.4325 | 2.0734 | 16.0203 |
| 103 O | 10.1162 | 1.9456 | 16.1054 |
| 104 C | 10.2763 | 4.3702 | 16.0160 |
| 105 C | 7.4949 | 4.4416 | 16.0322 |
| 106 C | 9.5515 | 3.1886 | 16.0422 |
| 107 C | 8.1585 | 3.2216 | 16.0300 |
| 108 C | 9.6127 | 5.5896 | 16.0122 |
| 109 C | 8.2201 | 5.6243 | 16.0426 |
| 110 H | 11.3413 | 4.3563 | 16.0236 |
| 111 H | 6.4303 | 4.4536 | 16.0511 |
| 112 H | 6.8041 | 6.8807 | 15.6575 |
| 113 H | 9.7218 | 7.4752 | 15.8698 |
| 114 H | 8.0467 | 1.3335 | 15.8913 |
| 115 H | 10.9893 | 1.9574 | 15.6864 |

**DHBQ on Cu, 4x4:**
E = -944.2071

| | | | |
|---|---|---|---|
| 0 Cu | 0.0000 | 0.0000 | 7.0000 |
| 1 Cu | 2.5385 | 0.0000 | 7.0000 |
| 2 Cu | 5.0770 | 0.0000 | 7.0000 |
| 3 Cu | 7.6155 | 0.0000 | 7.0000 |
| 4 Cu | 10.1541 | 0.0000 | 7.0000 |
| 5 Cu | 1.2693 | 2.1984 | 7.0000 |
| 6 Cu | 3.8078 | 2.1984 | 7.0000 |
| 7 Cu | 6.3463 | 2.1984 | 7.0000 |
| 8 Cu | 8.8848 | 2.1984 | 7.0000 |
| 9 Cu | 11.4233 | 2.1984 | 7.0000 |
| 10 Cu | 2.5385 | 4.3968 | 7.0000 |
| 11 Cu | 5.0770 | 4.3968 | 7.0000 |
| 12 Cu | 7.6155 | 4.3968 | 7.0000 |
| 13 Cu | 10.1541 | 4.3968 | 7.0000 |
| 14 Cu | 12.6926 | 4.3968 | 7.0000 |
| 15 Cu | 3.8078 | 6.5953 | 7.0000 |
| 16 Cu | 6.3463 | 6.5953 | 7.0000 |
| 17 Cu | 8.8848 | 6.5953 | 7.0000 |
| 18 Cu | 11.4233 | 6.5953 | 7.0000 |
| 19 Cu | 13.9618 | 6.5953 | 7.0000 |
| 20 Cu | 5.0770 | 8.7937 | 7.0000 |
| 21 Cu | 7.6155 | 8.7937 | 7.0000 |
| 22 Cu | 10.1541 | 8.7937 | 7.0000 |
| 23 Cu | 12.6926 | 8.7937 | 7.0000 |
| 24 Cu | 15.2311 | 8.7937 | 7.0000 |
| 25 Cu | 1.2678 | 0.7434 | 9.0481 |
| 26 Cu | 3.8071 | 0.7319 | 9.0327 |
| 27 Cu | 6.3414 | 0.7422 | 9.0399 |
| 28 Cu | 8.8779 | 0.7291 | 9.0415 |
| 29 Cu | 11.4169 | 0.7415 | 9.0465 |
| 30 Cu | 2.5337 | 2.9458 | 9.0392 |
| 31 Cu | 5.0691 | 2.9314 | 9.0373 |
| 32 Cu | 7.6208 | 2.9323 | 9.0368 |
| 33 Cu | 10.1585 | 2.9454 | 9.0456 |
| 34 Cu | 12.6911 | 2.9302 | 9.0550 |
| 35 Cu | 3.8192 | 5.1353 | 9.0528 |
| 36 Cu | 6.3440 | 5.1437 | 9.0483 |
| 37 Cu | 8.8764 | 5.1291 | 9.0422 |

