**Supporting Information: Computational Section**

Geometry optimizations of the parent zwitterion (ZI) adsorbed on the Cu(111) and Ag(111) surfaces were carried out using the ADF software package [1,2], the revPBE generalized gradient density functional [3-6], and Grimme's dispersion correction (DFT-D3) [7]. The metal surfaces were modeled using a finite cluster comprised of 166 atoms, where both layers were fixed at the experimental lattice parameters of 3.614 Å and 4.086 Å for Cu and Ag, respectively [8]. The basis functions on all of the atoms consisted of a triple-ζ Slater-type basis set with polarization functions (TZP) from the ADF basis set library. The core shells for C, N, O, Cu, and Ag up to 1s, 1s, 1s, 3p, and 4p, respectfully, were frozen.

The starting geometry employed in the DFT structural optimizations consisted of the ZI lying parallel to the metal surface. The only constraints employed in the optimization was that the system maintained C(s) symmetry throughout the computation. In addition, in one set of the calculations all of the surface atoms were fixed at the experimental geometry, whereas in the other set the top layer was allowed to relax. Thus, it was in principle possible for the ZI to optimize to a standing configuration. A parallel arrangement was not enforced during the optimization. However, we cannot guarantee that the geometry obtained corresponds to a local, rather than a global minimum. Since the experimentally determined spacing between the molecules correlates well with the intermolecular spacing of a flat-lying geometry, we deemed it not necessary to perform an expensive geometry optimization employing a standing configuration as a guess for the initial geometry.

The basis set superposition error (BSSE) was obtained using the Counterpoise method. The BSSE corrected binding energies of the ZI on Cu and Ag were determined to be 1.91 eV and 1.54 eV. The ZI donated a larger amount of charge to Cu than to Ag (0.14e vs. 0.02e). The stronger interaction was coupled by a shorter distance between the O and N atoms to the surface, 2.27 and 2.30 Å for Cu vs. 2.66 and 3.10 Å for Ag.

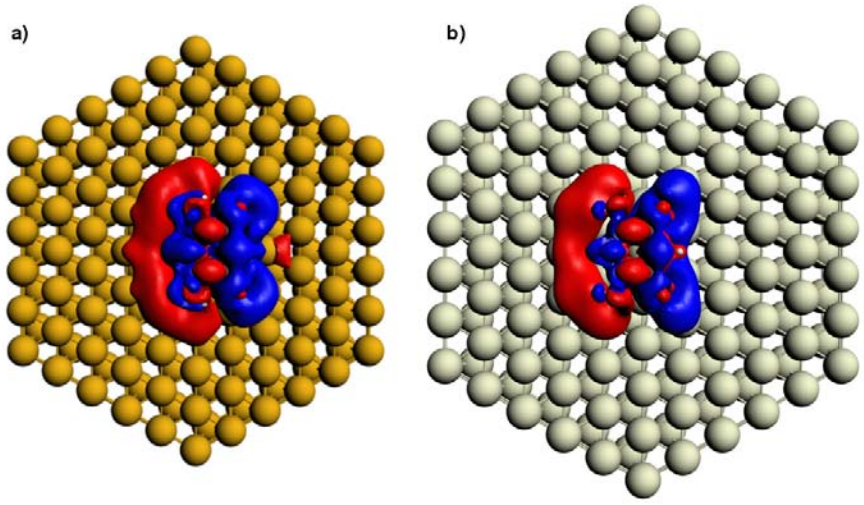



**Figure 1:** Charge Density Difference (CDD) isosurface plots (+/- 0.0003 au) of the ZI on a) Cu(111) and b) Ag(111). Red denotes a buildup and blue a depletion of charge upon adsorption. The plots have been scaled so that the size of the ZI is approximately the same in both. The ZI is aligned such that the O/N containing sides are on the left/right.

To clarify the nature of bonding a fragment orbital analysis [1] was performed using the distorted metal surface and the molecule as fragments. This analysis yields the composition of the molecular orbitals (MOs) in terms of occupied and unoccupied MOs of the ZI and the metal cluster. From this,

the charge density difference (CDD) plots were calculated. They indicate the rearrangement of electron density upon adsorption of the molecule to the surface. Moreover, this yielded approximate interaction diagrams [9-12] between the ZI and the substrate, see Figure 2. Charge was found to be donated from the HOMO of the ZI into the metal surface, and back donation from the surface into the LUMO of the adsorbate occurred. The larger band dispersion for Cu compared to Ag can be accounted for by the shorter metal-adsorbate distance, which gives rise to a larger overlap between the MOs of the surface and the adsorbate.

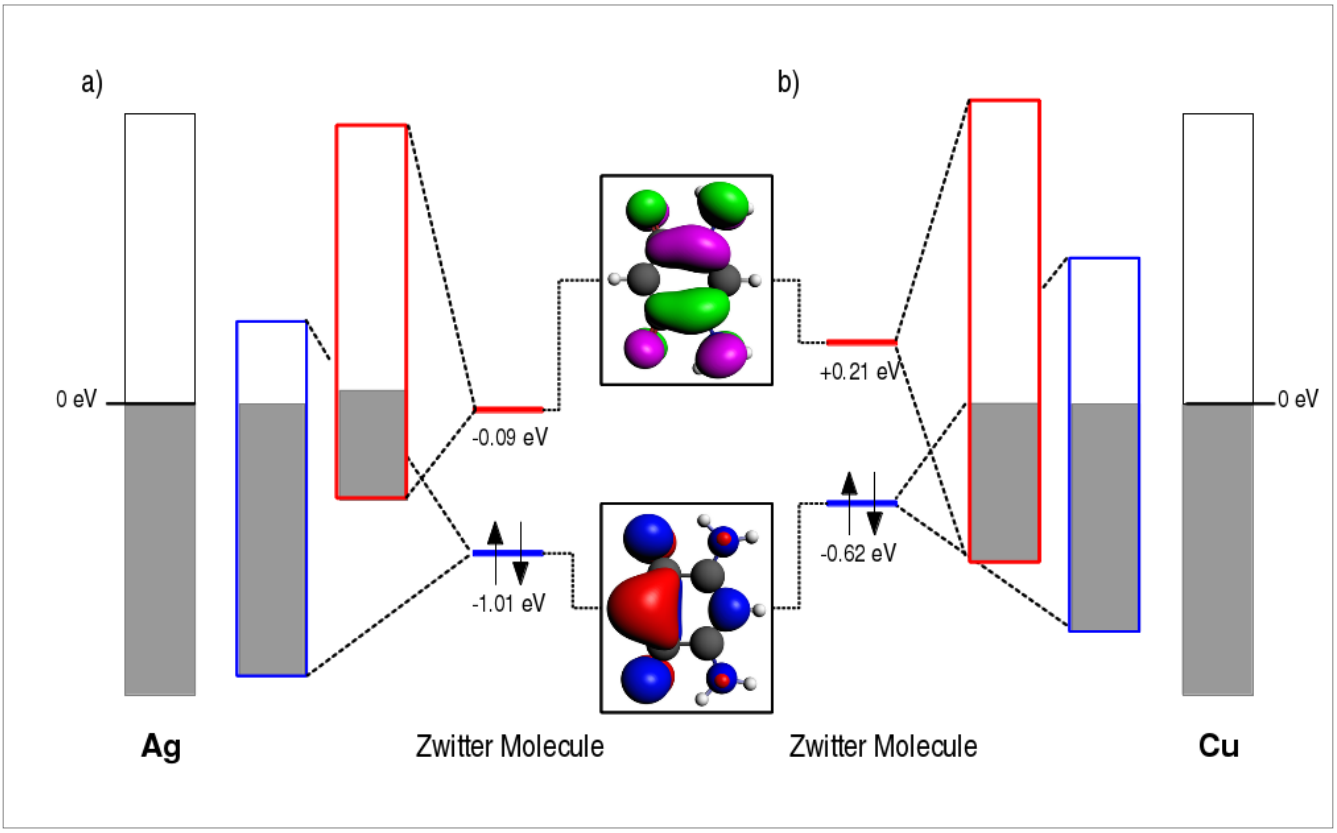



**Figure 2:** Schematic interaction diagram between the ZI and the a) Ag(111) and b) Cu(111) cluster model. The isosurfaces of the HOMO and LUMO (+/- 0.03 au) are displayed in red/blue and green/purple. The red/blue bands contain some LUMO/HOMO character as well as character from surface MOs. The HOMO/LUMO energies are given with respect to the Fermi-level of the a) Ag(111) and b) Cu(111) clusters.

