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Is 1-(4-fluorostyryl)-4-nitrostilbene a novel nonlinear optical crystal?

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Abstract

Many details including the reaction scheme of crystal synthesis in a recent paper reporting optical and mechanical properties of 1-(4-fluorostyryl)-4-nitrostilbene (FNS) single crystal, by Dinakaran and Kalainathan, (Optik, 2013), are very similar to those reported earlier by the same authors for another crystal namely 4-fluoro-4′-nitrostilbene (FONS). FNS is not a new NLO crystal but a new code for FONS with a different and obviously wrong chemical name. FNS crystal is a non-existent compound because substitution of a (4-fluorostyryl) moiety at the 1-position of 4-nitrostilbene will result in pentavalency for carbon.

Keywords: 1-(4-fluorostyryl)-4-nitrostilbene; 4-fluoro-4′-nitrostilbene; nonlinear optical; non-existent compound; dubious publication;

Comment

The authors of a recent paper (title paper hereinafter) claim to have prepared a new organic nonlinear optical (NLO) crystal namely 1-(4-fluorostyryl)-4-nitrostilbene abbreviated by the code FNS, as can be evidenced from the abstract '*A new organic nonlinear optical material 1-(4-fluorostyryl)-4-nitrostilbene (FNS) has been synthesized and single crystals of FNS were grown using solvent evaporation solution growth technique*' [1]. Unfortunately the authors of the title paper are unaware that the FNS crystal cannot actually exist because substitution of a (4-fluorostyryl) moiety at the 1-position of (E)-4-nitrostilbene will result in pentavalency for carbon (Fig. 1) and such pentavalent organic compounds are unheard of. Hence one cannot understand the research aim of a paper attempting to prepare a non-existent compound.

However, the authors claimed they could crystallize such a compound and displayed the picture of a large crystal in the title paper [1]. Hence the paper titled, '*Studies on the optical and mechanical properties of organic nonlinear optical 1-(4-fluorostyryl)-4-nitrostilbene (FNS) single crystal*' attracted our attention and was taken up for scrutiny.

