Supporting information

Guanine-Copper coordination polymers: Crystal analysis and application as thin film precursors

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Table S1: Selected hydrogen bonding distances (Å) and bond angles (°) in 1–3.

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>D—H…A</th>
<th>D…A</th>
<th>H…A</th>
<th>D—H…A</th>
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<tr>
<td>N(1)—H(1)...Cl(2)</td>
<td>3.145(3)</td>
<td>2.31</td>
<td>163</td>
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<tr>
<td>N(2A)—H(2A1)...Cl(2)</td>
<td>3.435(3)</td>
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<tr>
<td>N(1A)—H(1A)...O(6A)</td>
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<td>N(1B)—H(1B)...Cl(2)</td>
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<td>N(2A)—H(2A2)...O(6B)</td>
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<td>N(2)—H(2A)...Cl(3)</td>
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<td>C(11A)—H(11D)...Cl(1)</td>
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<td>C(11C)—H(11E)...O(1M)</td>
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<td>N(1)—H(1)...Br(2)</td>
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<td>C(9)—H(9A)...Br(1)</td>
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<td>C(11)—H(11)...O(6)</td>
<td>3.212(11)</td>
<td>2.28</td>
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#Symmetry of A: (i) -1+x,y,z (ii) 1-x,1-y,1-z (iii) 2-x,1-y,1-z (iv) x,-1+y,z (v) 1+x,y,z (vi) -1+x,-1+y,z (vii) 2-x,2-y,-z (viii) 1+x,1+y,z (ix) 1-x,-y,1-z (x) -1+x,1/2-y,-1/2+z (xi) 1-x,1/2+y,3/2-z (xii) 1+x,y,z (xiii) -1+x,1/2-y,-1/2+z (xiv) 1-x,1/2+y,1/2-z; where A= acceptor and D= donor
**Table S2:** Observed bond lengths (Å) between constituent atoms.

<table>
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<tr>
<th>Bond</th>
<th>( \text{N}_9\text{-propargyl} )</th>
<th>2</th>
<th>3</th>
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<tr>
<td>C2-N1</td>
<td>1.369</td>
<td>1.361</td>
<td>1.364</td>
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<td>C2-N2</td>
<td>1.335</td>
<td>1.337</td>
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<td>C2-N3</td>
<td>1.319</td>
<td>1.332</td>
<td>1.326</td>
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<tr>
<td>C4-C5</td>
<td>1.387</td>
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<td>C4-N9</td>
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<td>C4-N3</td>
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<td>C5-N7</td>
<td>1.390</td>
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<td>C5-C6</td>
<td>1.408</td>
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<td>C6-O6</td>
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<td>C6-N1</td>
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<td>1.403</td>
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<td>C8-N7</td>
<td>1.304</td>
<td>1.321</td>
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<tr>
<td>C8-N9</td>
<td>1.380</td>
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<td>C9-N9</td>
<td>1.467</td>
<td>1.473</td>
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<td>C9-C10</td>
<td>1.456</td>
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<td>C10-C11</td>
<td>1.183</td>
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<td>1.214</td>
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<td>Cu1-C10</td>
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<td>Cu1-C11</td>
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<td>Cu1-N3</td>
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<td>Cu2-N7</td>
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</table>
**Figure S1:** (a) Crystal lattice of 3 when viewed along $\alpha$-axis. (b) Corresponding bond lengths and distances (Å) in 3.

![Crystal lattice and bond lengths](image)

**Figure S2:** SEM images of thin films from 1–3 ($T_1 = 450 \, ^{\circ}\text{C}$; a, c, e), ($T_2 = 600 \, ^{\circ}\text{C}$; b, d, f). Scale: 1 µm.

![SEM images](image)
**Figure S3:** SEM images of thin films from CuCl$_2$, CuBr$_2$ on Si(100) (T$_1$ = 450 °C; a, c), (T$_2$ = 600 °C; b, d). scale: 2 µm.

**Figure S4:** AFM images of thin film from 1. (a) AFM image at T$_1$ [1.9×1.9 µm]. (b) AFM image at T$_2$ [5×5 µm]. (c & e) 3D image and diameter-height profile of panel [a] respectively. (d & f) 3D image and diameter-height profile of panel [b] respectively.
**Figure S5:** AFM images of thin film from 2. (a) AFM image at T₁ [1.9×1.9 µm]. (b) AFM image at T₂ [1.3×1.3 µm]. (c & e) 3D image and diameter-height profile of panel [a] respectively. (d & f) 3D image and diameter-height profile of panel [b] respectively.

![AFM images](image1)

**Figure S6:** AFM images of thin film from 3. (a) AFM image at T₁ [2.1×2.1 µm]. (b) AFM image at T₂ [0.9×1.3 µm]. (c & e) 3D image and diameter-height profile of panel [a] respectively. (d & f) 3D image and diameter-height profile of panel [b] respectively.

![AFM images](image2)
Figure S7: IR spectrum of N9-propargylguanine.
Figure S8: IR spectrum of 2.
Figure S9: IR spectrum of 3.
Figure S10: ESI-HRMS of 1.

\[(\text{IL-allyl})_2\text{Cu}^\text{II}+\text{MeO}\text{]+} \quad \text{(2L-2Cu}^\text{II}+\text{Cl)]}^+\]

- Calculated: 243.9896, 245.9878
- Found: 244.0065, 246.0057

\[\text{L = N9-allyl} \quad \text{guanine} \]
Figure S11: ESI-HRMS of 2.
Figure S12: ESI-HRMS of 3.
Figure S13: PXRD spectra of complexes.

(i) PXRD pattern of 1. (a) simulated pattern at 100 K (b) observed pattern at 298 K

(ii) PXRD pattern of 2. (a) simulated pattern at 100 K (b) observed pattern at 298 K
(iii) PXRD pattern of 3. (a) simulated pattern at 100 K (b) observed pattern at 298 K

The peak correspondence is marked with symbols. The reason for some of peaks are shifted may be attributed to difference in temperature for simulated and observed PXRD data, which causes a difference in the inter-planar distances, thus changing the $\theta$ values.