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On the existence of "diglycine ammonium sulphate"

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Abstract

We prove that a so-called "Semi Organic Non Linear Optical Crystal: Diglycine ammonium sulphate" reported by B. Helina, (*Optik - International Journal for Light and Electron Optics* (2015), http://dx.doi.org/10.1016/j.ijleo.2015.08.252) is not a new semi organic nonlinear optical crystal. Instead it is the well-known γ-glycine crystal.

Keywords: *γ-glycine; diglycine ammonium sulphate; improper characterization.*

Comment

The author of a recent paper [1] reports on the growth and characterization of a so called "diglycine ammonium sulphate, DGAS" as a new semi organic non-linear optical (NLO) crystal. According to [1] the "diglycine ammonium sulphate" is formed from an aqueous solution containing glycine and ammonium sulphate in the ratio 2:1. Although the author concludes by writing that "*The structure of the grown crystal of DGAS was found by single crystal XRD studies. The formation of DGAS was confirmed by Powder XRD pattern. Functional groups were confirmed by FTIR analysis*", only unit cell parameters and symmetry were presented but no other results of single crystal X-ray diffraction (*e.g.* CIF data) are provided. We find it strange that the author writes that a new crystal was obtained but at the same time reports that "*The obtained structural results in this work are found to be in good agreement with the reported value* [*10*]", where the cited "[*10*]" paper by Saha and Podder is [2] in the list of references, which has actually nothing to do with any amino acid especially "diglycine ammonium sulphate".

It was shown with the aid of many examples that incorrect interpretation of the unit cell parameters, powder diffraction patterns and infrared spectra without structure determination will lead to erroneous conclusions [3]. According to the author of [1] the infrared spectrum of the obtained crystal confirms the presence of sulphate anion in the structure. Sulphate anion is characterized by a very strong absorption band near 1100 cm^{-1} caused by asymmetric stretching vibration and the absence of this band indicates the absence of sulphate anion in the structure (see *e.g*. [4]). In the provided infrared spectrum [1] there are weak bands at 1129.96 cm^{-1} and 1052.73 cm^{-1}. The author assigned in text the first peak "to $(SO_4)^{2-}$ stretching vibration", while in Table 2 [1] this peak was assigned to NH_3^+ rocking vibration and the second small peak at 1052.73 cm^{-1} to S=O stretching. So, the infrared spectrum actually indicates the absence of sulphate anion and allows suggesting that the obtained crystal is one of the two components, namely, glycine. Indeed, a comparison of the unit cell metrics (a=b=7.051Å; c= 5.512 Å) [1] with that of the data for γ-glycine (a=b=7.037Å; c= 5.483Å) [5] unambiguously confirms that the title crystal is γ-glycine. In this regard it is worth mentioning that Azhagan and Ganesan [6] found that γ-glycine can be crystallized from an aqueous solution containing glycine and ammonium sulphate in equimolar (1:1) ratio. Powder diffraction pattern and unit cell parameters of γ-glycine in [6] correspond well to that of "diglycine ammonium sulphate", which allows to conclude that from solutions containing glycine and ammonium sulphate in 2:1 and 1:1 ratios γ-glycine is crystallized.

In summary, we have proved that a so called "diglycine ammonium sulphate" crystal reported by B. Helina [1] is not a new NLO crystal, but is actually the well-known γ-glycine crystal. Such an improper characterization is due to the incorrect interpretation of the obtained results in the absence of a single crystal structure determination.

References

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