In Figure 2 the computed HOMO and LUMO energies of the free ZI (but in the geometry of the molecule as optimized on the metal surface) is given with respect to the computed Fermi levels of the finite Ag(111) and Cu(111) cluster models (whose Fermi levels have been set to zero). The schematic interaction diagram is provided in order to illustrate the bonding interactions between the frontier orbitals of the molecule and the metal bands. Even though the Kohn Sham energies for the occupied molecular orbitals are typically in good agreement with those computed from more demanding $G_0W_0$ calculations, the HOMO-LUMO gap is often underestimated due to the dynamic polarization of the substrate which is not captured in DFT [13]. Despite the fact that DFT is not always able to describe the level alignment, for a comparison study such as this the results are consistent with experiment, and with the well-established trends of chemical reactivity of the metals [14].

We calculate the electric dipole of the free ZI as being 8.16 D. Upon surface adsorption, the dipole of the system changes dramatically. Table 1 and Table 2 provide the vector components of the dipole for the non-interacting ZI and surface models (with the same geometry as in the interacting system), and that of the interacting system. The magnitude of the electric dipole is given as well. The angles the dipoles make with the surface are illustrated in Figure 3.

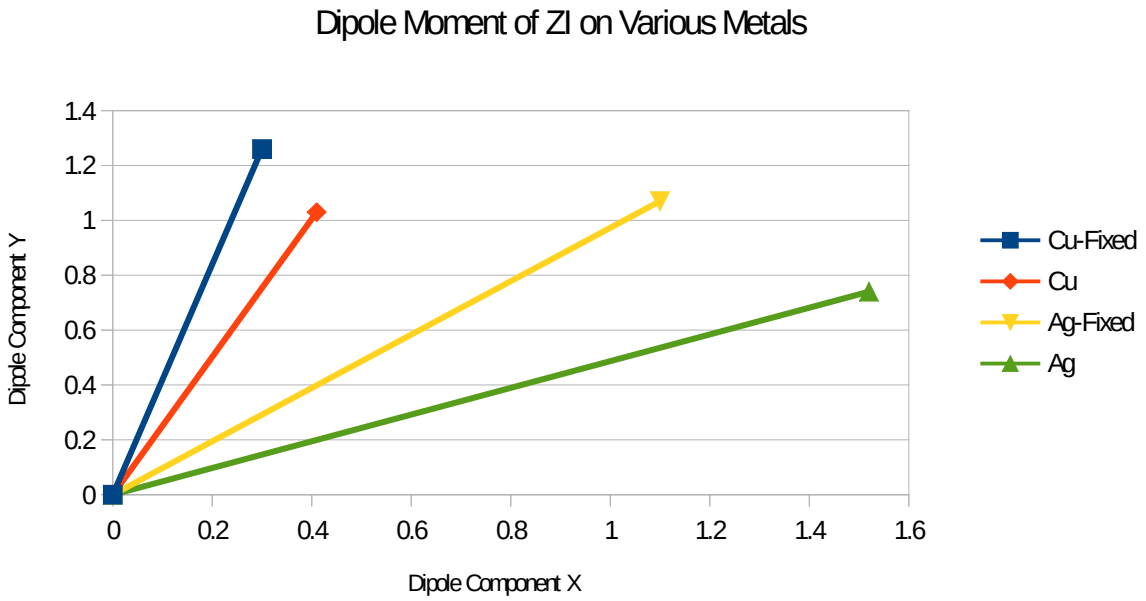
| | ZI-Cu | ZI | Cu |
|---|---|---|---|
| Dipole X | 0.30 | 8.33 | 0.01 |
| Dipole Y | 1.26 | 1.88 | -0.42 |
| Dipole Z | 0.00 | 0.02 | 0.00 |
| Dipole Mag | 1.29 | 8.54 | 0.42 |

**Table 1:** Electric dipole vector components of the ZI-Cu(111) system, as well as the non-interacting ZI, and Cu cluster in the distorted geometry of the ZI-Cu system. The values are reported in Debye.

| | ZI-Ag | ZI | Ag |
|---|---|---|---|
| Dipole X | 1.10 | 8.53 | 0.00 |
| Dipole Y | 1.07 | 0.56 | -0.44 |
| Dipole Z | 0.00 | 0.00 | 0.00 |
| Dipole Mag | 1.53 | 8.54 | 0.44 |

**Table 2:** As in Table 1 but for Ag(111).

Geometry optimizations were also performed in which only the bottom layer of the metal cluster was kept fixed at the experimental value (the top was allowed to relax), and the results were compared to those where both layers of the metal slab were kept fixed. The BSSE corrected BE, amount of charge transferred to the metal cluster (along with the CDD plots) and surface-adsorbate distances were relatively independent of the model used in the calculations (see Table 3). There was a slight variation of the angle that the dipole moment made with the surface plane. However, as Figure 3 shows, the difference between the two angles remained relatively constant in the two sets of calculations, with the angle on Cu(111) being greater than that on Ag(111).




| System | BE | Surface Charge | Dipole X | Dipole Y | Dipole Z | Dipole Mag | Dipole Angle | N Distance | O Distance |
|---|---|---|---|---|---|---|---|---|---|
| Cu-Fixed | 1.91 | -0.14 | 0.3 | 1.26 | 0.004 | 1.29 | 76.6 | 2.30 | 2.27 |
| Cu | 1.94 | -0.14 | 0.41 | 1.03 | 0 | 1.11 | 68.3 | 2.74 | 2.30 |
| Ag-Fixed | 1.54 | 0.02 | 1.1 | 1.07 | 0 | 1.54 | 44.2 | 3.10 | 2.66 |
| Ag | 1.52 | 0.03 | 1.52 | 0.74 | 0 | 1.7 | 26 | 3.11 | 2.65 |

