MS26-2-3 Dynamics and disorder: on the stability of pyrazinamide polymorphs
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Abstract
We focus on structures and the relative stability of four pyrazinamide polymorphs. We present new single crystal X-ray diffraction data collected for all forms at 10 K and 122 K. By combining periodic ab-initio DFT calculations with normal mode refinement against X-ray diffraction data, we calculate both enthalpic and entropic contributions to the free energy of all polymorphs. Based on the estimated free energies, we anticipate the stability order of the polymorphs at a given temperature and predict the phase transition temperatures. We conclude that α and γ forms have higher vibrational entropy than that of β and δ and therefore they are significantly more stabilized at higher temperatures. Due to the entropy, which arises from the disorder in γ form, it overcomes form α and is the most stable form at temperatures above c.a. 500 K. Our findings are in qualitative agreement with the experimental calorimetry results.

The four pyrazinamide polymorphs