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On the Existence of Structure and Space Group of L-Aspartate Single Crystals

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ABSTRACT

It is shown that the crystal structure and space group analyzed using powder X-ray diffraction and reported in the paper "Growth and Characterisation of L-Aspartate Single Crystals" A. Zamara et al., Archives of Physics Research, 2013, 4(3):56-60 is Monoclinic and $P2_12_12_1$ respectively as the authors believe. But actually, its crystal structure and space group is Monoclinic and $P2_1$ respectively.

Keywords: Nonlinear optical crystal, Powder X-ray diffraction, Space group.

INTRODUCTION

The paper makes all the scientific readers a great confusion on the space group corresponding to the monoclinic crystal system obtained [1]. The reason for giving this comment is to clear up the question and makes the readers utilize this article for further reference in their scientific research.

According to the title of the paper, the nonlinear optical crystal L-Aspartate was grown and subjected to various characterizations such as powder X-ray diffraction, absorption studies, Fourier Transform Infrared Spectroscopy for identifying the functional groups and molecules present in it, thermal studies by TGDTA analysis and second harmonic generation analysis by Hurtz-Perry powder technique. The unit cell parameters and space group were determined by powder X-ray diffraction method using Siemens D500 X-ray diffractometer with CuKα (λ=1.5418A°) radiation. It was reported in the paper that the L-Aspartate crystallizes into the monoclinic crystal system with a space group of $P2_12_12_1$ [1]. But the monoclinic crystal system does not consist of this space group. The powder X-ray diffraction was indexed and the lattice parameter was calculated and reported as a= 7.676 Å, b= 6.995 Å, c=5.211 Å, and Volume=275.93 A³ in the paper [1]. Thereafter the calculated values were compared with the reported values [2]. The ref. [2] explains the crystal and molecular structure of L-Aspartic acid and it confirms that the title compound crystallizes monoclinic with the space group of $P2_1$. According to the available international and geometric notation for all seven crystal systems, the symmetry operation $2_12_12_1$ is not associated with the monoclinic crystal structure [3]. The indexed powder X-ray diffraction pattern obtained in this paper is similar to the pattern of JCPDS PDF no. 391523 [4]. But this JCPDS data also confirm the compound L-Aspartic acid crystallizes monoclinic crystal system with $P2_1$ space group. Hence the crystal structure and space group formed in the L-Aspartic acid single crystal is monoclinic and $P2_1$ respectively.

In this article, the author has evaluated the crystal structure with well-defined lattice parameters by Powder X-ray diffraction [1]. The corresponding symmetry should be the relevant space group of that crystal system. But it is a false space group. In spite of the false space group, often a seemingly plausible structural model can be obtained, which may even be refined. The theory of symmetry is of special importance among the theories in crystallography. The symmetry of crystals, which also has an influence on the physical properties, is specified with the aid of space groups. So it is very important to report the appropriate space group for any crystal system [5]. From this evidence, it is very precisely reported in this article that the space group $P2_12_12_1$ does not correspond to the monoclinic crystal system rather it is $P2_1$ according to powder XRD analysis and Patterson vector shift method [2].

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