| | | | | |
|---|---|---|---|---|
| 38 | Cu | 11.4296 | 5.1275 | 9.0492 |
| 39 | Cu | 13.9708 | 5.1433 | 9.0444 |
| 40 | Cu | 5.0649 | 7.3296 | 9.0541 |
| 41 | Cu | 7.6229 | 7.3265 | 9.0455 |
| 42 | Cu | 10.1531 | 7.3243 | 9.0357 |
| 43 | Cu | 12.6902 | 7.3288 | 9.0449 |
| 44 | Cu | 15.2255 | 7.3460 | 9.0418 |
| 45 | Cu | 6.3440 | 9.5105 | 9.0479 |
| 46 | Cu | 8.8758 | 9.5333 | 9.0311 |
| 47 | Cu | 11.4097 | 9.5193 | 9.0343 |
| 48 | Cu | 13.9456 | 9.5326 | 9.0410 |
| 49 | Cu | 16.5011 | 9.5340 | 9.0479 |
| 50 | Cu | -0.0049 | 1.4944 | 11.1279 |
| 51 | Cu | 2.5309 | 1.4757 | 11.0820 |
| 52 | Cu | 5.0590 | 1.4827 | 11.0815 |
| 53 | Cu | 7.5960 | 1.4667 | 11.0800 |
| 54 | Cu | 10.1711 | 1.4638 | 11.0902 |
| 55 | Cu | 1.2874 | 3.6737 | 11.0894 |
| 56 | Cu | 3.8132 | 3.6909 | 11.0870 |
| 57 | Cu | 6.3423 | 3.6644 | 11.0889 |
| 58 | Cu | 8.8768 | 3.6882 | 11.0954 |
| 59 | Cu | 11.4089 | 3.6587 | 11.1240 |
| 60 | Cu | 2.5374 | 5.8753 | 11.0949 |
| 61 | Cu | 5.1079 | 5.8831 | 11.1367 |
| 62 | Cu | 7.5944 | 5.8716 | 11.1080 |
| 63 | Cu | 10.1608 | 5.8772 | 11.0881 |
| 64 | Cu | 12.6936 | 5.8636 | 11.0925 |
| 65 | Cu | 3.8089 | 8.0634 | 11.0961 |
| 66 | Cu | 6.3501 | 8.0702 | 11.1212 |
| 67 | Cu | 8.8770 | 8.0920 | 11.0715 |
| 68 | Cu | 11.4081 | 8.0752 | 11.0821 |
| 69 | Cu | 13.9675 | 8.0719 | 11.0913 |
| 70 | Cu | 5.0786 | 10.2683 | 11.0916 |
| 71 | Cu | 7.6104 | 10.2758 | 11.0840 |
| 72 | Cu | 10.1526 | 10.2869 | 11.0723 |
| 73 | Cu | 12.6789 | 10.2580 | 11.0775 |
| 74 | Cu | 15.2242 | 10.2760 | 11.0921 |
| 75 | Cu | 0.0070 | 0.0035 | 13.1457 |
| 76 | Cu | 2.5290 | 0.0437 | 13.1360 |
| 77 | Cu | 5.0542 | 0.0066 | 13.1351 |
| 78 | Cu | 7.5910 | -0.0321 | 13.1164 |
| 79 | Cu | 10.1476 | -0.0311 | 13.1525 |
| 80 | Cu | 1.2935 | 2.2359 | 13.1517 |
| 81 | Cu | 3.8150 | 2.2138 | 13.1361 |
| 82 | Cu | 6.3205 | 2.1634 | 13.1239 |
| 83 | Cu | 8.8899 | 2.1554 | 13.0508 |
| 84 | Cu | 11.4617 | 2.1929 | 13.2474 |
| 85 | Cu | 2.5403 | 4.4086 | 13.1493 |
| 86 | Cu | 5.0443 | 4.4118 | 13.1361 |
| 87 | Cu | 7.5732 | 4.3705 | 13.1098 |
| 88 | Cu | 10.1700 | 4.4592 | 13.1114 |
| 89 | Cu | 12.7128 | 4.4172 | 13.1299 |
| 90 | Cu | 3.8103 | 6.6185 | 13.1527 |
| 91 | Cu | 6.3307 | 6.6559 | 13.2665 |
| 92 | Cu | 8.8784 | 6.6563 | 13.0567 |
| 93 | Cu | 11.4716 | 6.6421 | 13.1315 |
| 94 | Cu | 13.9787 | 6.5990 | 13.1463 |
| 95 | Cu | 5.0549 | 8.8265 | 13.1460 |
| 96 | Cu | 7.6388 | 8.8483 | 13.1478 |
| 97 | Cu | 10.1634 | 8.8534 | 13.1109 |
| 98 | Cu | 12.6928 | 8.8202 | 13.1361 |
| 99 | Cu | 15.2177 | 8.7884 | 13.1431 |
| 100 | O | 7.5281 | 1.9984 | 15.6314 |
| 101 | O | 10.1919 | 1.9812 | 15.1327 |