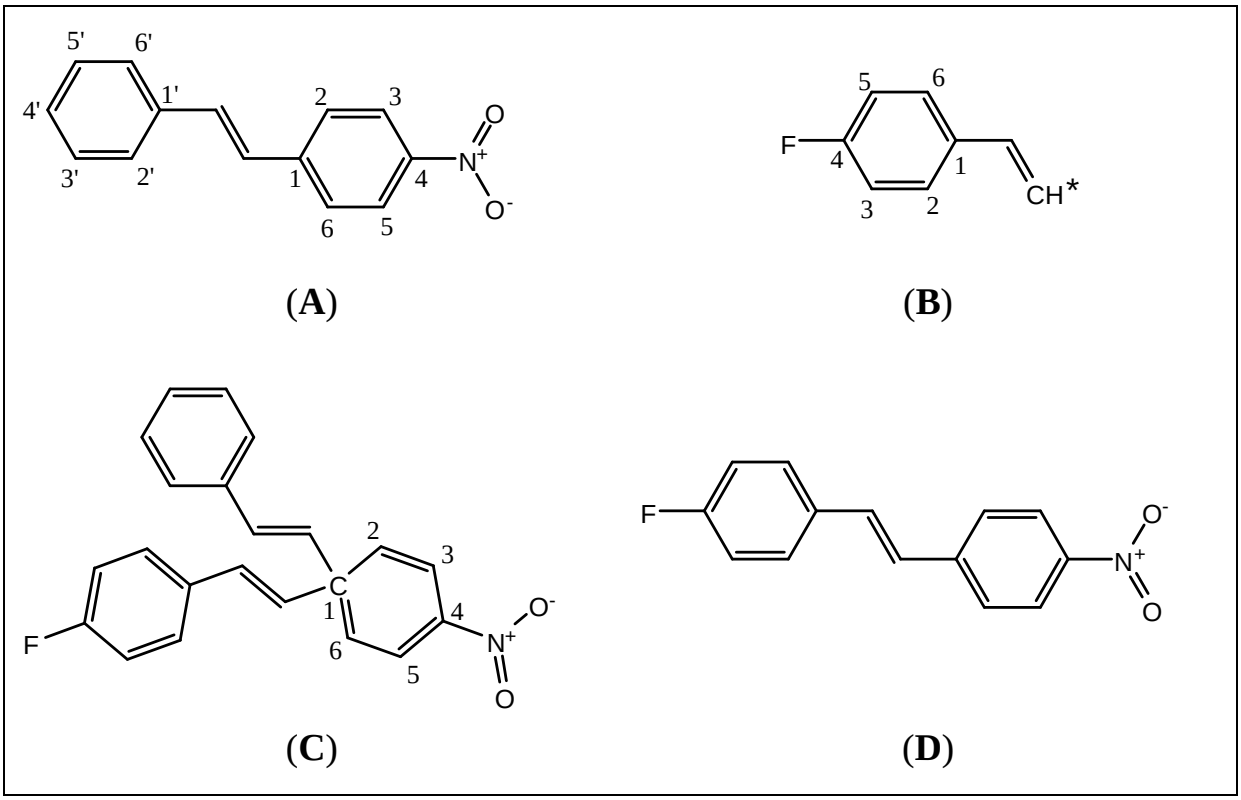

Fig. 1. (A) (*E*)-4-nitrostilbene; (B) (4-fluorostyryl) moiety; (C) 1-(4-fluorostyryl)-4-nitrostilbene; (D) (*E*)-4-fluoro-4′-nitrostilbene

An analysis of the reported results especially the reaction Scheme for the synthesis in the title paper reveals that the crystal grown by these authors is not a so called FNS crystal but actually a well-known compound (*E*)-4-fluoro-4′-nitrostilbene whose synthesis, spectra, SHG characteristics are well documented in the literature [2, 3] and also patented [4]. We note that the synthetic scheme in the title paper is identical in all aspects but for a change in the name of the product crystal, with a scheme reported by the same authors in another paper entitled, '*Synthesis, nucleation, growth, structural, spectral, thermal, linear and nonlinear optical studies of novel organic NLO crystal: 4-fluoro 4-nitrostilbene (FONS)*' in [5]. The scheme of

crystal synthesis in both these papers match so perfectly that both schemes show the same wrong structure for the diethyl(4-nitrobenzyl)phosphonate ester reactant which has already been pointed out in earlier comments [6, 7]. This error of a wrong structure for the phosphonate ester has so far been observed four times in four different papers by the same group reporting on so called 4-substituted-4′-nitrostilbene crystals and is observed once again in the title paper.

In addition to the perfect matching of the synthetic scheme but for product crystal name, the details of crystal growth, single crystal X-ray diffraction study, many equations, many figures and discussion pertaining to these figures, and nonlinear optical study given in the title paper for the FNS crystal are very nearly the same in the paper describing the growth of the FONS crystal. Thus, it can be confirmed that FNS is not a novel NLO crystal but a new code for FONS with a different and obviously wrong chemical name. Although it is not clear why a known compound is reported under a different name by the authors of the title paper, it is to be noted that a series of papers by the same research group on 4-substituted-4′-nitrostilbenes including FONS have been extensively criticized [6, 7].

Normally an error pertaining to the name of a compound in a published paper can be overlooked as an unintentional error of an author due to a researcher's non-familiarity in the nomenclature of chemical compounds. But in the case of FNS, the naming of 4-fluoro-4′-nitrostilbene (FONS) as 1-(4-fluorostyryl)-4-nitrostilbene by an author who has written a paper on FONS, should only be considered as an unacceptable scientific practice. It appears to be a deliberate attempt of the authors to mislead the reviewer and the editor to publish a second paper with almost the same data. However this (title paper) turned out to be more dubious than the first paper. It is disappointing to note that a paper was first submitted on the 4-fluoro-4′-nitrostilbene FONS crystal for publication to *Spectrochimica Acta PartA* and a few weeks later the title paper was submitted to *Optik* on the same FONS crystal by

deliberately changing its name to 1-(4-fluorostyryl)-4-nitrostilbene using a different code namely FNS. Such dubious papers do not add any new scientific information, instead create confusion in the literature.

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