Table of Contents

Figure 1. Thermal Ellipsoid Plot of Structure ....................... 3
Figure 2. Packing Diagram ........................................ 4
Comments ................................................................. 5
Experimental .............................................................. 5
Acknowledgements ....................................................... 6
References ................................................................. 6
Table 1. Crystal Data ...................................................... 7
Table 2. Atom Coordinates .............................................. 8
Table 3. Bond Distances and Angles ................................. 9
Table 4. Anisotropic Displacement Parameters ................... 11
Table 5. Hydrogen Atom Parameters ............................... 12
Table 6. Torsion Angles ................................................ 13
Table 7. Hydrogen Bond Details .................................... 14
Comment

The molecule was located on a 2-fold rotation axis. The displacement ellipsoids were drawn at the 50% probability level.

Experimental

A black, block-shaped crystal of dimensions 0.08 x 0.08 x 0.06 mm was selected for structural analysis. Intensity data for this compound were collected using a diffractometer with a Bruker APEX ccd area detector (1) and graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The sample was cooled to 100(2) K. Cell parameters were determined from a non-linear least squares fit of 5537 peaks in the range 2.68 < θ < 25.52°. A total of 35291 data were measured in the range 2.103 < θ < 25.780° using φ and ω oscillation frames. The data were corrected for absorption by the empirical method (2) giving minimum and maximum transmission factors of 0.786 and 0.833. The data were merged to form a set of 2096 independent data with R(int) = 0.0663 and a coverage of 100.0%.

The orthorhombic space group Pbcn was determined by systematic absences and statistical tests and verified by subsequent refinement. The structure was solved by direct methods and refined by full-matrix least-squares methods on F² (3). The positions of hydrogens were initially determined by geometry and were refined using a riding model. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atom displacement parameters were set to 1.2 times the isotropic equivalent displacement parameters of the bonded atoms. A total of 159 parameters were refined against 2096 data to give wR(F²) = 0.0705 and S = 1.001 for weights of w = 1/[σ²(F²) + (0.0400 P)² + 1.9000 P], where P = [F₀² + 2Fc²] / 3. The final R(F) was 0.0262 for the 1671 observed, [F > 4σ(F)], data. The largest shift/s.u. was 0.001 in the final refinement cycle. The final difference map had maxima and minima of 0.367 and -0.422 e/Å³, respectively.
Acknowledgment

The authors thank the National Science Foundation (grant CHE-0130835) and the University of Oklahoma for funds to purchase of the X-ray instrument and computers. This structure was determined by Douglas R. Powell.

References


Table 1. Crystal data and structure refinement for 2015-04-11-02.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C_{22}H_{16}Cl_2Cu_3N_6O_2</td>
</tr>
<tr>
<td>Formula weight</td>
<td>657.93</td>
</tr>
<tr>
<td>Crystal system</td>
<td>orthorhombic</td>
</tr>
<tr>
<td>Space group</td>
<td>Pbcn</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a = 15.219(4) Å, b = 7.4337(19) Å, c = 19.372(5) Å</td>
</tr>
<tr>
<td>Volume</td>
<td>2191.6(10) Å³</td>
</tr>
<tr>
<td>Z, Z'</td>
<td>4, 0.5</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>1.994 Mg/m³</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Temperature</td>
<td>100(2) K</td>
</tr>
<tr>
<td>F(000)</td>
<td>1308</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>3.165 mm⁻¹</td>
</tr>
<tr>
<td>Absorption correction</td>
<td>semi-empirical from equivalents</td>
</tr>
<tr>
<td>Max. and min. transmission</td>
<td>0.833 and 0.786</td>
</tr>
<tr>
<td>Theta range for data collection</td>
<td>2.103 to 25.780°</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>35291</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>2096 [R(int) = 0.0663]</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
<td>2096 / 0 / 159</td>
</tr>
<tr>
<td>wR(F² all data)</td>
<td>wR² = 0.0705</td>
</tr>
<tr>
<td>R(F obsd data)</td>
<td>R1 = 0.0262</td>
</tr>
<tr>
<td>Goodness-of-fit on F²</td>
<td>1.001</td>
</tr>
<tr>
<td>Observed data [I &gt; 2σ(I)]</td>
<td>1671</td>
</tr>
<tr>
<td>Largest and mean shift / s.u.</td>
<td>0.001 and 0.000</td>
</tr>
<tr>
<td>Largest diff. peak and hole</td>
<td>0.367 and -0.422 e/Å³</td>
</tr>
</tbody>
</table>

