

Isostructural copper-zinc mixed metal complexes for single source deposition of Cu-ZnO composite thin films

Muhammad Sultan,^{a,c} Asif Ali Tahir,^c Muhammad Mazhar,^{b,*} K. G. Upul Wijayantha,^c Matthias Zeller,^d

Received (in XXX, XXX) Xth XXXXXXXXXX 20XX, Accepted Xth XXXXXXXXXX 20XX

DOI: 10.1039/b000000x

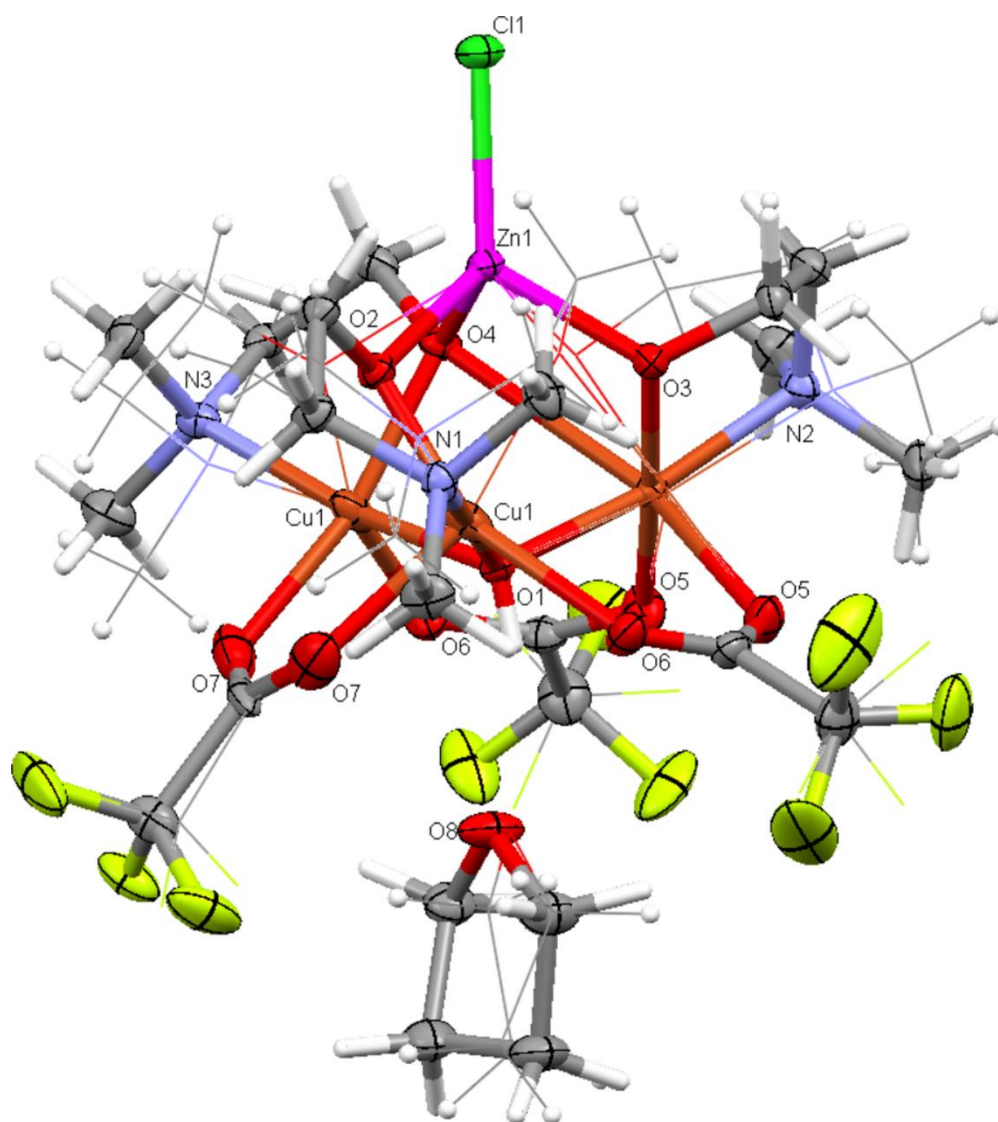


Fig. S1 Thermal displacement style plots of complex (2) the 50% thermal ellipsoid probability level. Atoms of the minor disordered moieties are shown as wireframe mesh for clarity and Labels for C, H and F atoms are omitted.

