

Could/Should/Would you publish a modulated metal-coordinated benzothiazole as an unremarkable structure?

Louise Dawe¹

¹*Wilfrid Laurier Univ*

ldawe@wlu.ca

In this short presentation, I will demonstrate how careful data reduction and the use of constraints, restraints, and the omission of 250 undesirable reflections during refinement yields an unremarkable metal-coordinated benzothiazole small molecule structure. I will address the questions: (1) Could you publish what is likely a modulated structure as unmodulated? (2) Should you use available tools to generate a nice-looking structure? (3) Would you publish this?