\[
\text{wR}^2 = \left\{ \frac{\sum [w(F_0^2 - F_c^2)^2]}{\sum [w(F_0^2)^2]} \right\}^{1/2}
\]
\[
R1 = \sum \frac{|F_o| - |F_c|}{\sum |F_o|}
\]
Table 2. Atomic coordinates and equivalent isotropic displacement parameters for 2015-04-11-02. U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>U(eq)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu(1)</td>
<td>0.54002(2)</td>
<td>0.54972(5)</td>
<td>0.69556(2)</td>
<td>0.01519(12)</td>
</tr>
<tr>
<td>Cu(2)</td>
<td>0.5000</td>
<td>0.89892(7)</td>
<td>0.7500</td>
<td>0.02160(15)</td>
</tr>
<tr>
<td>Cl(1)</td>
<td>0.54234(5)</td>
<td>0.90492(10)</td>
<td>0.64590(4)</td>
<td>0.02370(18)</td>
</tr>
<tr>
<td>O(1)</td>
<td>0.37370(13)</td>
<td>0.3312(3)</td>
<td>0.55869(10)</td>
<td>0.0226(5)</td>
</tr>
<tr>
<td>N(1)</td>
<td>0.35661(15)</td>
<td>0.5924(3)</td>
<td>0.74884(13)</td>
<td>0.0161(5)</td>
</tr>
<tr>
<td>N(2)</td>
<td>0.43039(15)</td>
<td>0.4803(3)</td>
<td>0.65476(12)</td>
<td>0.0147(5)</td>
</tr>
<tr>
<td>C(1)</td>
<td>0.28383(19)</td>
<td>0.6562(4)</td>
<td>0.78067(15)</td>
<td>0.0173(6)</td>
</tr>
<tr>
<td>C(2)</td>
<td>0.20201(18)</td>
<td>0.6517(4)</td>
<td>0.75160(16)</td>
<td>0.0185(6)</td>
</tr>
<tr>
<td>C(3)</td>
<td>0.1951(2)</td>
<td>0.5867(4)</td>
<td>0.68398(16)</td>
<td>0.0201(7)</td>
</tr>
<tr>
<td>C(4)</td>
<td>0.26892(18)</td>
<td>0.5323(4)</td>
<td>0.64934(15)</td>
<td>0.0181(6)</td>
</tr>
<tr>
<td>C(5)</td>
<td>0.35077(19)</td>
<td>0.5338(4)</td>
<td>0.68283(15)</td>
<td>0.0158(6)</td>
</tr>
<tr>
<td>C(6)</td>
<td>0.43496(19)</td>
<td>0.3877(4)</td>
<td>0.59395(15)</td>
<td>0.0175(6)</td>
</tr>
<tr>
<td>C(7)</td>
<td>0.52792(19)</td>
<td>0.3516(4)</td>
<td>0.57064(15)</td>
<td>0.0175(6)</td>
</tr>
<tr>
<td>C(8)</td>
<td>0.5420(2)</td>
<td>0.2486(4)</td>
<td>0.51227(15)</td>
<td>0.0220(7)</td>
</tr>
<tr>
<td>C(9)</td>
<td>0.6273(2)</td>
<td>0.2163(4)</td>
<td>0.49191(16)</td>
<td>0.0246(7)</td>
</tr>
<tr>
<td>C(10)</td>
<td>0.6961(2)</td>
<td>0.2906(4)</td>
<td>0.52951(15)</td>
<td>0.0234(7)</td>
</tr>
<tr>
<td>C(11)</td>
<td>0.6759(2)</td>
<td>0.3932(4)</td>
<td>0.58693(15)</td>
<td>0.0193(6)</td>
</tr>
</tbody>
</table>
Table 3. Bond lengths [Å] and angles [°] for 2015-04-11-02.