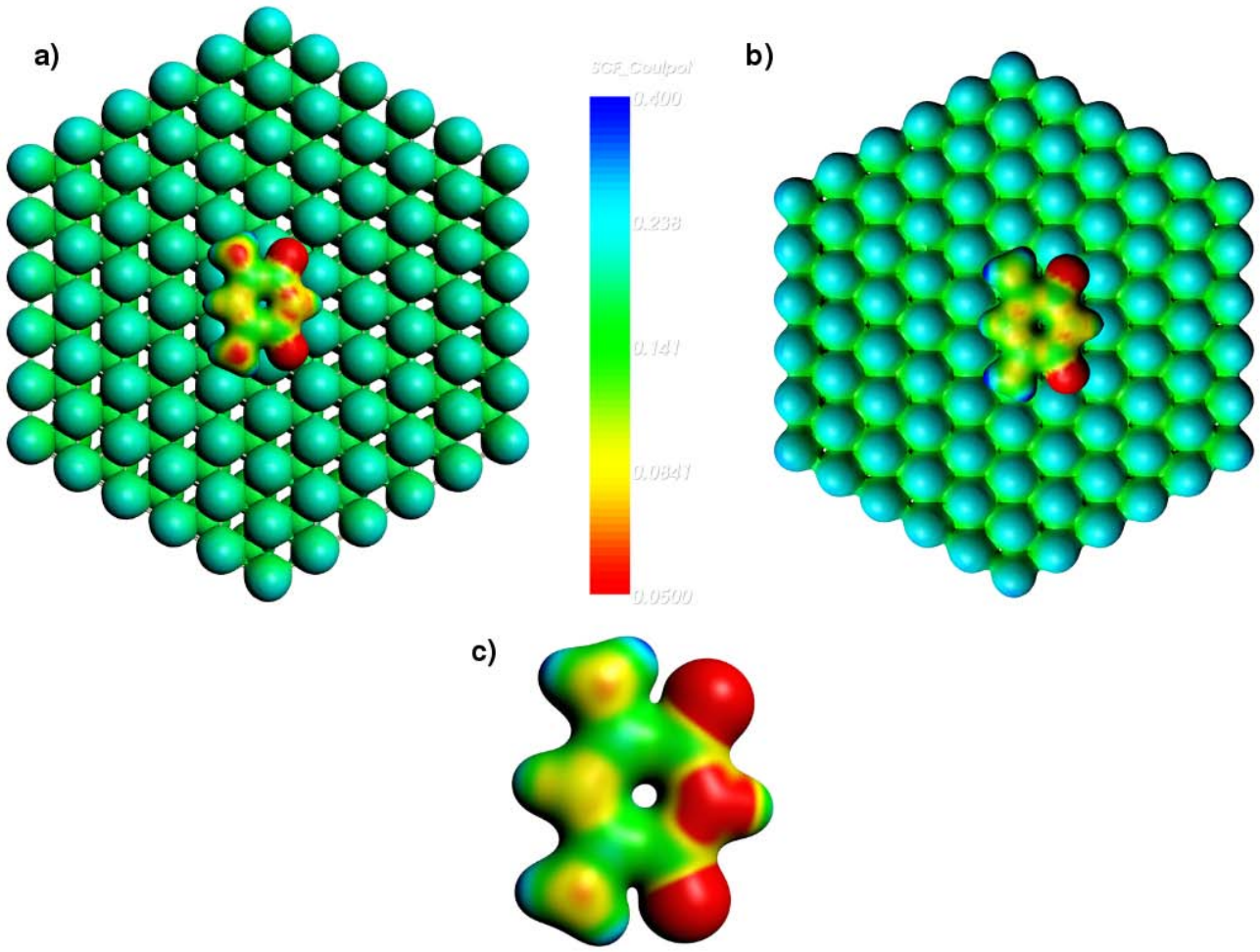



**Figure 4:** The charge density colored by the electrostatic potential (isovalue +/- 0.03 au) of (a) the ZI on the fixed Ag(111) surface, (b) the ZI on the fixed Cu(111) surface, (c) the free ZI molecule.

Gas phase calculations have been performed on a *N,N*'-diethyl derivatives 2 dimer arranged in a configuration which allowed for an H-bonding interaction. The two molecules were constrained to lie in the plane of the surface. The DFT calculations which did not employ a dispersion corrected functional showed that the C-O distance optimized to 3.660 A and the bonding energy (which must be a result of hydrogen bonding) was calculated as being 0.11eV. When the same calculation was carried out using a dispersion corrected functional the C-O bond length slightly decreased to 3.412 A and the bonding energy increased to 0.19 eV. This illustrates that for the gas phase ethyl ZI dimer the H-bonding interaction is weak, but of the same order of mangitude as the dispersion.

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**Coordinates:**

Parent Zwitterion Molecule
E= -102.30961755 eV
16

| | | | |
|---|---|---|---|
| C | -0.041680 | -0.768365 | 1.162528 |
| C | -0.193914 | -3.003888 | -0.002800 |
| C | -0.162066 | -2.314438 | 1.227483 |
| O | -0.220973 | -2.804240 | 2.387302 |
| N | -0.025157 | -0.217282 | 2.373570 |
| C | 0.002162 | -0.799554 | -1.221342 |
| C | 0.038411 | -0.058112 | -0.038062 |
| C | -0.121087 | -2.346704 | -1.249487 |
| O | -0.143392 | -2.867179 | -2.396758 |
| N | 0.066473 | -0.280498 | -2.444949 |
| H | 0.122710 | 1.033944 | -0.050702 |
| H | -0.279400 | -4.090350 | 0.009652 |
| H | 0.024020 | -0.978651 | -3.197910 |
| H | 0.152869 | 0.711333 | -2.628839 |
| H | 0.044874 | 0.779898 | 2.534120 |
| H | -0.093442 | -0.897814 | 3.141327 |

ZI on Fixed Ag(111)
E= -385.35728257 eV
182

| | | | |
|---|---|---|---|
| Ag | -1.668100 | -1.293210 | 2.889240 |
| Ag | -1.668100 | -1.293210 | 5.778480 |
| Ag | -1.668100 | -1.293210 | 8.667710 |
| Ag | -1.668100 | -1.293210 | 11.556950 |
| Ag | -1.668100 | -1.293210 | -11.556950 |
| Ag | -1.668100 | -1.293210 | -8.667710 |
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| Ag | -4.170250 | -1.293210 | -10.112330 |
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| Ag | 7.506460 | 1.065820 | -4.333860 |
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| Ag | 5.004310 | 1.065830 | -2.889240 |
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| Ag | 2.502160 | 1.065830 | 7.223100 |
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| Ag | 2.502150 | 1.065820 | 13.001570 |
| Ag | 2.502150 | 1.065820 | -13.001570 |
| Ag | 2.502160 | 1.065820 | -10.112330 |
| Ag | 2.502160 | 1.065830 | -7.223100 |
| Ag | 2.502150 | 1.065830 | -4.333860 |
| Ag | 2.502150 | 1.065830 | -1.444620 |
| Ag | 0.000000 | 1.065830 | 2.889240 |
| Ag | 0.000000 | 1.065830 | 5.778480 |
| Ag | 0.000000 | 1.065820 | 8.667710 |
| Ag | 0.000000 | 1.065820 | 11.556960 |
| Ag | 0.000000 | 1.065810 | 14.446190 |
| Ag | 0.000000 | 1.065810 | -14.446190 |
| Ag | 0.000000 | 1.065820 | -11.556960 |
| Ag | 0.000000 | 1.065820 | -8.667710 |
| Ag | 0.000000 | 1.065830 | -5.778480 |
| Ag | 0.000000 | 1.065830 | -2.889240 |
| Ag | 0.000000 | 1.065840 | 0.000000 |
| C | 1.007119 | 4.188488 | 1.211499 |
| C | -1.151804 | 3.903061 | 0.000000 |
| C | -0.480775 | 3.963328 | 1.249840 |
| O | -1.019041 | 3.725118 | 2.387040 |
| N | 1.608763 | 4.169545 | 2.420703 |
| C | 1.007119 | 4.188488 | -1.211499 |
| C | 1.706699 | 4.282066 | 0.000000 |
| C | -0.480775 | 3.963328 | -1.249840 |
| O | -1.019041 | 3.725118 | -2.387040 |
| N | 1.608763 | 4.169545 | -2.420703 |
| H | 2.797144 | 4.371975 | 0.000000 |
| H | -2.232456 | 3.759213 | 0.000000 |
| H | 1.005456 | 3.946034 | -3.213987 |
| H | 2.613402 | 4.071261 | -2.521383 |
| H | 2.613402 | 4.071261 | 2.521383 |
| H | 1.005456 | 3.946034 | 3.213987 |

