

New Insights into Organic Intergrown Polymorphic Materials

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The International Union for Crystallography defines an allotwin as a twin whose individuals are oriented crystal associations of different polytypes of the same compound. These structures exhibit locally identical but globally different components. These result when two polytypes grow together epitaxially to form domains sizable enough to yield sharp diffraction spots in an X-ray experiment.^{1–4} The phenomenon is normally characterized by “streaking” reflections. While this is not unknown for solid state inorganics, there are a limited number of molecular examples,¹ and each must be treated uniquely.⁴ We have recently found *N*-(4-methoxyphenyl)-*N'*-pyridin-2-ylthiourea to be a new molecule in this rare class of materials. The intergrown domains were sufficiently large to yield sharp diffraction spots (vs. streaking), but could not be observed by optical microscopy at room temperature. Synchrotron studies (X-ray microdiffraction) subsequently showed that a single domain could be fully indexed at room temperature, and the onset of the second domain was observed upon cooling. These were significant results, given that this type of investigation has never been previously reported for molecular crystals, and several challenges were anticipated. This, and other structural characterizations of this material will be discussed.

References

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