Monoclinic compound (1) itself exhibits whole molecule disorder of the $[\text{Zn}(\text{TFA})_3(\mu\text{-OH})\text{Cu}_3(\text{dmae})_3\text{Cl}]\cdot\text{THF}$ unit. The molecules in this structure are located on crystallographic mirror planes without being themselves mirror symmetric, thus necessarily leading to disorder of two equally occupied molecules over the same site in the crystal lattice. The similarity of the structures of (1) and (2) prompted us to test whether the structure of (1) might better be described in a triclinic setting

as in (2), but without the whole molecule disorder and being pseudo-merohedrally twinned instead. Attempts to refine the structure of (1) in a triclinic twinned setting as found for (2) were possible, but-despite of inclusion of pseudo-merohedral twinning -they did not give satisfactory results. Under exclusion of the whole molecule disorder the twinning ratio refined to 1:1, but R values of only slightly over 10% could be achieved, and major residual electron density peaks were present in positions that were in agreement with a second molecule mirror symmetric to the first. Inclusion of this second moiety led to a 1:1 disordered complex identical to that observed in the monoclinic structure of (1), but with worse refinement statistics. The structure of (1) thus seems to be indeed a monoclinic structure with randomly disordered molecules rather than a 1:1 twinned version of the structure of (2) with large ordered triclinic twin domains.

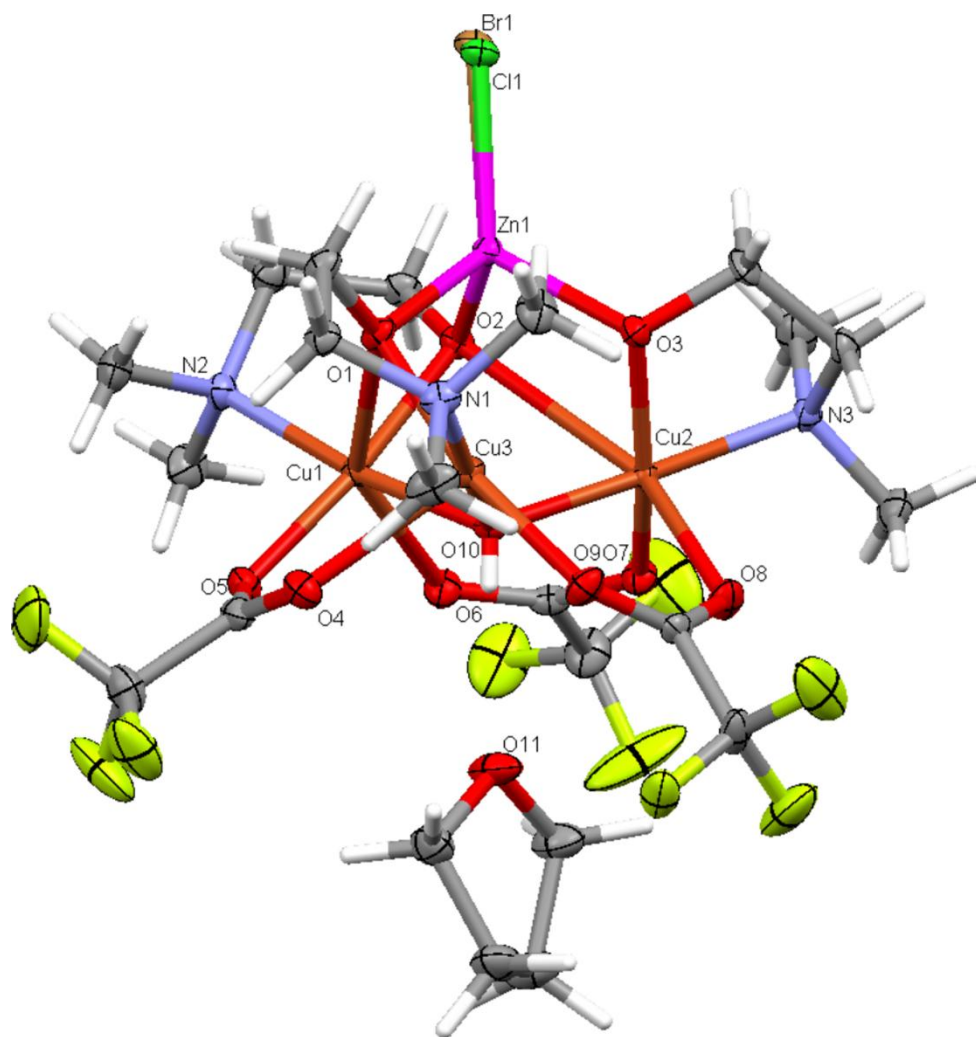


Fig. S2 Thermal displacement style plots of complex (3) the 50% thermal ellipsoid probability level. Atoms of the minor disordered moieties are shown as wireframe mesh for clarity and Labels for C, H and F atoms are omitted.

The structure of the mixed halogen compound (3) shows the highest degree of ordering. It indeed constitutes a superstructure of (1), created by ordering of the complex molecules along the c-axis. Rather than being randomly disordered across a mirror plane (as in (1)), the orientations of the complexes with respect to that mirror plane now do alternate along the c-axis. This ordering of the molecules destroys the mirror symmetry of the structure. Instead another glide plane is created and the unit cell volume is doubled, accompanied by a change of space group from $C2/m$ to $C2/c$. Apart from the disorder of the halogen atoms no disorder is observed in this most symmetric of the three structures.