<table>
<thead>
<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu(1)-N(2)</td>
<td>1.917(2)</td>
<td></td>
</tr>
<tr>
<td>Cu(1)-N(1)#1</td>
<td>1.933(2)</td>
<td>1.400(4)</td>
</tr>
<tr>
<td>Cu(1)-N(3)</td>
<td>2.098(2)</td>
<td>0.9500</td>
</tr>
<tr>
<td>Cu(1)-Cu(1)#1</td>
<td>2.4356(8)</td>
<td>1.369(4)</td>
</tr>
<tr>
<td>Cu(1)-Cu(2)</td>
<td>2.8673(8)</td>
<td>0.9500</td>
</tr>
<tr>
<td>Cu(2)-Cl(1)</td>
<td>2.1176(9)</td>
<td>1.405(4)</td>
</tr>
<tr>
<td>Cu(2)-Cl(1)#1</td>
<td>2.1176(9)</td>
<td>0.9500</td>
</tr>
<tr>
<td>Cu(2)-Cu(1)#1</td>
<td>2.8673(8)</td>
<td>1.509(4)</td>
</tr>
<tr>
<td>O(1)-C(6)</td>
<td>1.230(4)</td>
<td>1.382(4)</td>
</tr>
<tr>
<td>N(1)-C(5)</td>
<td>1.354(4)</td>
<td>1.378(4)</td>
</tr>
<tr>
<td>N(1)-C(1)</td>
<td>1.353(4)</td>
<td>0.9500</td>
</tr>
<tr>
<td>N(1)-Cu(1)#1</td>
<td>1.933(2)</td>
<td>1.389(5)</td>
</tr>
<tr>
<td>N(2)-C(6)</td>
<td>1.366(4)</td>
<td>0.9500</td>
</tr>
<tr>
<td>N(2)-C(5)</td>
<td>1.387(4)</td>
<td>1.383(4)</td>
</tr>
<tr>
<td>N(3)-C(11)</td>
<td>1.342(4)</td>
<td>0.9500</td>
</tr>
<tr>
<td>N(3)-C(7)</td>
<td>1.346(4)</td>
<td>0.9500</td>
</tr>
<tr>
<td>C(1)-C(2)</td>
<td>1.367(4)</td>
<td></td>
</tr>
<tr>
<td>N(2)-Cu(1)-N(1)#1</td>
<td>169.23(10)</td>
<td>C(7)-N(3)-Cu(1) 109.10(19)</td>
</tr>
<tr>
<td>N(2)-Cu(1)-N(3)</td>
<td>83.35(10)</td>
<td>N(1)-C(1)-C(2) 123.3(3)</td>
</tr>
<tr>
<td>N(1)-Cu(1)-N(3)</td>
<td>102.02(10)</td>
<td>N(1)-C(1)-H(1) 118.4</td>
</tr>
<tr>
<td>N(2)-Cu(1)-Cu(1)#1</td>
<td>85.51(7)</td>
<td>C(2)-C(1)-H(1) 118.4</td>
</tr>
<tr>
<td>N(1)-Cu(1)-Cu(1)#1</td>
<td>85.67(8)</td>
<td>C(1)-C(2)-C(3) 117.5(3)</td>
</tr>
<tr>
<td>N(3)-Cu(1)-Cu(1)#1</td>
<td>153.33(6)</td>
<td>C(1)-C(2)-H(2) 121.2</td>
</tr>
<tr>
<td>N(2)-Cu(1)-Cu(2)</td>
<td>102.16(7)</td>
<td>C(3)-C(2)-H(2) 121.2</td>
</tr>
<tr>
<td>N(1)-Cu(1)-Cu(2)</td>
<td>79.59(7)</td>
<td>C(4)-C(3)-C(2) 120.0(3)</td>
</tr>
<tr>
<td>N(3)-Cu(1)-Cu(2)</td>
<td>141.35(6)</td>
<td>C(4)-C(3)-H(3) 120.0</td>
</tr>
<tr>
