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NLO MATERIALS: BIS(2-METHYL-4-NITROANILINIUM) TIN(IV) HEXACHLORIDE MONOHYDRATE - EXPERIMENTAL INVESTIGATION AND CRYSTAL STRUCTURE PACKING

Samandarov E. Sh[1].,

Gulomov F[2].,

Ibragimov.A.B[1].,

C.Balakrishnan[1].

[1]Institute of General and Inorganic Chemistry of Uzbekistan Academy of Sciences,100170, Mirzo Ulug'bek str., 77a.
[2]Westminster International University in Tashkent, WIUT.

Abstrakt

2-Methyl-4-nitroaniline (2m4na) and Tin(IV) chloride formed a nonlinear optical material. The molecula obtained nonlinear optical material(NLO)=$(2m4na)_2SnCl_6 \cdot H_2O$-bis(2-Methyl-4-nitroanilinium)hexachloro-Tin(IV) monohydrate.In all the crystal structures presented, cations and anions are arranged alternatively to form chain and ring hydrogen-bonding patterns consisting of weak unconventional N−H•••Cl hydrogen bonds. The compound was first analyzed using single-crystal X-ray diffraction to determine its crystal structure.

Crystal packing

The transitioning to the compound bis(2-Methyl-4-nitroanilinium) hexachloro-Tin(IV) monohydrate, this complex compound consists of the cation bis(2-Methyl-4-nitroanilinium) and the anion hexachloro-Tin(IV) along with a water molecule forming a monohydrate. In the crystal structure of bis(2-Methyl-4-nitroanilinium) hexachloro-Tin(IV) monohydrate, the packing of molecules will be influenced by the interactions between the cation, anion, and the water molecule.

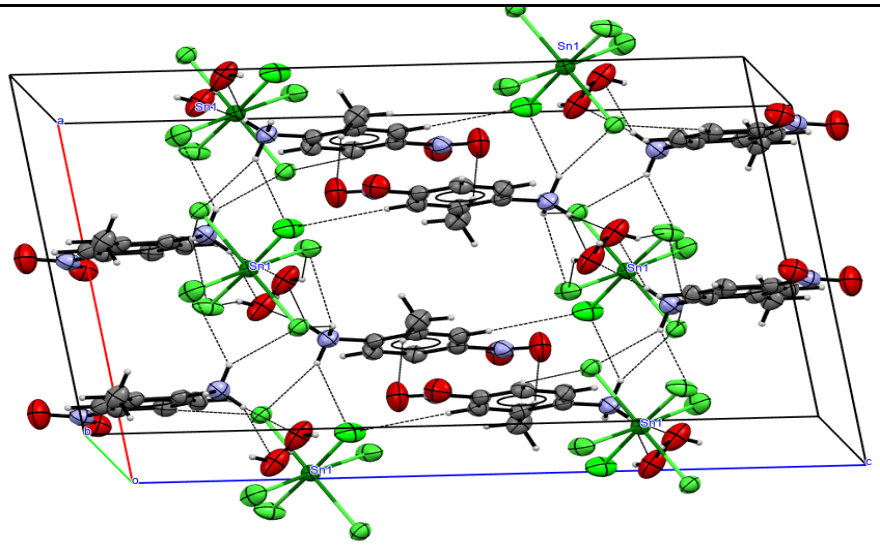


Fig-1. Packing of molecules in the structure of nonlinear optical (NLO) materials. bis(2-Methyl-4-nitroanilinium) hexachloro-Tin(IV) monohydrate

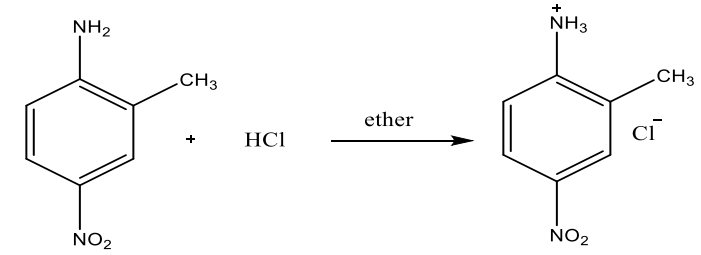
The coordination number of Tin(IV) in this compound is typically 6, indicating that Tin(IV) is surrounded by six chloride ions (Fig-1). In the crystal structure of 2-Methyl-4-Nitroanilinium Hexachloridostannate(IV), the layers are arranged in an ACC sequence due to the bivalent $SnCl_6^{2-}$ anion balancing two monovalent $2m4na^+$ ions. The aromatic rings of adjacent $2m4na^+$ ions are parallel to each other, as well as to the ions in the next layer. However, the vectors of neighboring ions are close to orthogonal, creating a unique geometric relationship.