| | | | | |
|---|---|---|---|---|
| 102 | O | 7.5506 | 6.7661 | 15.1563 |
| 103 | O | 10.2185 | 6.7444 | 15.6246 |
| 104 | C | 10.2782 | 4.3766 | 15.4346 |
| 105 | C | 7.4646 | 4.3679 | 15.4482 |
| 106 | C | 9.5605 | 5.5702 | 15.4829 |
| 107 | C | 8.1391 | 5.6087 | 15.3478 |
| 108 | C | 9.6021 | 3.1358 | 15.3399 |
| 109 | C | 8.1834 | 3.1735 | 15.4899 |
| 110 | H | 11.3353 | 4.3855 | 15.5646 |
| 111 | H | 6.4074 | 4.3574 | 15.5749 |
| 112 | H | 8.2053 | 1.2974 | 15.5668 |
| 113 | H | 9.5407 | 7.4455 | 15.5731 |

**DHB+2H(ads):**
E = -951.7786

| | | | | |
|---|---|---|---|---|
| 0 | Cu | 0.0000 | 0.0000 | 7.0000 |
| 1 | Cu | 2.5385 | 0.0000 | 7.0000 |
| 2 | Cu | 5.0770 | 0.0000 | 7.0000 |
| 3 | Cu | 7.6155 | 0.0000 | 7.0000 |
| 4 | Cu | 10.1541 | 0.0000 | 7.0000 |
| 5 | Cu | 1.2693 | 2.1984 | 7.0000 |
| 6 | Cu | 3.8078 | 2.1984 | 7.0000 |
| 7 | Cu | 6.3463 | 2.1984 | 7.0000 |
| 8 | Cu | 8.8848 | 2.1984 | 7.0000 |
| 9 | Cu | 11.4233 | 2.1984 | 7.0000 |
| 10 | Cu | 2.5385 | 4.3968 | 7.0000 |
| 11 | Cu | 5.0770 | 4.3968 | 7.0000 |
| 12 | Cu | 7.6155 | 4.3968 | 7.0000 |
| 13 | Cu | 10.1541 | 4.3968 | 7.0000 |
| 14 | Cu | 12.6926 | 4.3968 | 7.0000 |
| 15 | Cu | 3.8078 | 6.5953 | 7.0000 |
| 16 | Cu | 6.3463 | 6.5953 | 7.0000 |
| 17 | Cu | 8.8848 | 6.5953 | 7.0000 |
| 18 | Cu | 11.4233 | 6.5953 | 7.0000 |
| 19 | Cu | 13.9618 | 6.5953 | 7.0000 |
| 20 | Cu | 5.0770 | 8.7937 | 7.0000 |
| 21 | Cu | 7.6155 | 8.7937 | 7.0000 |
| 22 | Cu | 10.1541 | 8.7937 | 7.0000 |
| 23 | Cu | 12.6926 | 8.7937 | 7.0000 |
| 24 | Cu | 15.2311 | 8.7937 | 7.0000 |
| 25 | Cu | 1.2706 | 0.7404 | 9.0409 |
| 26 | Cu | 3.8115 | 0.7235 | 9.0352 |
| 27 | Cu | 6.3423 | 0.7410 | 9.0443 |
| 28 | Cu | 8.8763 | 0.7234 | 9.0505 |
| 29 | Cu | 11.4122 | 0.7409 | 9.0415 |
| 30 | Cu | 2.5321 | 2.9473 | 9.0406 |
| 31 | Cu | 5.0673 | 2.9295 | 9.0444 |
| 32 | Cu | 7.6193 | 2.9319 | 9.0417 |
| 33 | Cu | 10.1578 | 2.9442 | 9.0466 |
| 34 | Cu | 12.6894 | 2.9300 | 9.0502 |
| 35 | Cu | 3.8171 | 5.1341 | 9.0513 |
| 36 | Cu | 6.3388 | 5.1463 | 9.0601 |
| 37 | Cu | 8.8746 | 5.1246 | 9.0522 |
| 38 | Cu | 11.4311 | 5.1279 | 9.0638 |
| 39 | Cu | 13.9526 | 5.1294 | 9.0515 |
| 40 | Cu | 5.0664 | 7.3276 | 9.0521 |
| 41 | Cu | 7.6242 | 7.3242 | 9.0488 |
| 42 | Cu | 10.1556 | 7.3077 | 9.0428 |
| 43 | Cu | 12.6906 | 7.3287 | 9.0441 |
| 44 | Cu | 15.2266 | 7.3413 | 9.0394 |
| 45 | Cu | 6.3433 | 9.5076 | 9.0447 |
| 46 | Cu | 8.8794 | 9.5264 | 9.0312 |
| 47 | Cu | 11.4059 | 9.5134 | 9.0443 |