<td>Cu(1)-Cu(1)-Cu(2)</td>
<td>64.86(11)</td>
<td>C(2)-C(3)-H(3) 120.0</td>
</tr>
<tr>
<td>Cl(1)-Cu(2)-Cl(1)#1</td>
<td>177.59(5)</td>
<td>C(3)-C(4)-C(5) 119.9(3)</td>
</tr>
<tr>
<td>Cl(1)-Cu(2)-Cu(1)</td>
<td>66.68(2)</td>
<td>C(3)-C(4)-H(4) 120.1</td>
</tr>
<tr>
<td>Cl(1)-Cu(2)-Cu(1)#1</td>
<td>115.72(3)</td>
<td>C(5)-C(4)-H(4) 120.1</td>
</tr>
<tr>
<td>Cl(1)-Cu(2)-Cu(1)!1</td>
<td>66.68(2)</td>
<td>N(1)-C(5)-C(4) 119.8(3)</td>
</tr>
<tr>
<td>Cu(1)-Cu(2)-Cu(1)#1</td>
<td>50.27(2)</td>
<td>N(2)-C(5)-C(4) 126.3(3)</td>
</tr>
<tr>
<td>C(5)-N(1)-C(1)</td>
<td>119.3(2)</td>
<td>O(1)-C(6)-N(2) 127.8(3)</td>
</tr>
<tr>
<td>C(5)-N(1)-Cu(1)#1</td>
<td>121.80(19)</td>
<td>O(1)-C(6)-C(7) 118.9(3)</td>
</tr>
<tr>
<td>C(1)-N(1)-Cu(1)#1</td>
<td>118.0(2)</td>
<td>N(2)-C(6)-C(7) 113.3(2)</td>
</tr>
<tr>
<td>C(6)-N(2)-C(5)</td>
<td>121.8(2)</td>
<td>N(3)-C(7)-C(8) 123.3(3)</td>
</tr>
<tr>
<td>C(6)-N(2)-Cu(1)</td>
<td>116.55(19)</td>
<td>N(3)-C(7)-C(6) 117.5(3)</td>
</tr>
<tr>
<td>C(5)-N(2)-Cu(1)</td>
<td>121.44(19)</td>
<td>C(8)-C(7)-C(6) 119.3(3)</td>
</tr>
<tr>
<td>C(11)-N(3)-C(7)</td>
<td>117.3(3)</td>
<td>C(9)-C(8)-C(7) 118.5(3)</td>
</tr>
<tr>
<td>C(11)-N(3)-Cu(1)</td>
<td>133.3(2)</td>
<td>C(9)-C(8)-H(8) 120.7</td>
</tr>
<tr>
<td>Bond</td>
<td>Angle</td>
<td>Bond</td>
</tr>
<tr>
<td>----------------------</td>
<td>-------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>C(7)-C(8)-H(8)</td>
<td>120.7</td>
<td>C(11)-C(10)-H(10)</td>
</tr>
<tr>
<td>C(8)-C(9)-C(10)</td>
<td>119.3(3)</td>
<td>C(9)-C(10)-H(10)</td>
</tr>
<tr>
<td>C(8)-C(9)-H(9)</td>
<td>120.3</td>
<td>N(3)-C(11)-C(10)</td>
</tr>
<tr>
<td>C(10)-C(9)-H(9)</td>
<td>120.3</td>
<td>N(3)-C(11)-H(11)</td>
</tr>
<tr>
<td>C(11)-C(10)-C(9)</td>
<td>118.3(3)</td>
<td>C(10)-C(11)-H(11)</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#1 -x+1, y, -z+3/2
Table 4. Anisotropic displacement parameters (Å$^2 \times 10^3$) for 2015-04-11-02. The anisotropic displacement factor exponent takes the form:

