

Table 1. Structural determination details.

|                                                   |                                                                 |                                                   |
|---------------------------------------------------|-----------------------------------------------------------------|---------------------------------------------------|
| Compound                                          | 1                                                               | 2                                                 |
| Empirical formula                                 | C <sub>24</sub> H <sub>30</sub> CuN <sub>2</sub> O <sub>9</sub> | C <sub>15</sub> H <sub>19</sub> CuNO <sub>7</sub> |
| Crystal Form                                      |                                                                 |                                                   |
| Crystal System                                    | Monoclinic                                                      | Orthorhombic                                      |
| Space group                                       | C2/c (#14)                                                      | Pbca, (#36)                                       |
| T (°C)                                            | 20.0                                                            | 20.0                                              |
| Scan Method                                       | $\omega$                                                        | $\omega$                                          |
| Solution                                          | Direct Methods (ShelXS)                                         | Direct Methods (ShelXS)                           |
| Refinement Method                                 | Full-matrix least-squares                                       | Full-matrix least-squares                         |
| a, (Å)                                            | 17.835(13)                                                      | 12.218(3)                                         |
| b, (Å)                                            | 5.528(4)                                                        | 15.098(6)                                         |
| c, (Å)                                            | 26.72(2)                                                        | 18.008(6)                                         |
| $\alpha$ , (°)                                    | 90                                                              | 90                                                |
| $\beta$ , (°)                                     | 98.68(6)                                                        | 90                                                |
| $\gamma$ , (°)                                    | 90                                                              | 90                                                |
| Z                                                 | 4                                                               | 8                                                 |
| V (Å <sup>3</sup> )                               | 2604(4)                                                         | 3322(2)                                           |
| Density <sub>(calc)</sub> , (Mg/m <sup>3</sup> )  | 1.413                                                           | 1.555                                             |
| Size (mm)                                         | 0.15 x 0.15 x 0.10                                              | 0.15 x 0.15 x 0.10                                |
| Formula weight (amu)                              | 388.85                                                          | 397.86                                            |
| Independent reflections                           | 2999                                                            | 2929                                              |
| No. of Parameters                                 | 164                                                             | 219                                               |
| Final R indices (obs)                             | R <sub>1</sub> = 5.43%<br>wR <sub>2</sub> = 11.85%              | R <sub>1</sub> = 3.84%<br>wR <sub>2</sub> = 6.41% |
| R indices (all. data)                             | R <sub>1</sub> = 9.40%<br>wR <sub>2</sub> = 14.04%              | R <sub>1</sub> = 9.65%<br>wR <sub>2</sub> = 6.91% |
| Goodness-of-fit                                   | 0.882                                                           | 0.626                                             |
| Extinction coefficient                            | ----                                                            | 0.0073(12)                                        |
| Largest diff. peak and hole, (e.Å <sup>-3</sup> ) | 0.659 and -0.63                                                 | 0.350 and -0.302                                  |

$$R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad wR_2 = \left[ \frac{\sum (wF_o^2 - F_c^2)^2}{\sum (wF_o^4)} \right]^{1/2}$$

$$\text{Goodness-of-Fit} = \left[ \frac{\sum (w|F_o| - |F_c|)^2}{(n_o - n_v)} \right]^{1/2}$$

where  $n_o$  = number of observations,  $n_v$  = number of parameters and  $w$  = weights.

$$\text{weight} = 1/\sigma^2(F_o^2) + (0.0000 \cdot P)^2 + 0 \cdot P, \quad \text{where } P = (\max(F_o^2, 0) + 2 \cdot F_c^2)/3$$