

Poster Presentation

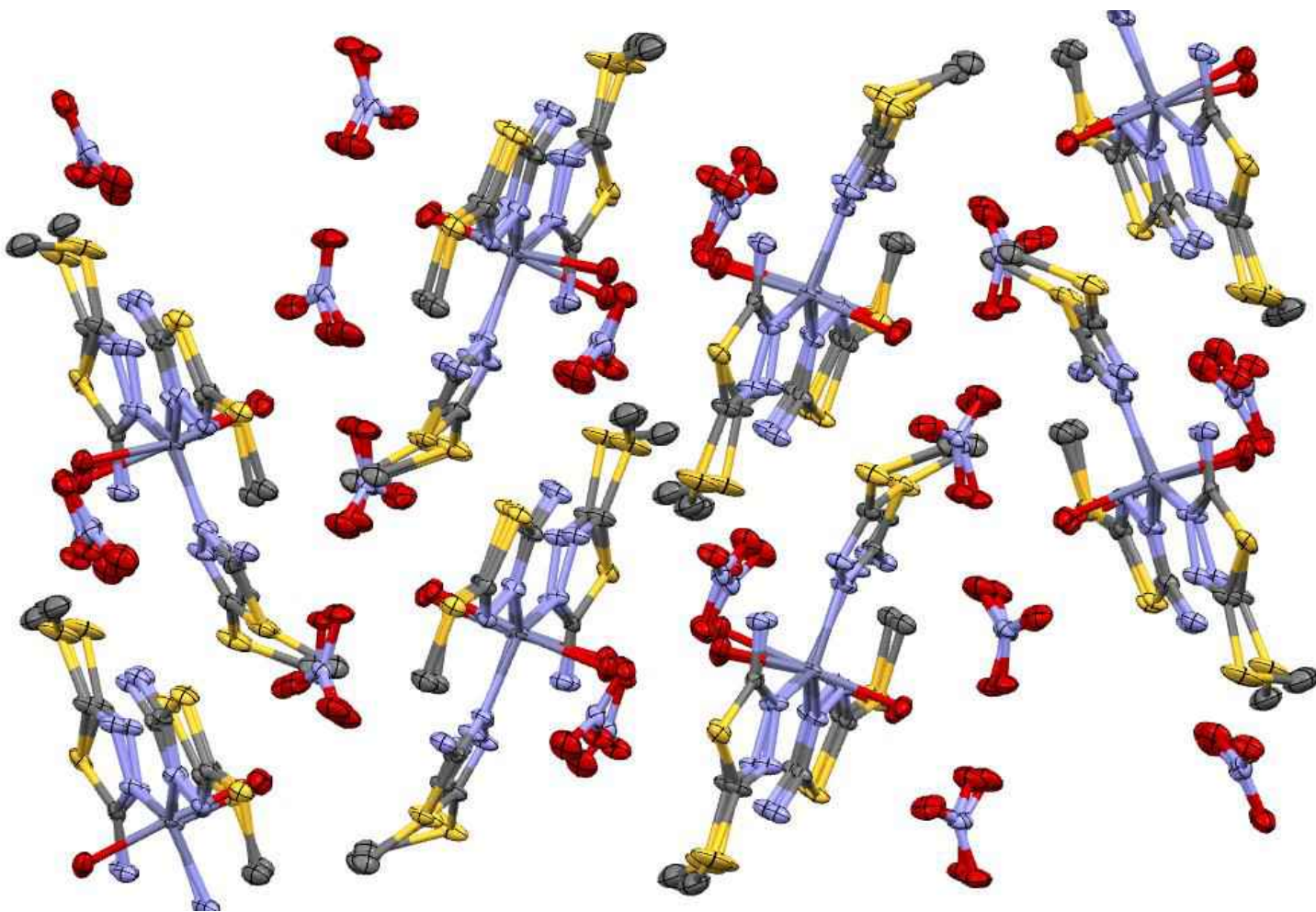
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Incommensurate modulation and phase transformation in a zinc tetra-thiadiazol complex

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The complex of zinc nitrate with 5-(methylthio)-1,3,4-thiadiazol-2-amine crystallizes in a monoclinic setting, space group P2₁/n, as the tetra-thiadiazol complex [(C₃H₅N₃S₂)₄(OH₂)₂Zn](NO₃)₂, with the water molecules in the apical positions of the pseudo-octahedral complex. At room temperature, the structure is characterized by large thermal libration and disorder of the thiomethyl groups, the nitrate counterions and also of one of the zinc coordinated water molecules. Upon cooling to less than 200 K, disorder and thermal libration reversibly transition to incommensurate modulation, with a q-vector of 0.337 a + 0.460 b and space group P2₁/n(a0g)s. At 100 K satellites up to second order are visible, and disorder and libration is completely replaced by pronounced modulation. Phase transformation, refinement strategy and parameters and modulation functions used will be presented, and the correlation between disorder above 200 K and modulation functions below this temperature will be discussed.



Keywords: Incommensurate Modulation, Phase Change, Zinc Complex