Theoretical prediction of 5,5'-bistetrazole-1,1’-diolate (TKX-50) crystal structure

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5,5'-Bistetrazole-1,1'-diolate(TKX-50) is a new generation of energetic material which has both low sensitivity and high energy. After TKX-50 was firstly prepared in 2012 [1], many researches have been reported about its properties experimentally and theoretically [2-3]. To find more crystal structures of TKX-50 is important for us. Quantum calculation was performed to optimize geometrical structure of TKX-50’s ionic pairs with Gaussian 09 software. The Gaussian electrostatic potential (ESP) charges of all atoms were obtained. The crystal structure prediction, based on the embedded ESP charges, was performed by using Monte Carlo methods and further optimized by DFT-D method. Our simulation showed that the density of predicted crystal structures are in a range from 1.818 g/cm^3 to 1.851 g/cm^3 which is comparable to the reported density of 1.91 g/cm^3 [4]. The DOS of the predicted crystal structures are in good agreement with that from the experimental TKX-50 structure. Our simulations showed that one of the predicted structures is comparable to the reported TKX-50 crystal.

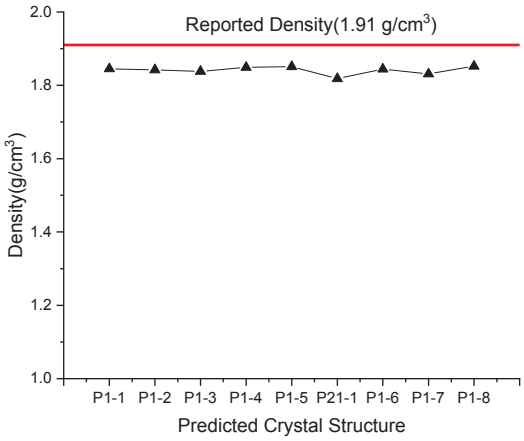

Fig. 1 The density of predicted TKX-50 crystal structures

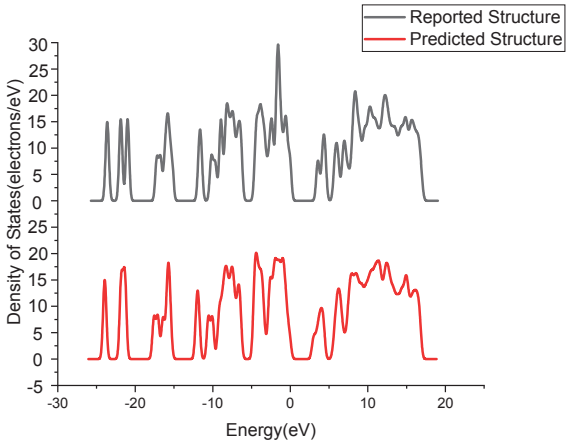

Fig. 2 The DOS of predicted TKX-50 crystal structures

Keywords: TKX-50; Crystal Prediction; Density; Density of States

References:

1. Fischer, N.; Fischer, D.; Klapötke, T. M.; et al. Pushing the limits of energetic materials–the synthesis and characterization of dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate. J. Mater. Chem., 2012, 22, 20418–20422
2. Tidey J P, Zhurov V V, Gianopoulos C G, et al. Experimental Charge-Density Study of the Intra- and Intermolecular Bonding in TKX-50. J. Phys. Chem. A, 2017, 121(46), 8962-8972.
3. Hu N, Chen S, Shu Q, et al. Preparation, characterization and thermal risk evaluation of dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate based polymer bonded explosive. J. Hazard. Mater., 2017, 338, 208-217.

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