

W0112

Subtle Crystal Environmental Influence on Pseudo-Jahn-Teller Effect Expression. Larry R. Falvello, Inmaculada Escorihuela, Rosa M. Llusar,^a Tatiana Soler^b, Milagros Tomás, Dept. of Inorganic Chemistry and I.C.M.A., Univ. of Zaragoza - C.S.I.C., Plaza San Francisco s/n E-50009 Zaragoza, Spain, ^aDept. de Ciències Experimentals, Univ. Jaume I, Campus de Riu Sec, P.O. Box 224, Castelló, Spain, ^bServicios Técnicos de Investigación, Facultad de Ciencias, Univ. de Alicante, 03080 Alicante, Spain.

A parametric study has been conducted on crystals with two independent pseudo-Jahn-Teller active monocations, $[\text{Cu}(\text{NO}_3)(\text{bipy})_2]^+$ (bipy = 2,2'-bipyridyl), crystallized with a large dianion, $[\text{Pt}(\text{C}_6\text{F}_5)_4]^{2-}$. In crystals with one molecule of acetone in the asymmetric unit, one of the independent cations is dynamic at all temperatures studied, while the other has static distortion at low temperature and suffers increasing amounts of disorder as the temperature is raised. When this system is crystallized with one molecule of CH_2Cl_2 instead of acetone, the Jahn-Teller behavior changes although the gross aspects of the crystal structure -- unit cell, space group, molecular arrangement -- remain essentially the same. In the CH_2Cl_2 -containing crystals both of the cation sites have a component of static behavior at low temperature. This represents a change in expression of the JT effect that could not be achieved at any attainable temperature for the acetone solvate.