$-2 \pi^2 [ h^2 a^* a^* U_{11} + \ldots + 2 h k a^* b^* U_{12} ]$

<table>
<thead>
<tr>
<th></th>
<th>U$_{11}$</th>
<th>U$_{22}$</th>
<th>U$_{33}$</th>
<th>U$_{23}$</th>
<th>U$_{13}$</th>
<th>U$_{12}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu(1)</td>
<td>15(1)</td>
<td>18(1)</td>
<td>12(1)</td>
<td>-1(1)</td>
<td>0(1)</td>
<td>0(1)</td>
</tr>
<tr>
<td>Cu(2)</td>
<td>27(1)</td>
<td>20(1)</td>
<td>18(1)</td>
<td>0</td>
<td>-3(1)</td>
<td>0</td>
</tr>
<tr>
<td>Cl(1)</td>
<td>30(1)</td>
<td>24(1)</td>
<td>18(1)</td>
<td>1(1)</td>
<td>-4(1)</td>
<td>-1(1)</td>
</tr>
<tr>
<td>O(1)</td>
<td>23(1)</td>
<td>28(1)</td>
<td>17(1)</td>
<td>-5(1)</td>
<td>-3(1)</td>
<td>-4(1)</td>
</tr>
<tr>
<td>N(1)</td>
<td>17(1)</td>
<td>16(1)</td>
<td>14(1)</td>
<td>-2(1)</td>
<td>1(1)</td>
<td>-1(1)</td>
</tr>
<tr>
<td>N(2)</td>
<td>16(1)</td>
<td>16(1)</td>
<td>13(1)</td>
<td>0(1)</td>
<td>0(1)</td>
<td>-1(1)</td>
</tr>
<tr>
<td>N(3)</td>
<td>20(1)</td>
<td>17(1)</td>
<td>15(1)</td>
<td>1(1)</td>
<td>-1(1)</td>
<td>2(1)</td>
</tr>
<tr>
<td>C(1)</td>
<td>21(2)</td>
<td>17(1)</td>
<td>14(2)</td>
<td>1(1)</td>
<td>2(1)</td>
<td>1(1)</td>
</tr>
<tr>
<td>C(2)</td>
<td>17(2)</td>
<td>16(2)</td>
<td>22(2)</td>
<td>2(1)</td>
<td>3(1)</td>
<td>1(1)</td>
</tr>
<tr>
<td>C(3)</td>
<td>19(2)</td>
<td>16(2)</td>
<td>25(2)</td>
<td>5(1)</td>
<td>-2(1)</td>
<td>-1(1)</td>
</tr>
<tr>
<td>C(4)</td>
<td>21(2)</td>
<td>17(1)</td>
<td>17(2)</td>
<td>2(1)</td>
<td>-2(1)</td>
<td>-3(1)</td>
</tr>
<tr>
<td>C(5)</td>
<td>21(2)</td>
<td>11(1)</td>
<td>16(2)</td>
<td>4(1)</td>
<td>3(1)</td>
<td>-1(1)</td>
</tr>
<tr>
<td>C(6)</td>
<td>23(2)</td>
<td>16(1)</td>
<td>13(2)</td>
<td>5(1)</td>
<td>0(1)</td>
<td>-1(1)</td>
</tr>
<tr>
<td>C(7)</td>
<td>25(2)</td>
<td>14(1)</td>
<td>14(2)</td>
<td>4(1)</td>
<td>0(1)</td>
<td>2(1)</td>
</tr>
<tr>
<td>C(8)</td>
<td>29(2)</td>
<td>22(2)</td>
<td>15(2)</td>
<td>-2(1)</td>
<td>0(1)</td>
<td>0(1)</td>
</tr>
<tr>
<td>C(9)</td>
<td>33(2)</td>
<td>25(2)</td>
<td>15(2)</td>
<td>-1(1)</td>
<td>4(1)</td>
<td>5(1)</td>
</tr>
<tr>
<td>C(10)</td>
<td>26(2)</td>
<td>24(2)</td>
<td>21(2)</td>
<td>5(1)</td>
<td>6(1)</td>
<td>9(1)</td>
</tr>
<tr>
<td>C(11)</td>
<td>20(2)</td>
<td>22(2)</td>
<td>16(2)</td>
<td>4(1)</td>
<td>1(1)</td>
<td>3(1)</td>
</tr>
</tbody>
</table>
Table 5. Hydrogen coordinates and isotropic displacement parameters for 2015-04-11-02.

