MS34-04 | Computational Protocol for Simulating the Anisotropic Lattice Expansion in Organic Crystals

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The anisotropic lattice expansion is a different variation of one crystallographic axis respect the other ones. In a temperature dependent X-Ray Powder Diffraction experiment, the anisotropic lattice expansion can be visualized as a significant shift of a set of peaks while others practically did not move. As a consequence, the anisotropic expansion could lead wrong conclusions on the purity and/or composition of a crystalline phase.

We observed anisotropic lattice expansion for metoprolol succinate salt (metoprolol = (±)-1-isopropylamino-3-[4-(2-methoxy-ethyl)-phenoxy]-propan-2-ol) salt. For the related and structural close, metoprolol tartrate salt no such behavior was found. [1] Moreover also the metoprolol free base is subject to anisotropic expansion while the related betaxolol, with similar solid state arrangement and very small structural difference, expands isotropically. [2]

In this work, we show that semiempirical HF-3c method [3] is able to reproduce the experimental observations at a reasonable computational cost within the standard error in reproducing crystal structures. [4] Our protocol could help to shed some light on the anisotropic lattice expansion in organic crystals and to rationalize the factor responsible for the phenomenon.

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