<u>ZI on relaxed Ag(111)</u>
E= -402.29814005 eV
182

| | | | |
|---|---|---|---|
| Ag | -1.668100 | -1.293210 | 2.889240 |
| Ag | -1.668100 | -1.293210 | 5.778480 |
| Ag | -1.668100 | -1.293210 | 8.667710 |
| Ag | -1.668100 | -1.293210 | 11.556950 |
| Ag | -1.668100 | -1.293210 | -11.556950 |
| Ag | -1.668100 | -1.293210 | -8.667710 |
| Ag | -1.668100 | -1.293210 | -5.778480 |
| Ag | -1.668100 | -1.293210 | -2.889240 |
| Ag | -1.668100 | -1.293220 | 0.000000 |
| Ag | -4.170260 | -1.293210 | 4.333860 |
| Ag | -4.170260 | -1.293210 | 7.223100 |
| Ag | -4.170250 | -1.293210 | 10.112330 |
| Ag | -4.170250 | -1.293210 | -10.112330 |
| Ag | -4.170260 | -1.293210 | -7.223100 |
| Ag | -4.170260 | -1.293210 | -4.333860 |
| Ag | -4.170260 | -1.293220 | -1.444620 |
| Ag | -4.170260 | -1.293220 | 1.444620 |
| Ag | -6.672410 | -1.293210 | 5.778480 |
| Ag | -6.672410 | -1.293210 | 8.667700 |
| Ag | -6.672410 | -1.293210 | -8.667700 |
| Ag | -6.672410 | -1.293210 | -5.778480 |
| Ag | -6.672410 | -1.293220 | -2.889240 |
| Ag | -6.672410 | -1.293220 | 0.000000 |
| Ag | -6.672410 | -1.293220 | 2.889240 |
| Ag | -9.174560 | -1.293210 | 7.223090 |
| Ag | -9.174560 | -1.293210 | -7.223090 |

| | | | |
|---|---|---|---|
| Ag | -9.174560 | -1.293230 | -4.333850 |
| Ag | -9.174560 | -1.293230 | -1.444620 |
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| Ag | -9.174560 | -1.293230 | 4.333850 |
| Ag | -11.676720 | -1.293230 | -5.778480 |
| Ag | -11.676710 | -1.293230 | -2.889240 |
| Ag | -11.676710 | -1.293230 | 0.000000 |
| Ag | -11.676710 | -1.293230 | 2.889240 |
| Ag | -11.676720 | -1.293230 | 5.778480 |
| Ag | 10.842660 | -1.293210 | -4.333850 |
| Ag | 10.842660 | -1.293210 | -1.444620 |
| Ag | 10.842660 | -1.293210 | 1.444620 |
| Ag | 10.842660 | -1.293210 | 4.333850 |
| Ag | 10.842660 | -1.293230 | 7.223100 |
| Ag | 10.842660 | -1.293230 | -7.223100 |
| Ag | 8.340510 | -1.293210 | -2.889240 |
| Ag | 8.340510 | -1.293210 | 0.000000 |
| Ag | 8.340510 | -1.293210 | 2.889240 |
| Ag | 8.340510 | -1.293230 | 5.778480 |
| Ag | 8.340510 | -1.293230 | 8.667710 |
| Ag | 8.340510 | -1.293230 | -8.667710 |
| Ag | 8.340510 | -1.293230 | -5.778480 |
| Ag | 5.838360 | -1.293210 | -1.444620 |
| Ag | 5.838360 | -1.293210 | 1.444620 |
| Ag | 5.838360 | -1.293220 | 4.333860 |
| Ag | 5.838360 | -1.293230 | 7.223100 |
| Ag | 5.838350 | -1.293230 | 10.112330 |
| Ag | 5.838350 | -1.293230 | -10.112330 |
| Ag | 5.838360 | -1.293230 | -7.223100 |
| Ag | 5.838360 | -1.293220 | -4.333860 |
| Ag | 3.336200 | -1.293210 | 0.000000 |
| Ag | 3.336210 | -1.293220 | 2.889240 |
| Ag | 3.336210 | -1.293220 | 5.778480 |
| Ag | 3.336210 | -1.293230 | 8.667710 |
| Ag | 3.336200 | -1.293230 | 11.556940 |
| Ag | 3.336200 | -1.293230 | -11.556940 |
| Ag | 3.336210 | -1.293230 | -8.667710 |
| Ag | 3.336210 | -1.293220 | -5.778480 |
| Ag | 3.336210 | -1.293220 | -2.889240 |
| Ag | 0.834050 | -1.293220 | 1.444620 |
| Ag | 0.834050 | -1.293220 | 4.333860 |
| Ag | 0.834050 | -1.293220 | 7.223090 |
| Ag | 0.834050 | -1.293230 | 10.112330 |
| Ag | 0.834050 | -1.293230 | 13.001570 |
| Ag | 0.834050 | -1.293230 | -13.001570 |
| Ag | 0.834050 | -1.293230 | -10.112330 |
| Ag | 0.834050 | -1.293220 | -7.223090 |
| Ag | 0.834050 | -1.293220 | -4.333860 |
| Ag | 0.834050 | -1.293220 | -1.444620 |
| Ag | -2.767169 | 1.705530 | 4.533961 |
| Ag | -2.811580 | 1.574825 | 7.543740 |
| Ag | -2.904538 | 1.626658 | 10.550053 |
| Ag | -3.258490 | 0.470420 | 13.402980 |
| Ag | -3.258490 | 0.470420 | -13.402980 |
| Ag | -2.904538 | 1.626658 | -10.550053 |
| Ag | -2.811580 | 1.574825 | -7.543740 |
| Ag | -2.767169 | 1.705530 | -4.533961 |
| Ag | -2.779112 | 1.477041 | -1.526054 |
| Ag | -2.779112 | 1.477041 | 1.526054 |
| Ag | -5.466367 | 1.580972 | 5.991053 |
| Ag | -5.538232 | 1.600203 | 8.974992 |
| Ag | -5.845165 | 0.509091 | 11.831731 |
| Ag | -5.845165 | 0.509091 | -11.831731 |
| Ag | -5.538232 | 1.600203 | -8.974992 |
| Ag | -5.466367 | 1.580972 | -5.991053 |
| Ag | -5.456019 | 1.563216 | -3.009480 |
| Ag | -5.419330 | 1.574762 | 0.000000 |
| Ag | -5.456019 | 1.563216 | 3.009480 |
| Ag | -8.186063 | 1.647589 | 7.466927 |
| Ag | -8.486385 | 0.508739 | 10.296085 |
| Ag | -8.486385 | 0.508739 | -10.296085 |
| Ag | -8.186063 | 1.647589 | -7.466927 |
| Ag | -8.146837 | 1.564168 | -4.498982 |
| Ag | -8.104874 | 1.564145 | -1.501973 |
| Ag | -8.104874 | 1.564145 | 1.501973 |
| Ag | -8.146837 | 1.564168 | 4.498982 |
| Ag | -11.094167 | 0.462799 | 8.810293 |
| Ag | -11.094167 | 0.462799 | -8.810293 |
| Ag | -10.835980 | 1.674112 | -5.961246 |
| Ag | -10.802798 | 1.597111 | -2.987229 |
| Ag | -10.759749 | 1.575351 | 0.000000 |
| Ag | -10.802798 | 1.597111 | 2.987229 |
| Ag | -10.835980 | 1.674112 | 5.961246 |
| Ag | -13.665418 | 0.936799 | -7.371839 |
| Ag | -13.607181 | 0.945188 | -4.416905 |
| Ag | -13.611520 | 0.937354 | -1.478381 |
| Ag | -13.611520 | 0.937354 | 1.478381 |
| Ag | -13.607181 | 0.945188 | 4.416905 |
| Ag | -13.665418 | 0.936799 | 7.371839 |
| Ag | 13.126455 | 0.611906 | -4.694278 |
| Ag | 13.079606 | 0.657823 | -1.618486 |
| Ag | 13.079606 | 0.657823 | 1.618486 |
| Ag | 13.126455 | 0.611906 | 4.694278 |
| Ag | 13.015286 | 0.955197 | 7.682954 |
| Ag | 13.015286 | 0.955197 | -7.682954 |
| Ag | 10.454506 | 1.608530 | -3.108693 |