| | | | | |
|---|---|---|---|---|
| 48 | Cu | 13.9512 | 9.5336 | 9.0385 |
| 49 | Cu | 16.5066 | 9.5375 | 9.0556 |
| 50 | Cu | -0.0060 | 1.4949 | 11.1051 |
| 51 | Cu | 2.5309 | 1.4726 | 11.0738 |
| 52 | Cu | 5.0585 | 1.4758 | 11.0856 |
| 53 | Cu | 7.5931 | 1.4628 | 11.0856 |
| 54 | Cu | 10.1682 | 1.4604 | 11.0889 |
| 55 | Cu | 1.2813 | 3.6633 | 11.1111 |
| 56 | Cu | 3.8094 | 3.6919 | 11.0874 |
| 57 | Cu | 6.3405 | 3.6653 | 11.0932 |
| 58 | Cu | 8.8805 | 3.6644 | 11.1127 |
| 59 | Cu | 11.4072 | 3.6595 | 11.1239 |
| 60 | Cu | 2.5315 | 5.8749 | 11.0860 |
| 61 | Cu | 5.0689 | 5.9047 | 11.1591 |
| 62 | Cu | 7.5858 | 5.8651 | 11.1176 |
| 63 | Cu | 10.1571 | 5.8689 | 11.1039 |
| 64 | Cu | 12.7036 | 5.8929 | 11.1186 |
| 65 | Cu | 3.8065 | 8.0787 | 11.0884 |
| 66 | Cu | 6.3499 | 8.0679 | 11.1169 |
| 67 | Cu | 8.8782 | 8.0732 | 11.0760 |
| 68 | Cu | 11.4092 | 8.0710 | 11.0845 |
| 69 | Cu | 13.9741 | 8.0757 | 11.0845 |
| 70 | Cu | 5.1106 | 10.2838 | 11.1099 |
| 71 | Cu | 7.6186 | 10.2685 | 11.0722 |
| 72 | Cu | 10.1383 | 10.2830 | 11.1001 |
| 73 | Cu | 12.6801 | 10.2522 | 11.0757 |
| 74 | Cu | 15.2294 | 10.2619 | 11.1132 |
| 75 | Cu | 0.0147 | 0.0038 | 13.1699 |
| 76 | Cu | 2.5251 | 0.0370 | 13.1740 |
| 77 | Cu | 5.0503 | 0.0003 | 13.1346 |
| 78 | Cu | 7.5825 | -0.0415 | 13.1136 |
| 79 | Cu | 10.1539 | -0.0457 | 13.1413 |
| 80 | Cu | 1.2687 | 2.1928 | 13.1753 |
| 81 | Cu | 3.8209 | 2.2138 | 13.1239 |
| 82 | Cu | 6.3164 | 2.1596 | 13.1309 |
| 83 | Cu | 8.8742 | 2.1244 | 13.0665 |
| 84 | Cu | 11.4137 | 2.1783 | 13.2160 |
| 85 | Cu | 2.5292 | 4.3745 | 13.1394 |
| 86 | Cu | 5.0431 | 4.4111 | 13.1348 |
| 87 | Cu | 7.5706 | 4.3609 | 13.1188 |
| 88 | Cu | 10.1637 | 4.4525 | 13.1230 |
| 89 | Cu | 12.7092 | 4.4124 | 13.1235 |
| 90 | Cu | 3.7939 | 6.6197 | 13.1875 |
| 91 | Cu | 6.3260 | 6.6482 | 13.2600 |
| 92 | Cu | 8.8722 | 6.6469 | 13.0666 |
| 93 | Cu | 11.4721 | 6.6372 | 13.1394 |
| 94 | Cu | 13.9872 | 6.5959 | 13.1853 |
| 95 | Cu | 5.0784 | 8.8260 | 13.1241 |
| 96 | Cu | 7.6423 | 8.8330 | 13.1322 |
| 97 | Cu | 10.1616 | 8.8220 | 13.1138 |
| 98 | Cu | 12.6815 | 8.8180 | 13.1253 |
| 99 | Cu | 15.2172 | 8.7790 | 13.1887 |
| 100 | O | 7.5282 | 1.9992 | 15.6378 |
| 101 | O | 10.1871 | 1.9807 | 15.1333 |
| 102 | O | 7.5525 | 6.7651 | 15.1608 |
| 103 | O | 10.2191 | 6.7440 | 15.6326 |
| 104 | C | 10.2814 | 4.3777 | 15.4385 |
| 105 | C | 7.4619 | 4.3664 | 15.4430 |
| 106 | C | 9.5606 | 5.5698 | 15.4916 |
| 107 | C | 8.1387 | 5.6079 | 15.3555 |
| 108 | C | 9.6033 | 3.1369 | 15.3470 |
| 109 | C | 8.1834 | 3.1742 | 15.4899 |
| 110 | H | 11.3389 | 4.3862 | 15.5698 |
| 111 | H | 6.4051 | 4.3577 | 15.5806 |