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>U(eq)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(1)</td>
<td>0.2899</td>
<td>0.7067</td>
<td>0.8255</td>
<td>0.021</td>
</tr>
<tr>
<td>H(2)</td>
<td>0.1517</td>
<td>0.6911</td>
<td>0.7764</td>
<td>0.022</td>
</tr>
<tr>
<td>H(3)</td>
<td>0.1393</td>
<td>0.5805</td>
<td>0.6621</td>
<td>0.024</td>
</tr>
<tr>
<td>H(4)</td>
<td>0.2647</td>
<td>0.4936</td>
<td>0.6027</td>
<td>0.022</td>
</tr>
<tr>
<td>H(8)</td>
<td>0.4940</td>
<td>0.2012</td>
<td>0.4868</td>
<td>0.026</td>
</tr>
<tr>
<td>H(9)</td>
<td>0.6390</td>
<td>0.1439</td>
<td>0.4526</td>
<td>0.029</td>
</tr>
<tr>
<td>H(10)</td>
<td>0.7554</td>
<td>0.2714</td>
<td>0.5161</td>
<td>0.028</td>
</tr>
<tr>
<td>H(11)</td>
<td>0.7229</td>
<td>0.4441</td>
<td>0.6127</td>
<td>0.023</td>
</tr>
</tbody>
</table>
Table 6. Torsion angles [°] for 2015-04-11-02.

