Group-subgroup Relations, Twinning, and Rigid-body Vibration (TLS) in a Bio-crystal: Analogy to Inorganic Structures

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The crystal structure of native methylenetetrahydromethanopterin dehydrogenase, **Mtd-nat**, from *Methanopyrus kandleri* (a= 120 Å, b= 151 Å, c= 220 Å, β =90.0°, *mmm* Laue symmetry due to twinning) was shown to own monoclinic symmetry (C2) by group theory arguments. The structure is closely related to that of the Se-methionine labelled protein, **Mtd-Se**, (a= 120 Å, b=151 Å, c= 110 Å, C222₁, structure solution by MAD) differing only by small reorientations of about 1° of the hexameric structural units. Standard tests for twinning were negative; the twinning was recognized using l=odd reflections only.

The structural units in the Mtd-Se crystals feature a striking anisotropic rigid body libration of the hexameric units as shown by TLS refinement (at 1.55 Å resolution) which is consistent with the static reorientation in the Mtd-nat crystals [1].

The relation between the two crystal structures, the rigid body libration in one, as well as the characteristic twinning of the other suggest an analogy to the structural changes at certain kinds of phase transitions described by group-subgroup relations which imply twinning, 'soft' lattice vibration modes, and which are well studied in inorganic structural chemistry and solid state physics.

[1] Warkentin E., Hagemeier C. H., Shima S., Thauer R. K., Ermler U., *Acta Cryst.*, 2005, D61, 198-202.

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