Rung-Defected Ladder of Azido-Bridged Cu(II) Chains Linked by [Cu(picolinate)₂] Units

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Table S1. Bond lengths [Å] and angles [deg] for Complexes 1.

| | Com | plex 1 | |
|-------------------|-----------|-------------------|-----------|
| Cu(1)-N(13) | 1.979(12) | (12) Cu(6)-O(2) | |
| Cu(1)-N(7) | 2.013(10) | Cu(6)-N(3b) | 1.955(12) |
| Cu(1)-N(10) | 2.030(10) | O(6)-Cu(6b) | 1.916(9) |
| Cu(1)-N(4) | 2.058(10) | N(3)-Cu(6b) | 1.955(12) |
| Cu(1)-O(3) | 2.253(9) | N(22)-Cu(4c) | 2.014(10) |
| Cu(2)-N(19) | 1.991(12) | N(25)-Cu(4c) | 2.025(10) |
| Cu(2)-N(13) | 2.003(11) | Cu(4)-O(5) | 2.249(10) |
| Cu(2)-N(10) | 2.000(10) | Cu(5)-O(4b) | 1.941(9) |
| Cu(2)-N(16) | 2.037(10) | Cu(5)-O(4) | 1.941(9) |
| Cu(2)-O(1) | 2.265(10) | Cu(5)-N(2) | 1.947(12) |
| Cu(3)-N(22) | 1.967(11) | Cu(5)-N(2b) | 1.947(12) |
| Cu(3)-N(16) | 1.974(10) | Cu(6)-O(6b) | 1.916(9) |
| Cu(3)-N(25) | 2.003(10) | Cu(6)-N(1) | 1.928(11) |
| Cu(3)-N(19) | 2.007(10) | N(17)-N(18) | 1.146(18) |
| Cu(4)-N(7) | 1.988(10) | N(19)-N(20) | 1.190(15) |
| Cu(4)-N(22a) | 2.014(10) | N(20)-N(21) | 1.139(16) |
| Cu(4)-N(4) | 2.018(10) | N(22)-N(23) | 1.210(16) |
| Cu(4)-N(25a) | 2.025(10) | N(26)-N(27) | 1.160(16) |
| | | | |
| N(13)-Cu(1)-N(7) | 102.9(4) | N(10)-Cu(2)-O(1) | 97.2(4) |
| N(13)-Cu(1)-N(10) | 78.3(4) | N(16)-Cu(2)-O(1) | 88.2(4) |
| N(7)-Cu(1)-N(10) | 171.9(4) | N(22)-Cu(3)-N(16) | 101.0(4) |
| N(13)-Cu(1)-N(4) | 164.5(4) | N(22)-Cu(3)-N(25) | 81.2(4) |
| N(7)-Cu(1)-N(4) | 78.2(4) | N(16)-Cu(3)-N(25) | 167.4(4) |
| N(10)-Cu(1)-N(4) | 98.6(4) | N(22)-Cu(3)-N(19) | 177.0(5) |