112 H 8.2032 1.2970 15.5692
113 H 9.5427 7.4457 15.5746
114 H 15.2215 7.3342 14.1695
115 H 1.2561 0.7371 14.1544

**Cu slab, 4x4:**
E = -829.9448

0 Cu 0.0000 0.0000 7.0000
1 Cu 2.5385 0.0000 7.0000
2 Cu 5.0770 0.0000 7.0000
3 Cu 7.6155 0.0000 7.0000
4 Cu 10.1541 0.0000 7.0000
5 Cu 1.2693 2.1984 7.0000
6 Cu 3.8078 2.1984 7.0000
7 Cu 6.3463 2.1984 7.0000
8 Cu 8.8848 2.1984 7.0000
9 Cu 11.4233 2.1984 7.0000
10 Cu 2.5385 4.3968 7.0000
11 Cu 5.0770 4.3968 7.0000
12 Cu 7.6155 4.3968 7.0000
13 Cu 10.1541 4.3968 7.0000
14 Cu 12.6926 4.3968 7.0000
15 Cu 3.8078 6.5953 7.0000
16 Cu 6.3463 6.5953 7.0000
17 Cu 8.8848 6.5953 7.0000
18 Cu 11.4233 6.5953 7.0000
19 Cu 13.9618 6.5953 7.0000
20 Cu 5.0770 8.7937 7.0000
21 Cu 7.6155 8.7937 7.0000
22 Cu 10.1541 8.7937 7.0000
23 Cu 12.6926 8.7937 7.0000
24 Cu 15.2311 8.7937 7.0000
25 Cu 1.2756 0.7365 9.0676
26 Cu 3.8116 0.7240 9.0656
27 Cu 6.3457 0.7373 9.0686
28 Cu 8.8787 0.7237 9.0655
29 Cu 11.4148 0.7366 9.0673
30 Cu 2.5328 2.9390 9.0656
31 Cu 5.0670 2.9255 9.0674
32 Cu 7.6232 2.9260 9.0672
33 Cu 10.1582 2.9391 9.0657
34 Cu 12.6916 2.9267 9.0720
35 Cu 3.8114 5.1268 9.0686
36 Cu 6.3456 5.1389 9.0672
37 Cu 8.8794 5.1265 9.0683
38 Cu 11.4237 5.1312 9.0673
39 Cu 13.9572 5.1300 9.0670
40 Cu 5.0661 7.3274 9.0655
41 Cu 7.6244 7.3277 9.0657
42 Cu 10.1556 7.3276 9.0673
43 Cu 12.6917 7.3276 9.0729
44 Cu -0.00009 -0.00654 -0.03061
45 Cu 0.00175 0.02717 -0.02204
46 Cu 0.04067 -0.02160 -0.03335
47 Cu -0.00067 -0.00112 -0.03094
48 Cu -0.00571 0.00320 -0.03060
49 Cu -0.03929 -0.02269 -0.03347
50 Cu -0.00120 -0.03842 -0.04870
51 Cu 0.02583 0.01491 -0.06127
52 Cu 0.00605 -0.00718 -0.04539
53 Cu 0.00218 -0.00036 -0.04544
54 Cu -0.02688 0.01444 -0.06169

