

Refinable correlation coefficients to describe crystals with alternative structures .

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Our recent structure refinement of tricarbonyl(ϵ -4,2,5-bis-trimethylsilylcyclopenta-2,4-dienone)iron showed layers of Pbc21m symmetry that could be inversion related to their adjacent layers to form either of two Pbcm structures consistent with the observed diffraction pattern and unit cell. There was a $\frac{1}{4}$ b translation between the two possible sets of inversion centres that created alternative molecule sites $\frac{1}{2}$ b apart. Data merged assuming Pbcm symmetry could be successfully modeled as a 1: 1 twin of a disordered Pbc21m structure provided separate scales Kodd and Keven were used for reflections with k odd and k even. This resulted with a value for Kodd/Keven greater than 1 but not great enough for the structure to be described as an allo twin that would have no correlation between the alternative structures. The k odd reflections show no correlation between the two possible structures but this is not so for the k even reflections. This becomes more of a modeling problem the bigger the difference between the layers of the two structures.

The crystal data was shown to be consistent with a P1 : P2 = 0.651(4) : 0.349 disorder involving the two possible structures each with a single origin choice and an implied correlation coefficient of 0.59(2) that lies between the values of 1.0 corresponding to a disordered structure that is everywhere the same with a volume ratio of P1 to P2 and 0.0 corresponding to an allo twin with a volume ratio of P1 squared to P2 squared.

Keywords: [alternative layer stackings](#), [correlation coefficients](#), [structure refinement](#)