| N(13)-Cu(1)-O(3) | 102.4(4) | N(16)-Cu(3)-N(19) | 79.7(4) |
|-------------------|------------|---------------------|-----------|
| N(7)-Cu(1)-O(3) | 99.5(4) | N(25)-Cu(3)-N(19) | 97.5(4) |
| N(10)-Cu(1)-O(3) | 88.0(4) | N(7)-Cu(4)-N(22a) | 164.2(5) |
| N(4)-Cu(1)-O(3) | 92.6(4) | N(7)-Cu(4)-N(4) | 79.7(4) |
| N(19)-Cu(2)-N(13) | 102.9(4) | N(22a)-Cu(4)-N(4) | 98.5(4) |
| N(19)-Cu(2)-N(10) | 173.6(4) | N(7)-Cu(4)-N(25a) | 98.6(4) |
| N(13)-Cu(2)-N(10) | 78.5(4) | N(22a)-Cu(4)-N(25a) | 79.5(4) |
| N(19)-Cu(2)-N(16) | 78.6(4) | N(4)-Cu(4)-N(25a) | 166.8(4) |
| N(13)-Cu(2)-N(16) | 172.9(4) | N(7)-Cu(4)-O(5) | 103.6(4) |
| N(10)-Cu(2)-N(16) | 99.3(4) | N(22a)-Cu(4)-O(5) | 92.1(4) |
| N(19)-Cu(2)-O(1) | 88.9(4) | N(4)-Cu(4)-O(5) | 92.9(4) |
| N(13)-Cu(2)-O(1) | 98.7(4) | N(25a)-Cu(4)-O(5) | 100.2(4) |
| O(4b)-Cu(5)-O(4) | 180.000(2) | C(12)-N(2)-Cu(5) | 129.2(9) |
| O(4b)-Cu(5)-N(2) | 96.1(4) | C(8)-N(2)-Cu(5) | 112.7(9) |
| O(4)-Cu(5)-N(2) | 83.9(4) | C(18)-N(3)-C(14) | 118.7(13) |
| O(4b)-Cu(5)-N(2b) | 83.9(4) | C(18)-N(3)-Cu(6b) | 129.4(10) |
| O(4)-Cu(5)-N(2b) | 96.1(4) | C(14)-N(3)-Cu(6b) | 111.9(9) |
| N(2)-Cu(5)-N(2b) | 180.0(4) | N(5)-N(4)-Cu(4) | 119.8(9) |
| O(6b)-Cu(6)-N(1) | 96.3(4) | N(5)-N(4)-Cu(1) | 120.2(8) |
| O(6b)-Cu(6)-O(2) | 170.6(5) | Cu(4)-N(4)-Cu(1) | 98.9(4) |
| N(1)-Cu(6)-O(2) | 83.9(4) | N(8)-N(7)-Cu(4) | 125.6(8) |
| O(6b)-Cu(6)-N(3b) | 84.5(4) | N(8)-N(7)-Cu(1) | 127.0(8) |
| N(1)-Cu(6)-N(3b) | 168.6(5) | Cu(4)-N(7)-Cu(1) | 101.5(5) |
| O(2)-Cu(6)-N(3b) | 97.2(4) | N(11)-N(10)-Cu(2) | 123.7(8) |
| C(1)-O(1)-Cu(2) | 132.6(10) | N(11)-N(10)-Cu(1) | 121.9(9) |
| C(1)-O(2)-Cu(6) | 114.5(9) | Cu(2)-N(10)-Cu(1) | 100.3(5) |
| C(7)-O(3)-Cu(1) | 124.2(9) | N(14)-N(13)-Cu(1) | 130.9(9) |
| C(7)-O(4)-Cu(5) | 114.9(8) | N(14)-N(13)-Cu(2) | 123.9(9) |
| C(13)-O(5)-Cu(4) | 126.2(10) | Cu(1)-N(13)-Cu(2) | 101.9(5) |
| C(13)-O(6)-Cu(6b) | 114.0(8) | Cu(3)-N(22)-Cu(4c) | 100.5(5) |
| C(6)-N(1)-C(2) | 116.7(13) | N(26)-N(25)-Cu(3) | 116.3(8) |
| C(6)-N(1)-Cu(6) | 129.7(10) | N(26)-N(25)-Cu(4c) | 123.9(8) |
| C(2)-N(1)-Cu(6) | 113.5(10) | Cu(3)-N(25)-Cu(4c) | 98.9(4) |
| C(12)-N(2)-C(8) | 118.0(12) | | |

Symmetry codes: a) x,y-1,z; b) -x,-y+1,-z+1; c) x,y+1,z.

| Table S2 | . Hydrogen | bond geome | etrical parame | ters for 1 (i | in Å for t | he distances | and $^{\circ}$ |
|------------|------------|------------|----------------|---------------|------------|--------------|----------------|
| for the an | igles). | | | | | | |

| <u>D–H</u> … <u>A</u> | | <u>d(D–H)</u> | <u>d(H</u> … <u>A)</u> | <u>d(D</u> … <u>A)</u> | <u><(DHA)</u> | |
|----------------------------------|-------------------|---------------|------------------------|------------------------|------------------|--|
| <u>C(5)-H(5A)</u> … <u>N(21)</u> | [<u>1455.01]</u> | <u>0.93</u> | <u>2.56</u> | <u>3.28(3)</u> | <u>135</u> | |
| C(6)-H(6A)…N(27) | [2576.01] | 0.93 | 2.39 | 3.28(2) | 159 | |

Translation of ARU-Code to CIF and Equivalent Position Code: $[2576.01] = [2_576] = -x, 2-y, 1-z; [1455.01] = [1_455] = -1+x, y, z.$