

The missing link: first successful structural analysis of 2-ethylimidazole, a ZIF linker

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ZIFs, or zeolitic imidazolate frameworks, are a particular class of metal organic frameworks in which metal centers are linked by imidazole-based organic molecules such as 2-ethylimidazole. Despite its utility as a link in well-ordered structures, the crystal structure of pure 2-ethylimidazole has remained elusive. Here, we present the first successful structure determination of 2-ethylimidazole and illuminate the reasons for its characteristically poor crystallinity. A phase transition occurs between 150 K and room temperature with the low temperature (100 K) structure appearing more ordered (orthorhombic) than the high temperature structure (triclinic). Though ostensibly more ordered, the low temperature structure is plagued by whole-molecule disorder and probable inversion twinning that lead to a host of pseudo symmetry operations. The low temperature structure, its intriguing ambiguities, and its relationship to the high temperature structure will be discussed.