Correlation between structural studies and third order NLO properties of three new semi-organic compounds

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The study of semi-organic compounds has been of growing interest for a few years. In addition to their fundamental interest in the nature of the bonds occurring between inorganic anions and organic cations, these compounds also have remarkable physico-chemical and optical properties. Recently, the variety of semi-organic hybrid crystals has been developed for NLO applications. The combination of organic compounds, especially amino acids with mineral acids, gives rise to new hybrid crystals with strong NLO properties.Semi-organic compounds play an important role in cell metabolism; they intervene in transfer of energy because of their richness in hydrogen bonds. Inter-ionic interactions through the hydrogen bridges present in this type of semi-organic compounds can serve as mimes explaining some bio-inorganic mechanisms.

Measurement of nonlinear third order electrical susceptibilities was performed for three new compounds (Table 1) by the Third Harmonic Generation (THG) technique. Figure 1 shows the intensity of the THG signal as a function of the angle of incidence, it exhibits the same behavior as the silica.

Table 1. Experimental values of nonlinear susceptibility of the third order.

Compouds	Space group	$\chi_{THG}^{<3>}$ [m^2V^{-2}] 10^{-22}
ortho ammonium benzoic acid hydrogenselenite (o-AAB)$^+$, $(HSeO_3)^-$	P 2_1, chiral	96,3
meta-ammonium benzoic acid hydrogenselenite (m-AAB)$^+$, $(HSeO_3)^-$	P 2_1/n, achiral	67,7
para-ammonium benzoic acid hydrogenselenite (p-AAB)$^+$, $(HSeO_3)^-$	P -1, achiral	43,2

The third order nonlinear electrical susceptibility values $\chi_{THG}^{<3>}$ of studied compounds are stronger than that of silica (reference material). The largest value is observed for the first compound, $\chi_{THG}^{<3>} = 9.63\times10^{-21}$ m^2/V^2 (Table 1) due to the increase in charge transfer and the large number of hydrogen bonding which increases the dipole moment of the compound.

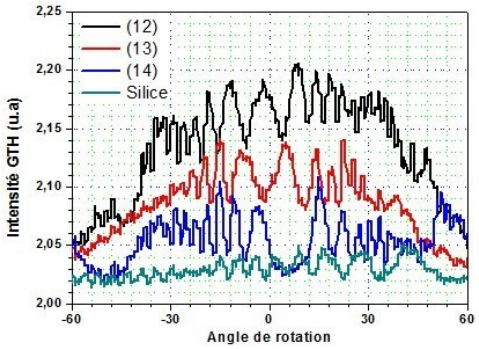

Figure 1. Intensity of the third harmonic for the three samples

These optical measurements revealed different optical behaviors of the three compounds studied. It is therefore very interesting to analyze and discuss the different structural factors correlated with these interesting physical properties. Several structural parameters affect the physical and optical properties of these materials such as: atomic arrangement, intra- and intermolecular interactions, crystal symmetry and electron density distribution.

Keywords: semi-organic compounds - NLO properties - THG technique