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Variable Low-Temperature Data Collection and Hierarchical Refinement to Study an Order-Disorder Phase Transition. Weenawan Somphon¹, Kenneth J. Haller¹, A. David Rae², ¹School of Chemistry, Inst. of Science, Suranaree Univ. of Technology, Nakhon Ratchasima 30000 Thailand, ²Research School of Chemistry, The Australian National Univ., Canberra, ACT 0200 Australia.

The polymorphic structure of Ag(bipy)NO₃, which undergoes a reversible order-disorder transformation at ~150 K, was studied by variable temperature (100-296 K). Synthetic precession photographs show *Fddd* symmetry and diffuse scattering above 150 K, but a loss of systematic absences below 150 K, indicating *F12/d1* (*i.e.* *C2/c*) symmetry, and essential disappearance of the diffuse scattering. The 100 K structure is an ordered structure with twin components related by a rotation around *c**. Features of the program RAELS (including refinable local coordinates relative to refinable orthonormal axial systems, refinable *TL* and *TLX* thermal models to describe rigid body motions, and constraints and restraints that can be used to impose more rational models and control refinement pathways by decreasing the effective number of refinable variables) were used to define and control the hierarchical refinements. Bruker-Nonius KappaCCD data collection; Oxford Cryosystems low temperature device; unit cells from phi/chi scan data; EvalCCD data reduction; SORTAV absorption corrections and data merging.