| | | | | |
|---|---|---|---|---|
| 55 | Cu | -0.05097 | -0.00737 | -0.03735 |
| 56 | Cu | -0.00319 | 0.00882 | -0.04539 |
| 57 | Cu | -0.00173 | -0.00100 | -0.03468 |
| 58 | Cu | 0.00408 | 0.00841 | -0.04572 |
| 59 | Cu | 0.04813 | -0.00542 | -0.03726 |
| 60 | Cu | 0.03549 | -0.02130 | -0.03401 |
| 61 | Cu | 0.00078 | 0.00207 | -0.04544 |
| 62 | Cu | 0.00933 | -0.00067 | -0.04572 |
| 63 | Cu | -0.03674 | -0.02121 | -0.03382 |
| 64 | Cu | -0.00185 | 0.03272 | -0.04710 |
| 65 | Cu | -0.02112 | 0.04420 | -0.03863 |
| 66 | Cu | -0.00094 | -0.03049 | -0.06169 |
| 67 | Cu | 0.01937 | 0.04440 | -0.03726 |
| 68 | Cu | 0.02741 | -0.01796 | -0.04710 |
| 69 | Cu | -0.02922 | -0.01687 | -0.04754 |
| 70 | Cu | 0.03102 | 0.01791 | -0.05022 |
| 71 | Cu | -0.03387 | 0.01818 | -0.04870 |
| 72 | Cu | -0.03187 | -0.04045 | -0.03735 |
| 73 | Cu | -0.00071 | 0.04139 | -0.03401 |
| 74 | Cu | 0.02772 | -0.04039 | -0.03863 |
| 75 | Cu | 0.00085 | 0.00049 | -0.00876 |
| 76 | Cu | 0.00682 | 0.00281 | -0.00476 |
| 77 | Cu | 0.04824 | 0.00052 | -0.01512 |
| 78 | Cu | -0.04749 | 0.00117 | -0.01623 |
| 79 | Cu | -0.00486 | 0.00369 | -0.00596 |
| 80 | Cu | 0.00584 | 0.00450 | -0.00476 |
| 81 | Cu | -0.04219 | -0.02436 | -0.00414 |
| 82 | Cu | 0.00109 | 0.02818 | -0.00973 |
| 83 | Cu | 0.04238 | -0.02364 | -0.00344 |
| 84 | Cu | -0.00239 | 0.00380 | -0.00437 |
| 85 | Cu | 0.02457 | 0.04151 | -0.01512 |
| 86 | Cu | 0.02494 | -0.01315 | -0.00973 |
| 87 | Cu | -0.02305 | -0.01331 | -0.00893 |
| 88 | Cu | -0.02432 | 0.04290 | -0.01543 |
| 89 | Cu | 0.00042 | -0.04814 | -0.00728 |
| 90 | Cu | -0.02273 | -0.04171 | -0.01623 |
| 91 | Cu | 0.00072 | 0.04852 | -0.00344 |
