Poster

What we have learned about negative linear compressibility studying cocrystal of 1,2-bis(4-pyridyl)ethane and fumaric acid

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Negative linear compressibility (NLC) is an unusual and counterintuitive behaviour of crystals in response to increased pressure, where crystal expands along one of principal axis. Although, at first it seems this phenomenon contradicts laws of thermodynamics they can be satisfied as long the volume of crystal decreases due to adequate positive linear compressibility (PLC) along two remaining principal axes compensating prolongation along the third one [1,2].

This exceptional property may be useful in many fields of engineering including optical sensors [3], micromechanical controls [4] or body armour [5]. The multitude of potential applications requires constant expansion of the collection of diverse materials, however among reported cases of NLC still prevail framework materials. As a relatively uniform group they may share similar disadvantages like, expensive or environmentally-unfriendly synthesis, limitation of metal hinges and sensitivity to presence of solvent molecules [6].

In this work we present the organic cocrystal of 1,2-bis(4-pyridyl)ethane and fumaric acid - an alternative, metal-free NLC material synthesised with no waste using only green solvent (methanol) and substrates which can be easily recycle. The crystal was investigated up to 3.6 GPa using high-pressure X-ray diffraction technique. We have discovered it exhibits exceptional NLC (Fig. 1) compared to other metal-free NLC materials [2,6]. Moreover, we believe that our study can serve as guideline for the design of NLC materials of wine-rack topology that do not require metal cations as hinges.

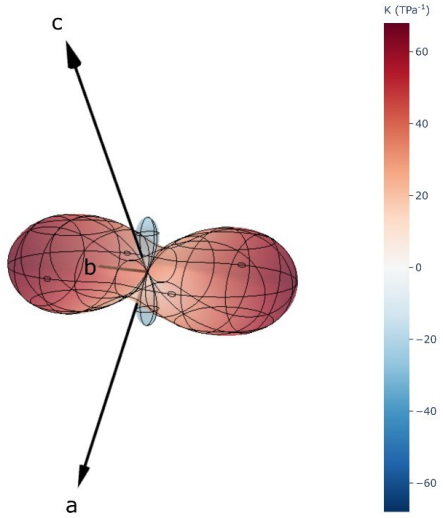

Figure 1. Indicatrix plot of compressibility tensor for cocrystal of 1,2-bis(4-pyridyl)ethane and fumaric acid calculated for 0.1 MPa-3.6 GPa pressure range.

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