| | | | |
|---|---|---|---|
| Ag | 10.461894 | 1.566817 | 0.000000 |
| Ag | 10.454506 | 1.608530 | 3.108693 |
| Ag | 10.419966 | 1.661177 | 6.164957 |
| Ag | 10.439179 | 1.131829 | 9.348518 |
| Ag | 10.439179 | 1.131829 | -9.348518 |
| Ag | 10.419966 | 1.661177 | -6.164957 |
| Ag | 7.831880 | 1.575244 | -1.546631 |
| Ag | 7.831880 | 1.575244 | 1.546631 |
| Ag | 7.820772 | 1.580713 | 4.636231 |
| Ag | 7.800383 | 1.606643 | 7.725327 |
| Ag | 7.819621 | 1.141087 | 10.869226 |
| Ag | 7.819621 | 1.141087 | -10.869226 |
| Ag | 7.800383 | 1.606643 | -7.725327 |
| Ag | 7.820772 | 1.580713 | -4.636231 |
| Ag | 5.171401 | 1.595999 | 0.000000 |
| Ag | 5.192703 | 1.552969 | 3.073683 |
| Ag | 5.178119 | 1.549117 | 6.145141 |
| Ag | 5.127139 | 1.558765 | 9.210354 |
| Ag | 5.136200 | 1.183231 | 12.343740 |
| Ag | 5.136200 | 1.183231 | -12.343740 |
| Ag | 5.127139 | 1.558765 | -9.210354 |
| Ag | 5.178119 | 1.549117 | -6.145141 |
| Ag | 5.192703 | 1.552969 | -3.073683 |
| Ag | 2.555436 | 1.468802 | 1.529963 |
| Ag | 2.527901 | 1.608188 | 4.597967 |
| Ag | 2.492331 | 1.533882 | 7.668470 |
| Ag | 2.427669 | 1.608759 | 10.749605 |
| Ag | 2.411104 | 1.225822 | 13.807911 |
| Ag | 2.411104 | 1.225822 | -13.807911 |
| Ag | 2.427669 | 1.608759 | -10.749605 |
| Ag | 2.492331 | 1.533882 | -7.668470 |
| Ag | 2.527901 | 1.608188 | -4.597967 |
| Ag | 2.555436 | 1.468802 | -1.529963 |
| Ag | -0.102837 | 1.421761 | 3.060493 |
| Ag | -0.127638 | 1.541975 | 6.110537 |
| Ag | -0.189784 | 1.528889 | 9.143801 |
| Ag | -0.282759 | 1.671381 | 12.128044 |
| Ag | -0.639683 | 0.508257 | 14.913473 |
| Ag | -0.639683 | 0.508257 | -14.913473 |
| Ag | -0.282759 | 1.671381 | -12.128044 |
| Ag | -0.189784 | 1.528889 | -9.143801 |
| Ag | -0.127638 | 1.541975 | -6.110537 |
| Ag | -0.102837 | 1.421761 | -3.060493 |
| Ag | -0.090902 | 1.280221 | 0.000000 |
| C | 0.720760 | 4.497615 | -1.210970 |
| C | -1.440451 | 4.224264 | 0.000000 |
| C | -0.770062 | 4.280515 | -1.248898 |
| O | -1.310934 | 4.071358 | -2.389828 |
| N | 1.313310 | 4.529520 | -2.423594 |
| C | 0.720760 | 4.497615 | 1.210970 |
| C | 1.423150 | 4.576663 | 0.000000 |
| C | -0.770062 | 4.280515 | 1.248898 |
| O | -1.310934 | 4.071358 | 2.389828 |
| N | 1.313310 | 4.529520 | 2.423594 |
| H | 2.512681 | 4.676546 | 0.000000 |
| H | -2.523353 | 4.097042 | 0.000000 |
| H | 0.704524 | 4.333098 | 3.219835 |
| H | 2.317734 | 4.443559 | 2.535267 |
| H | 2.317734 | 4.443559 | -2.535267 |
| H | 0.704524 | 4.333098 | -3.219835 |

ZI on Fixed Cu(111)
E= -532.14468447 eV
182

| | | | |
|---|---|---|---|
| Cu | 8.105765 | -6.381640 | -1.142575 |
| Cu | 8.105765 | 6.381640 | -1.142575 |
| Cu | 1.473780 | -10.210618 | -1.142575 |
| Cu | 1.473780 | 10.210618 | -1.142575 |
| Cu | -9.579545 | 3.828978 | -1.142575 |
| Cu | -9.579545 | -3.828978 | -1.142575 |
| Cu | 5.895106 | -7.657964 | -1.142573 |
| Cu | 5.895106 | 7.657964 | -1.142573 |
| Cu | 3.684439 | -8.934294 | -1.142573 |
| Cu | 3.684439 | 8.934294 | -1.142573 |
| Cu | -9.579545 | 1.276329 | -1.142573 |
| Cu | -9.579545 | -1.276329 | -1.142573 |
| Cu | 5.895105 | -5.105304 | -1.142571 |
| Cu | 5.895105 | 5.105304 | -1.142571 |
| Cu | 1.473770 | -7.657963 | -1.142571 |
| Cu | 1.473770 | 7.657963 | -1.142571 |
| Cu | -7.368876 | 2.552659 | -1.142571 |
| Cu | -7.368876 | -2.552659 | -1.142571 |
| Cu | 10.316433 | 5.105310 | -1.142569 |
| Cu | 10.316433 | -5.105310 | -1.142569 |
| Cu | 3.684438 | -6.381633 | -1.142569 |
| Cu | 3.684438 | 6.381633 | -1.142569 |
| Cu | -0.736888 | -11.486948 | -1.142569 |
| Cu | -0.736888 | 11.486948 | -1.142569 |
| Cu | -7.368876 | 0.000000 | -1.142569 |
| Cu | -9.579545 | -6.381637 | -1.142569 |
| Cu | -9.579545 | 6.381637 | -1.142569 |
| Cu | 3.684442 | -3.828982 | -1.142567 |
| Cu | 3.684442 | 3.828982 | -1.142567 |
| Cu | 1.473774 | -5.105311 | -1.142567 |
| Cu | 1.473774 | 5.105311 | -1.142567 |

