Space group ambiguity in Tb_2(Porphyrin)$_3$

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A triple-decker Tb_2(Porphyrin)$_3$ sandwich complex refines in both *I*4/*m* and *I*-4. In *I*4/*m*, the molecule has 4/*m* point symmetry, the refinement is stable, and the outer porphyrins are ordered, but significant disorder is modeled in the center porphyrin. Alternatively, in *I*-4, with molecular point symmetry -4, no disorder model is required, but heavy restraints/constraints are needed for the portion of the molecule that has 4/*m* point symmetry. This talk aims to stimulate discussion from the different schools of thought about which is the preferred space group choice for modeling the structure.