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Jahn Teller Effects In Cubic ScF3[1] DOMITILER ORORI, The Catholic University of Eastern Africa, ELICAH WABULULU COLLABORATION, CAROLYNE SONGA COLLABORATION, JAMES SIFUNA COLLABORATION
— Jahn-Teller effects arise in a crystal if distortions are considered on either the octahedral or tetrahedra complexes. This is a non-volatile approach in tailoring materials properties. ScF3 is a material that has arouse special interests based on its Negative thermal expansion (NTE) behaviour. To this date, little is understood on the interplay between Jahn-Teller effects and NTE. The researchers herein, give a focus on how the Jahn-Teller interactions alter the chemistry of this crystal. We employed Density Functional theory as implemented in the Siesta method coupled with mild distortions on the octahedra complex. The results herein go along way in exploring non-volatile approaches in engineering materials. Experimentalists can use this as a back bench in designing materials for novelty. Key words: DFT, ScF3 , NTE, Jahn-Teller distortions.

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