| | | | |
|---|---|---|---|
| Cu | -5.158216 | 1.276329 | -1.142567 |
| Cu | -5.158216 | -1.276329 | -1.142567 |
| Cu | 8.105764 | 3.828979 | -1.142566 |
| Cu | 8.105764 | -3.828979 | -1.142566 |
| Cu | -0.736889 | -8.934287 | -1.142566 |
| Cu | -0.736889 | 8.934287 | -1.142566 |
| Cu | -7.368876 | -5.105308 | -1.142566 |
| Cu | -7.368876 | 5.105308 | -1.142566 |
| Cu | 10.316432 | 2.552650 | -1.142565 |
| Cu | 10.316432 | -2.552650 | -1.142565 |
| Cu | -2.947556 | -10.210617 | -1.142565 |
| Cu | -2.947556 | 10.210617 | -1.142565 |
| Cu | -7.368876 | -7.657967 | -1.142565 |
| Cu | -7.368876 | 7.657967 | -1.142565 |
| Cu | 5.895101 | -2.552657 | -1.142564 |
| Cu | 5.895101 | 2.552657 | -1.142564 |
| Cu | -0.736884 | -6.381636 | -1.142564 |
| Cu | -0.736884 | 6.381636 | -1.142564 |
| Cu | -5.158216 | -3.828978 | -1.142564 |
| Cu | -5.158216 | 3.828978 | -1.142564 |
| Cu | 8.105768 | -1.276328 | -1.142563 |
| Cu | 8.105768 | 1.276328 | -1.142563 |
| Cu | 1.473774 | -2.552651 | -1.142563 |
| Cu | 1.473774 | 2.552651 | -1.142563 |
| Cu | -2.947547 | 0.000000 | -1.142563 |
| Cu | -2.947552 | -7.657965 | -1.142563 |
| Cu | -2.947552 | 7.657965 | -1.142563 |
| Cu | -5.158216 | -6.381637 | -1.142563 |
| Cu | -5.158216 | 6.381637 | -1.142563 |
| Cu | 3.684441 | -1.276321 | -1.142562 |
| Cu | 3.684441 | 1.276321 | -1.142562 |
| Cu | -0.736894 | -3.828980 | -1.142562 |
| Cu | -0.736894 | 3.828980 | -1.142562 |
| Cu | -2.947547 | -2.552659 | -1.142562 |
| Cu | -2.929936 | 2.540996 | -1.290662 |
| Cu | 10.316427 | 0.000000 | -1.142561 |
| Cu | -5.158214 | -8.934288 | -1.142561 |
| Cu | -5.158214 | 8.934288 | -1.142561 |
| Cu | 5.895100 | 0.000000 | -1.142560 |
| Cu | 1.473778 | 0.000000 | -1.142560 |
| Cu | -0.736889 | -1.276329 | -1.142560 |
| Cu | -0.736889 | 1.276329 | -1.142560 |
| Cu | -2.947550 | -5.105306 | -1.142560 |
| Cu | -2.947550 | 5.105306 | -1.142560 |
| Cu | 8.842651 | -7.657964 | 0.941652 |
| Cu | 8.842651 | 7.657964 | 0.941652 |
| Cu | 2.210666 | -11.486943 | 0.941652 |
| Cu | 2.210666 | 11.486943 | 0.941652 |
| Cu | -11.053317 | 3.828978 | 0.941652 |
| Cu | -11.053317 | -3.828978 | 0.941652 |
| Cu | 6.631992 | -8.934289 | 0.941654 |
| Cu | 6.631992 | 8.934289 | 0.941654 |
| Cu | 4.421325 | -10.210618 | 0.941654 |
| Cu | 4.421325 | 10.210618 | 0.941654 |
| Cu | -11.053317 | 1.276329 | 0.941654 |
| Cu | -11.053317 | -1.276329 | 0.941654 |
| Cu | 6.631996 | -6.381637 | 0.941656 |
| Cu | 6.631996 | 6.381637 | 0.941656 |
| Cu | 2.210661 | -8.934296 | 0.941656 |
| Cu | 2.210661 | 8.934296 | 0.941656 |
| Cu | -8.842658 | 2.552659 | 0.941656 |
| Cu | -8.842658 | -2.552659 | 0.941656 |
| Cu | 11.053319 | 6.381635 | 0.941658 |
| Cu | 11.053319 | -6.381635 | 0.941658 |
| Cu | 4.421329 | -7.657966 | 0.941658 |
| Cu | 4.421329 | 7.657966 | 0.941658 |
| Cu | -0.000002 | -12.763272 | 0.941658 |
| Cu | -0.000002 | 12.763272 | 0.941658 |
| Cu | -8.842658 | 0.000000 | 0.941658 |
| Cu | -11.053317 | -6.381637 | 0.941658 |
| Cu | -11.053317 | 6.381637 | 0.941658 |
| Cu | 4.421328 | -5.105306 | 0.941660 |
| Cu | 4.421328 | 5.105306 | 0.941660 |
| Cu | 2.210661 | -6.381635 | 0.941660 |
| Cu | 2.210661 | 6.381635 | 0.941660 |
| Cu | -6.631989 | 1.276329 | 0.941660 |
| Cu | -6.631989 | -1.276329 | 0.941660 |
| Cu | 8.842655 | 5.105312 | 0.941661 |
| Cu | 8.842655 | -5.105312 | 0.941661 |
| Cu | 0.000003 | -10.210620 | 0.941661 |
| Cu | 0.000003 | 10.210620 | 0.941661 |
| Cu | -8.842658 | -5.105308 | 0.941661 |
| Cu | -8.842658 | 5.105308 | 0.941661 |
| Cu | 11.053323 | 3.828983 | 0.941662 |
| Cu | 11.053323 | -3.828983 | 0.941662 |
| Cu | -2.210665 | -11.486950 | 0.941662 |
| Cu | -2.210665 | 11.486950 | 0.941662 |
| Cu | -8.842658 | -7.657967 | 0.941662 |
| Cu | -8.842658 | 7.657967 | 0.941662 |
| Cu | 6.631987 | 3.828981 | 0.941663 |
| Cu | 6.631987 | -3.828981 | 0.941663 |
| Cu | 0.000002 | -7.657960 | 0.941663 |
| Cu | 0.000002 | 7.657960 | 0.941663 |
| Cu | -6.631989 | -3.828978 | 0.941663 |
| Cu | -6.631989 | 3.828978 | 0.941663 |
| Cu | 2.210665 | -3.828984 | 0.941664 |