<table>
<thead>
<tr>
<th>Torsion Angle</th>
<th>Torsion Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(5)-N(1)-C(1)-C(2)</td>
<td>5.5(4)</td>
</tr>
<tr>
<td>Cu(1)#1-N(1)-C(1)-C(2)</td>
<td>-163.9(2)</td>
</tr>
<tr>
<td>N(1)-C(1)-C(2)-C(3)</td>
<td>-3.7(4)</td>
</tr>
<tr>
<td>C(1)-C(2)-C(3)-C(4)</td>
<td>-0.6(4)</td>
</tr>
<tr>
<td>C(2)-C(3)-C(4)-C(5)</td>
<td>3.0(4)</td>
</tr>
<tr>
<td>C(1)-N(1)-C(5)-N(2)</td>
<td>176.9(2)</td>
</tr>
<tr>
<td>Cu(1)#1-N(1)-C(5)-N(2)</td>
<td>-14.1(3)</td>
</tr>
<tr>
<td>C(1)-N(1)-C(5)-C(4)</td>
<td>-2.8(4)</td>
</tr>
<tr>
<td>Cu(1)#1-N(1)-C(5)-C(4)</td>
<td>166.2(2)</td>
</tr>
<tr>
<td>C(6)-N(2)-C(5)-N(1)</td>
<td>167.9(2)</td>
</tr>
<tr>
<td>Cu(1)-N(2)-C(5)-N(1)</td>
<td>-17.3(3)</td>
</tr>
<tr>
<td>C(6)-N(2)-C(5)-C(4)</td>
<td>-12.4(4)</td>
</tr>
<tr>
<td>Cu(1)-N(2)-C(5)-C(4)</td>
<td>162.5(2)</td>
</tr>
<tr>
<td>C(3)-C(4)-C(5)-N(1)</td>
<td>-1.3(4)</td>
</tr>
<tr>
<td>C(3)-C(4)-C(5)-N(2)</td>
<td>179.0(3)</td>
</tr>
<tr>
<td>C(5)-N(2)-C(6)-O(1)</td>
<td>-4.5(5)</td>
</tr>
<tr>
<td>Cu(1)-N(2)-C(6)-O(1)</td>
<td>-179.5(2)</td>
</tr>
<tr>
<td>C(5)-N(2)-C(6)-C(7)</td>
<td>176.8(2)</td>
</tr>
<tr>
<td>Cu(1)-N(2)-C(6)-C(7)</td>
<td>1.7(3)</td>
</tr>
<tr>
<td>C(11)-N(3)-C(7)-C(8)</td>
<td>-0.4(4)</td>
</tr>
<tr>
<td>Cu(1)-N(3)-C(7)-C(8)</td>
<td>-175.4(2)</td>
</tr>
<tr>
<td>C(11)-N(3)-C(7)-C(6)</td>
<td>-179.6(2)</td>
</tr>
<tr>
<td>Cu(1)-N(3)-C(7)-C(6)</td>
<td>5.5(3)</td>
</tr>
<tr>
<td>O(1)-C(6)-C(7)-N(3)</td>
<td>176.0(3)</td>
</tr>
<tr>
<td>N(2)-C(6)-C(7)-N(3)</td>
<td>-5.1(4)</td>
</tr>
<tr>
<td>O(1)-C(6)-C(7)-C(8)</td>
<td>-3.2(4)</td>
</tr>
<tr>
<td>N(2)-C(6)-C(7)-C(8)</td>
<td>175.7(3)</td>
</tr>
<tr>
<td>N(3)-C(7)-C(8)-C(9)</td>
<td>1.2(4)</td>
</tr>
<tr>
<td>C(6)-C(7)-C(8)-C(9)</td>
<td>-179.7(3)</td>
</tr>
<tr>
<td>C(7)-C(8)-C(9)-C(10)</td>
<td>-1.3(4)</td>
</tr>
<tr>
<td>C(8)-C(9)-C(10)-C(11)</td>
<td>0.8(4)</td>
</tr>
<tr>
<td>C(7)-N(3)-C(11)-C(10)</td>
<td>-0.1(4)</td>
</tr>
<tr>
<td>Cu(1)-N(3)-C(11)-C(10)</td>
<td>173.3(2)</td>
</tr>
<tr>
<td>C(9)-C(10)-C(11)-N(3)</td>
<td>0.0(4)</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#1  -x+1, y, -z+3/2
Table 7. Hydrogen bonds for 2015-04-11-02[Å and °].

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>d(D-H)</th>
<th>d(H...A)</th>
<th>d(D...A)</th>
<th>&lt;(DHA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C(4)-H(4)...O(1)</td>
<td>0.95</td>
<td>2.22</td>
<td>2.804(4)</td>
<td>118.7</td>
</tr>
<tr>
<td>C(8)-H(8)...Cl(1)#2</td>
<td>0.95</td>
<td>2.74</td>
<td>3.513(3)</td>
<td>138.5</td>
</tr>
<tr>
<td>C(10)-H(10)...O(1)#3</td>
<td>0.95</td>
<td>2.43</td>
<td>3.324(4)</td>
<td>155.9</td>
</tr>
</tbody>
</table>

Symmetry transformations used to generate equivalent atoms:
#2 -x+1, -y+1, -z+1  #3 x+1/2, -y+1/2, -z+1