2. Experimental. Synthesis of bis(2-Methyl-4-nitroanilinium) hexachloro-Tin(IV) monohydrate.

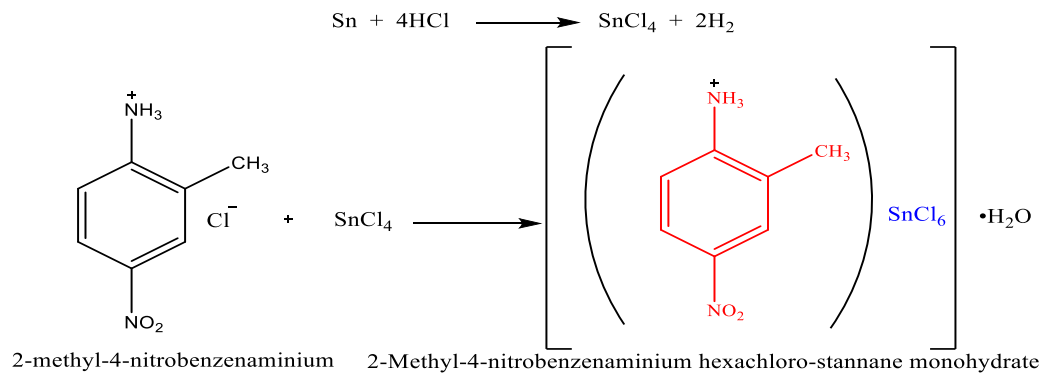
Synthesis: The initial compounds, 2-Methyl-4-nitroaniline All reagents and solvents used in the synthesis were of reagent grade and employed without additional purification. Yellow powder 2-Methyl-4-nitroaniline [Aldrich, purum > 98% (NT)], (0.152g 10 mM) and hydrochloric acid (Aldrich, 35 % in H_2O, 99.95%), (2 mL) were mixed in diethyl ether (10 mL) at room temperature to form a 2-Methyl-4-nitroanilinium chloride precursor solution. The solution was heated to 60 ^{0}C and kept at this temperature for 10 min. Upon cooling, 2-Methyl-4-nitroanilinium chloride precipitated in the solution. The precipitate was then washed with diethyl ether and dissolved in ethanol. Tin shots, weighing 0.118 g (5 mM), were dissolved

in 5 mL of 37 % hydrochloric acid at room temperature over seven hours to produce form **tin chloride** ($SnCl_4$). The tin chloride solution was added to the freshly prepared ethanolic solution of the 2-Methyl-4-nitroanilinium chloride precursor while continuously stirring (Scheme-1).

The solution was placed in a thermostat at 25°C for 20-22 days, resulting in the formation of a new crystal (Scheme-2).

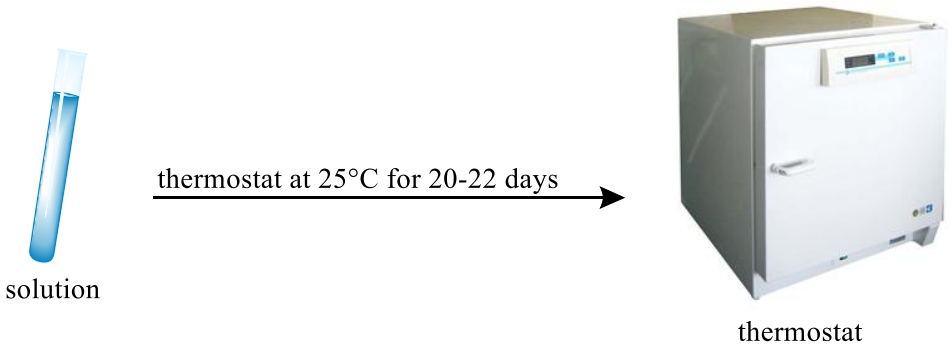


2-methyl-4-nitroaniline 2-methyl-4-nitrobenzenaminium



2-methyl-4-nitrobenzenaminium 2-Methyl-4-nitrobenzenaminium hexachloro-stannane monohydrate

(Scheme-1). Synthesis of bis(2-Methyl-4-nitroanilinium) hexachloro-Tin(IV) monohydrate.



solution thermostat

(Scheme-2). Synthesis of bis(2-Methyl-4-nitroanilinium) hexachloro-Tin(IV) monohydrate.

The compound was first analyzed using single-crystal X-ray diffraction to determine its crystal structure. Subsequently, FTIR (Fourier-transform infrared spectroscopy) and UV-visible absorption spectroscopy studies were conducted to provide insights into the compound's chemical composition and electronic transitions.

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