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| Cu | 2.210665 | 3.828984 | 0.941664 |
| Cu | -4.421330 | 0.000000 | 0.941664 |
| Cu | 8.842655 | 2.552652 | 0.941665 |
| Cu | 8.842655 | -2.552652 | 0.941665 |
| Cu | 4.421332 | -2.552654 | 0.941665 |
| Cu | 4.421332 | 2.552654 | 0.941665 |
| Cu | -0.000003 | -5.105313 | 0.941665 |
| Cu | -0.000003 | 5.105313 | 0.941665 |
| Cu | -2.210666 | -8.934289 | 0.941665 |
| Cu | -2.210666 | 8.934289 | 0.941665 |
| Cu | -4.421330 | -2.552659 | 0.941665 |
| Cu | -4.421330 | 2.552659 | 0.941665 |
| Cu | -6.631989 | -6.381637 | 0.941665 |
| Cu | -6.631989 | 6.381637 | 0.941665 |
| Cu | 11.053313 | 1.276327 | 0.941666 |
| Cu | 11.053313 | -1.276327 | 0.941666 |
| Cu | -4.421325 | -10.210614 | 0.941666 |
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| Cu | 6.631991 | -1.276330 | 0.941667 |
| Cu | 6.631991 | 1.276330 | 0.941667 |
| Cu | -2.210662 | -6.381638 | 0.941667 |
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| Cu | -4.421330 | -5.105308 | 0.941667 |
| Cu | -4.421330 | 5.105308 | 0.941667 |
| Cu | 8.842659 | 0.000000 | 0.941668 |
| Cu | 2.210664 | -1.276323 | 0.941668 |
| Cu | 2.210664 | 1.276323 | 0.941668 |
| Cu | -0.000004 | -2.552653 | 0.941668 |
| Cu | -0.000004 | 2.552653 | 0.941668 |
| Cu | -2.210660 | -1.276329 | 0.941668 |
| Cu | -2.210660 | 1.276329 | 0.941668 |
| Cu | -4.421329 | -7.657967 | 0.941668 |
| Cu | -4.421329 | 7.657967 | 0.941668 |
| Cu | 4.421323 | 0.000000 | 0.941669 |
| Cu | -2.210661 | -3.828978 | 0.941669 |
| Cu | -2.210661 | 3.828978 | 0.941669 |
| Cu | 0.000000 | 0.000000 | 0.941670 |
| C | -0.580758 | -1.241294 | 3.508926 |
| C | -2.724497 | -0.021946 | 3.463838 |
| C | -2.038966 | -1.278087 | 3.440669 |
| O | -2.632412 | -2.423270 | 3.213722 |
| N | 0.050146 | -2.473619 | 3.246232 |
| C | -0.584706 | 1.207932 | 3.510435 |
| C | 0.121089 | -0.015198 | 3.515162 |
| C | -2.043802 | 1.237708 | 3.444941 |
| O | -2.641902 | 2.380454 | 3.225027 |
| N | 0.039617 | 2.444860 | 3.253823 |
| H | 1.215800 | -0.013300 | 3.483453 |
| H | -3.816963 | -0.024152 | 3.466601 |
| H | -0.555998 | 3.234408 | 3.514151 |
| H | 1.010696 | 2.543851 | 3.541272 |
| H | 1.023074 | -2.566725 | 3.529907 |
| H | -0.538964 | -3.268026 | 3.506886 |

ZI on relaxed Cu(111)
E= -534.39781461 eV
182

| | | | |
|---|---|---|---|
| Cu | 8.110000 | -1.138500 | 6.374200 |
| Cu | 8.110000 | -1.138500 | -6.374200 |
| Cu | 1.465200 | -1.138500 | 10.210600 |
| Cu | 1.465200 | -1.138500 | -10.210600 |
| Cu | -9.575300 | -1.138500 | -3.836400 |
| Cu | -9.575300 | -1.138500 | 3.836400 |
| Cu | 5.895900 | -1.140800 | 7.649700 |
| Cu | 5.895900 | -1.140800 | -7.649700 |
| Cu | 3.676900 | -1.140800 | 8.930800 |
| Cu | 3.676900 | -1.140800 | -8.930800 |
| Cu | -9.572800 | -1.140800 | -1.281100 |
| Cu | -9.572800 | -1.140800 | 1.281100 |
| Cu | 5.890100 | -1.149500 | 5.098900 |
| Cu | 5.890100 | -1.149500 | -5.098900 |
| Cu | 1.470700 | -1.149500 | 7.650500 |
| Cu | 1.470700 | -1.149500 | -7.650500 |
| Cu | -7.360900 | -1.149500 | -2.551500 |
| Cu | -7.360900 | -1.149500 | 2.551500 |
| Cu | 10.318700 | -1.133000 | -5.102000 |
| Cu | 10.318700 | -1.133000 | 5.102000 |
| Cu | 3.685300 | -1.152500 | 6.383100 |
| Cu | 3.685300 | -1.152500 | -6.383100 |
| Cu | -0.740900 | -1.133000 | 11.487200 |
| Cu | -0.740900 | -1.133000 | -11.487200 |
| Cu | -7.370500 | -1.152500 | 0.000000 |
| Cu | -9.577800 | -1.133000 | 6.385200 |
| Cu | -9.577800 | -1.133000 | -6.385200 |
| Cu | 3.681300 | -1.138200 | 3.827500 |
| Cu | 3.681300 | -1.138200 | -3.827500 |
| Cu | 1.474100 | -1.138200 | 5.101800 |
| Cu | 1.474100 | -1.138200 | -5.101800 |
| Cu | -5.155400 | -1.138200 | -1.274300 |
| Cu | -5.155400 | -1.138200 | 1.274300 |
| Cu | 8.106900 | -1.160800 | -3.826800 |
| Cu | 8.106900 | -1.160800 | 3.826800 |
| Cu | -0.739300 | -1.160800 | 8.934200 |

