Whole Molecule Disorder in the Crystal Structures of 7-Chloro & 7-Methyl Indole.

J. M. Tanski, Department of Chemistry, Vassar College, Poughkeepsie, NY 12604 USA.

The crystal structures of 7-chloroindole and 7-methylindole both exhibit whole molecule disorder. In the case of the methyl derivative, the disorder is easily modeled in two parts and refines well. $P2_1/c$, with a = 14.283(3), b = 5.3045(10), c = 9.3195(16) Å, β = 90.005(3)° and *R1* = 0.0373. On the other hand, the similarly disordered chloro derivative appears to be orthorhombic, Pnma, with comparable metrical parameters. Refinement of the whole molecule disorder of 7-chloroindole in the orthorhombic space group would require modeling two half molecules about the symmetry element. However, if the structure is solved and refined in the lower symmetry monoclinic unit cell, the modeling is straight forward. $P2_1/n$, with a = 5.218(2), b = 9.287(4), c = 14.353(6) Å, β = 89.993(7)° and *R1* = 0.0462. Appropriate?

This work was supported by grants from the U.S. National Science Foundation, # 0521237 & 0911324.