

A Few Important Facts about Small Molecule X-ray Crystallography Data

- 1.) X-ray crystallography gives information about a compound in the solid state.
 - a.) Any close contacts, classical (or non-classical) interactions, or other features observed in the solid state may not carry over into a solution.
 - b.) This is important for unusual coordination geometries. Sometimes the way molecules pack in the crystalline lattice relative to each other has a bigger effect on the coordination geometry than the orbital electronics of the compound.
- 2.) While the R1 factor is important, C-C_(esds) are just as important.
 - a.) Even novice crystallographers know tricks to lower the R1, but the bond length and angle statistics do not lie.
- 3.) Bond lengths need to be outside of 3x the e.s.d. of a bond to be considered statistically different.
 - a.) For example: 1.356(4) Å and 1.370(4) Å would be considered the same statistically.
 - b.) On the other hand: 1.356(4) Å and 1.391(4) Å would be considered statistically different.
- 4.) When including bond lengths and angles in your written exam (or in a paper for that matter) be sure to include the error associated with the length or angle.
 - a.) Reporting a C-C bond length of 1.345 Å does not mean much; however a C-C bond length of 1.345(2) Å indicates a good structure, while 1.345(9) Å would indicate a structure of lower quality.
- 5.) The previous guidelines apply to small molecules. Protein crystal structures are governed by a different set of standards.
 - a.) For example: the resolution of a small molecule structure is typically 0.84 Å to 0.77 Å, while the best protein structures have resolutions of 2.0 Å to 1.9 Å. This means that C-C(esds) are not as accurate; though connectivity is fine.