**Table 1** Crystal data and structure refinement parameters for complexes **1** and **2**

|  |  |  |
| --- | --- | --- |
| Complex | 1 | 2 |
| Empirical formula | C9H6CuN3O2 | C16H11CdClN4O2 |
| Formula weight | 251.71 | 439.15 |
| Crystal system | Monoclinic | Monoclinic |
| Space group | *P21/c* | *P21/c* |
| *a* (Ǻ) | 5.3384(9) | 10.3623(4) |
| *b* (Ǻ) | 14.499(2) | 16.2454(5) |
| *c* (Ǻ) | 10.905(3) | 10.3291(5) |
| *α* (o) | 90 | 90 |
| *β* (o) | 95.724(19) | 110.599(4) |
| *γ* (°) | 90 | 90 |
| *V* (Ǻ3) | 839.8(3) | 1627.63(12) |
| Z | 4 | 4 |
| *D*c(gcm–3) | 1.991 | 1.792 |
| μ (mm-1) | 2.577 | 1.522 |
| F(000) | 504 | 864 |
| Refl. collected | 3938 | 5054 |
| Unique refl. | 2024 | 2739 |
| *R*int | 0.044 | 0.015 |
| GOF | 1.15 | 1.04 |
| *R*1[*I* ≥ 2σ(*I*)] | 0.0865 | 0.0188 |
| *wR*2 [*I* ≥ 2σ(*I*)]a | 0.3144 | 0.0422 |
| *R*1(all data) | 0.1086 | 0.0234 |
| *wR*2(all data) | 0.3324 | 0.0437 |

*R*1 =Σ|*|F*o|-|*F*c||/Σ|*F*o|, *wR*2 = [Σ*w*(*F*o2-*F*c2)2/Σ*w*(*F*o2)2]1/2