

Title

# Search for Crystal Structures using the Generalized Scaled Hypersphere Search Method.

Author and Affiliation

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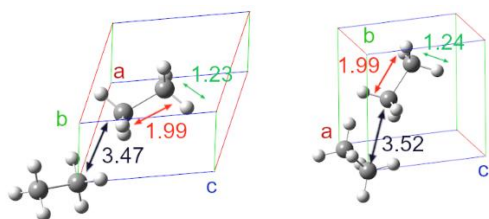
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Abstract

The authors have been trying to explore crystal structures using the Scaled Hypersphere Search (SHS) method, which was developed by K. Ohno and S. Maeda and using the Generalized Scaled Hypersphere Search (GSHS) method, which was developed by K. Ohno, Y. Osada and S. Maeda. In this presentation, the author presents several examples of crystal structure searches by applying the GSHS method to volume of unit cell containing quasi rigid body approximated atoms and molecules. The author also introduces about using the Rapid Nuclear Motion (RNM) method and the Picking up Discrete reaction Center Atoms (PDrCA) method with the GSHS method.



**Figure.** Initial MIN-0 (left) and MIN-10 (right) structures of ethane. Among all evaluated structures, MIN-10 is the most similar to the actual structure. [Ref. Midoro et al., *Chem. Lett.* **2021**, 50, 1559-1561]