Poster

Temperature related bending of isothiouronium hippurate trihydrate crystals

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The isothiouronium salts are formed by S-alkylation of thiourea [1]. Various thiourea derivatives as well as various alkyl substituents can be used for fine tuning of resulting compound's properties. As isothiouronium group usually possesses hydrogen atoms on positively charged nitrogen atoms, they tend to form strong charge assisted hydrogen bonds. These features led to their use in anion receptor design [2], recently they were investigated for inducible nitric oxide synthase inhibition [3] and leukemia treatment [4].

In my studies with tuning the isothiouronium salt properties using anion exchange, I have encountered the unusual behaviour of of 2- ((naphthalen-2-ylmethyl)thio)-4,5-dihydro-1H-imidazol-3-ium hippurate. Upon insertion into cold flow of our cooling device, the plate like crystals bent and twisted, when the crystals were recovered, they quickly straightened. Such behaviour was not observed among the prism like crystals. I have measured the crystals of both habiti and confirmed they have the same structure. The samples were measured in temperature range from 290 K to 95 K, revealing no phase transition. However, I was able to find a significant anisotropy of linear thermal expansion coefficient. While lattice parameter *a* remained almost unchanged during the sample heating (expansion of 0.04 %), the lattice parameter *b* and *c* expanded considerably, with expansions of 2.40 % and 0.89 %. Since the prism like crystals were formed by single crystals and plate like crystals were twinned, I assume the bending is the result of thermal coefficient anisotropy, with twinned crystals acting similarly to a bimetallic strip.

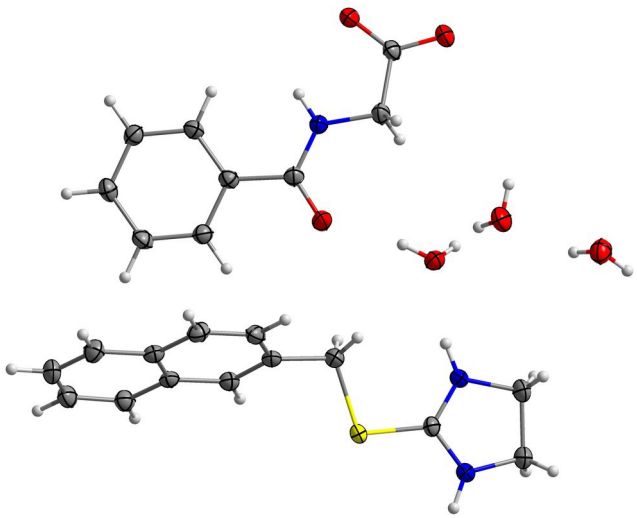

Figure 1. Crystal structure of 2-((naphthalen-2-ylmethyl)thio)-4,5-dihydro-1H-imidazol-3-ium hippurate trihydrate

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