An Easy Method to Prepare D$_3$ and C$_2$-TATP Crystals

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Abstract

D3 and C2 TATP structures interconvert at room temperature. Herein, an easy method to isolate both conformers is shown that consists of multiple recrystallization steps using different solvent and heating to boiling. Spectroscopic and physical measurements, such as Raman spectroscopy, X-ray diffraction, and melting point analysis, showed that clear and opaque crystals, respectively, represent different conformations of TATP. Additionally, the transition energy between both conformers was estimated using the Raman shifts.

Keywords

D3 and C2 TATP, ConformersRaman, X-ray diffractogram