| 92 | Cu | 0.02499 | -0.04251 | -0.01543 |
| 93 | Cu | 0.02620 | 0.01513 | -0.01365 |
| 94 | Cu | -0.02381 | 0.01384 | -0.01462 |
| 95 | Cu | 0.00076 | -0.00605 | -0.00596 |
| 96 | Cu | 0.00209 | -0.00397 | -0.00437 |
| 97 | Cu | -0.04148 | 0.02443 | -0.00728 |
| 98 | Cu | 0.00009 | -0.02754 | -0.01462 |
| 99 | Cu | 0.04338 | 0.02505 | -0.00596 |

**THB gas phase:**
E = -121.4169

| | | | | |
|---|---|---|---|---|
| 0 | O | 21.4641 | 12.3017 | 11.9510 |
| 1 | O | 21.4094 | 9.5852 | 11.9510 |
| 2 | O | 16.6781 | 12.4029 | 11.9510 |
| 3 | O | 16.6235 | 9.6871 | 11.9510 |
| 4 | C | 19.0455 | 9.6102 | 11.9510 |
| 5 | C | 19.0423 | 12.3783 | 11.9510 |
| 6 | C | 17.8517 | 10.3034 | 11.9510 |
| 7 | C | 17.8418 | 11.6915 | 11.9510 |
| 8 | C | 20.2458 | 10.2974 | 11.9510 |
| 9 | C | 20.2360 | 11.6852 | 11.9510 |
| 10 | H | 19.0583 | 8.5452 | 11.9510 |
| 11 | H | 19.0293 | 13.4433 | 11.9510 |
| 12 | H | 21.3269 | 13.2522 | 11.9510 |
| 13 | H | 22.1388 | 10.2139 | 11.9510 |
| 14 | H | 15.9503 | 11.7721 | 11.9510 |

15 H 16.7599 8.7363 11.9510

**DHB gas phase:**
E = -113.4823

0 O 21.3952 12.3327 11.9510
1 O 21.3795 9.7473 11.9510
2 O 16.6983 12.2371 11.9510
3 O 16.6826 9.6515 11.9510
4 C 19.0268 9.5343 11.9510
5 C 19.0510 12.4500 11.9510
6 C 17.8709 10.2270 11.9510
7 C 17.8198 11.7295 11.9510
8 C 20.2580 10.2548 11.9510
9 C 20.2070 11.7573 11.9510
10 H 19.0504 8.4717 11.9510
11 H 19.0273 13.5125 11.9510
12 H 22.0330 11.5903 11.9510
13 H 16.0447 10.3939 11.9510

**$H_2$ gas phase**:
E = -7.1843

0 H 18.6780 11.0054 11.9510
1 H 19.3997 10.9787 11.9510

## Notes and references


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