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**The Crystal Structure of a Stable N-heterocyclic Carbene.** G.D. Enright, K.E. Krahulic, R Roesler, Steacie Inst. for Molecular Sciences, National Research Council, Ottawa (ONT.), and Chemistry Dept., Univ. of Calgary, Canada.

We report on a small molecule crystal structure that has proven to be a significant challenge. Although weak satellite peaks characteristic of a modulated structure were observed we decided to collect and solve the primary unit cell structure, expecting significant disorder. We were not disappointed. Researchers at the University of Calgary had been studying a five-membered inorganic heterocyclic carbene that has significance as a spectator ligand in catalysis. They were only able to solve a structure of a protonated form. As the free carbene is not air stable a low temperature data set was collected. The crystal chosen for the data collection diffracted well and a primary F-centered orthorhombic unit cell was indicated. Initial attempts to solve the structure in the indicated space group (Fdd2) using standard programs failed. Attempts at lower symmetry also failed to yield a reasonable starting structure. Eventually, by greatly expanding the number of trial sets (TREF > 300000) a suitable starting electron density map was obtained. The molecule was modeled as fully disordered about a two-fold axis. Numerous restraints were needed to stabilize the refinement. Enlarged thermal ellipsoids indicate further unresolved disorder.