| | | | |
|---|---|---|---|
| Cu | -0.739300 | -1.160800 | -8.934200 |
| Cu | -7.367600 | -1.160800 | 5.107300 |
| Cu | -7.367600 | -1.160800 | -5.107300 |
| Cu | 10.341500 | -1.148000 | -2.559000 |
| Cu | 10.341500 | -1.148000 | 2.559000 |
| Cu | -2.954600 | -1.148000 | 10.235500 |
| Cu | -2.954600 | -1.148000 | -10.235500 |
| Cu | -7.387000 | -1.148000 | 7.676500 |
| Cu | -7.387000 | -1.148000 | -7.676500 |
| Cu | 5.893800 | -1.128300 | 2.554700 |
| Cu | 5.893800 | -1.128300 | -2.554700 |
| Cu | -0.734500 | -1.128300 | 6.381500 |
| Cu | -0.734500 | -1.128300 | -6.381500 |
| Cu | -5.159300 | -1.128300 | 3.826800 |
| Cu | -5.159300 | -1.128300 | -3.826800 |
| Cu | 8.108300 | -1.149400 | 1.274500 |
| Cu | 8.108300 | -1.149400 | -1.274500 |
| Cu | 1.479100 | -1.148400 | 2.561900 |
| Cu | 1.479100 | -1.148400 | -2.561900 |
| Cu | -2.958200 | -1.148400 | 0.000000 |
| Cu | -2.950400 | -1.149400 | 7.659200 |
| Cu | -2.950400 | -1.149400 | -7.659200 |
| Cu | -5.157900 | -1.149400 | 6.384700 |
| Cu | -5.157900 | -1.149400 | -6.384700 |
| Cu | 3.671900 | -1.143700 | 1.263600 |
| Cu | 3.671900 | -1.143700 | -1.263600 |
| Cu | -0.741600 | -1.143700 | 3.811700 |
| Cu | -0.741600 | -1.143700 | -3.811700 |
| Cu | -2.930300 | -1.143700 | 2.548100 |
| Cu | -2.930300 | -1.143700 | -2.548100 |
| Cu | 10.339600 | -1.145500 | 0.000000 |
| Cu | -5.169800 | -1.145500 | 8.954300 |
| Cu | -5.169800 | -1.145500 | -8.954300 |
| Cu | 5.896500 | -1.138200 | 0.000000 |
| Cu | 1.475800 | -1.153300 | 0.000000 |
| Cu | -0.737900 | -1.153300 | 1.278100 |
| Cu | -0.737900 | -1.153300 | -1.278100 |
| Cu | -2.948200 | -1.138200 | 5.106500 |
| Cu | -2.948200 | -1.138200 | -5.106500 |
| Cu | 8.854400 | 0.959800 | 7.661700 |
| Cu | 8.854400 | 0.959800 | -7.661700 |
| Cu | 2.215400 | 0.962100 | 11.487300 |
| Cu | 2.215400 | 0.962100 | -11.487300 |
| Cu | -11.068600 | 0.958000 | -3.835600 |
| Cu | -11.068600 | 0.958000 | 3.835600 |
| Cu | 6.643200 | 0.945700 | 8.930800 |
| Cu | 6.643200 | 0.945700 | -8.930800 |
| Cu | 4.422700 | 0.944700 | 10.209900 |
| Cu | 4.422700 | 0.944700 | -10.209900 |
| Cu | -11.060000 | 0.944200 | -1.282100 |
| Cu | -11.060000 | 0.944200 | 1.282100 |
| Cu | 6.639900 | 1.069900 | 6.369000 |
| Cu | 6.639900 | 1.069900 | -6.369000 |
| Cu | 2.202700 | 1.068300 | 8.925500 |
| Cu | 2.202700 | 1.068300 | -8.925500 |
| Cu | -8.840700 | 1.069300 | -2.562900 |
| Cu | -8.840700 | 1.069300 | 2.562900 |
| Cu | 11.056500 | 0.967500 | -6.380500 |
| Cu | 11.056500 | 0.967500 | 6.380500 |
| Cu | 4.420500 | 1.067100 | 7.647100 |
| Cu | 4.420500 | 1.067100 | -7.647100 |
| Cu | 0.004700 | 0.968200 | 12.747700 |
| Cu | 0.004700 | 0.968200 | -12.747700 |
| Cu | -8.841500 | 1.071600 | 0.000000 |
| Cu | -11.057000 | 0.967200 | 6.381200 |
| Cu | -11.057000 | 0.967200 | -6.381200 |
| Cu | 4.417200 | 1.108300 | 5.092800 |
| Cu | 4.417200 | 1.108300 | -5.092800 |
| Cu | 2.203300 | 1.115700 | 6.367200 |
| Cu | 2.203300 | 1.115700 | -6.367200 |
| Cu | -6.630600 | 1.110800 | -1.276700 |
| Cu | -6.630600 | 1.110800 | 1.276700 |
| Cu | 8.859600 | 1.095900 | -5.104300 |
| Cu | 8.859600 | 1.095900 | 5.104300 |
| Cu | -0.004400 | 1.096500 | 10.211300 |
| Cu | -0.004400 | 1.096500 | -10.211300 |
| Cu | -8.852100 | 1.096700 | 5.120400 |
| Cu | -8.852100 | 1.096700 | -5.120400 |
| Cu | 11.096200 | 0.992300 | -3.826600 |
| Cu | 11.096200 | 0.992300 | 3.826600 |
| Cu | -2.227800 | 1.003300 | 11.506400 |
| Cu | -2.227800 | 1.003300 | -11.506400 |
| Cu | -8.860500 | 1.001200 | 7.694600 |
| Cu | -8.860500 | 1.001200 | -7.694600 |
| Cu | 6.642400 | 1.087000 | -3.825000 |
| Cu | 6.642400 | 1.087000 | 3.825000 |
| Cu | -0.008300 | 1.088200 | 7.650900 |
| Cu | -0.008300 | 1.088200 | -7.650900 |
| Cu | -6.638900 | 1.087300 | 3.839400 |
| Cu | -6.638900 | 1.087300 | -3.839400 |
| Cu | 2.207200 | 1.098600 | 3.815200 |
| Cu | 2.207200 | 1.098600 | -3.815200 |
| Cu | -4.438200 | 1.025500 | 0.000000 |
| Cu | 8.855200 | 1.106700 | -2.556800 |
| Cu | 8.855200 | 1.106700 | 2.556800 |
| Cu | 4.429800 | 1.120200 | 2.552200 |

| | | | |
|---|---|---|---|
| Cu | 4.429800 | 1.120200 | -2.552200 |
| Cu | -0.004100 | 1.114600 | 5.102800 |
| Cu | -0.004100 | 1.114600 | -5.102800 |
| Cu | -2.213100 | 1.104800 | 8.936000 |
| Cu | -2.213100 | 1.104800 | -8.936000 |
| Cu | -4.443400 | 1.135600 | 2.558100 |
| Cu | -4.443400 | 1.135600 | -2.558100 |
| Cu | -6.647500 | 1.106400 | 6.387200 |
| Cu | -6.647500 | 1.106400 | -6.387200 |
| Cu | 11.083500 | 0.993200 | -1.281200 |
| Cu | 11.083500 | 0.993200 | 1.281200 |
| Cu | -4.431100 | 0.994800 | 10.231700 |
| Cu | -4.431100 | 0.994800 | -10.231700 |
| Cu | -6.655500 | 0.989800 | 8.958500 |
| Cu | -6.655500 | 0.989800 | -8.958500 |
| Cu | 6.637700 | 1.078800 | 1.271300 |
| Cu | 6.637700 | 1.078800 | -1.271300 |
| Cu | -2.216000 | 1.082000 | 6.369000 |
| Cu | -2.216000 | 1.082000 | -6.369000 |
| Cu | -4.420200 | 1.065700 | 5.106100 |
| Cu | -4.420200 | 1.065700 | -5.106100 |
| Cu | 8.859800 | 1.103400 | 0.000000 |
| Cu | 2.221500 | 1.052200 | 1.273000 |
| Cu | 2.221500 | 1.052200 | -1.273000 |
| Cu | 0.009000 | 0.967500 | 2.558700 |
| Cu | 0.009000 | 0.967500 | -2.558700 |
| Cu | -2.222900 | 0.975000 | 1.270500 |
| Cu | -2.222900 | 0.975000 | -1.270500 |
| Cu | -4.432000 | 1.096700 | 7.666200 |
| Cu | -4.432000 | 1.096700 | -7.666200 |
| Cu | 4.423800 | 1.113800 | 0.000000 |
| Cu | -2.207100 | 1.192500 | 3.816100 |
| Cu | -2.207100 | 1.192500 | -3.816100 |
| Cu | 0.012600 | 1.030600 | 0.000000 |
| C | -0.474800 | 3.738400 | -1.220000 |
| C | -2.646500 | 3.641500 | 0.000000 |
| C | -1.969400 | 3.655700 | -1.252400 |
| O | -2.539400 | 3.490200 | -2.394100 |
| N | 0.128200 | 3.718700 | -2.433800 |
| C | -0.474800 | 3.738400 | 1.220000 |
| C | 0.232000 | 3.714600 | 0.000000 |
| C | -1.969400 | 3.655700 | 1.252400 |
| O | -2.539400 | 3.490200 | 2.394100 |
| N | 0.128200 | 3.718700 | 2.433800 |
| H | 1.326300 | 3.711000 | 0.000000 |
| H | -3.737000 | 3.590200 | 0.000000 |
| H | -0.487900 | 3.570600 | 3.237500 |
| H | 1.114700 | 3.481600 | 2.535400 |
| H | 1.114700 | 3.481600 | -2.535400 |
| H | -0.487900 | 3.570600 | -3.237500 |