squares to a final R value of 0.077 using 1900 reflections. The α-MONA is a centrosymmetric. Its crystal structure is triclinic, with space group P-1, a=1.1912(3), b=1.2110(3), c=1.4818(4)nm, α =99.53(2), ß =113.02(2), γ =92.81(2)° , V=1.92476nm³, Mr=253.26, Z=6, Dx=1.311g/cm³, h =0.87 cm-1, F(000)=792. The relationship between the crystal growth and crystal structure is discussed.

1 Stiegman A E. Graham Eva Perry K j. et al. " The Electronic structure and secondorder nonlinear optical properties of Donor-Acceptor acetylenes: A detailed investigation of structure-property relationship," J. Am. Chem. Soc. 1991, 113, 7658-7666.

PS06.00.36 MORPHOLOGY AND GROWTH OF THE NMDA IN THE DIFFERENT SOLVENTS.

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In actual practice a crystal growth method can not give suitable for different organic crystals. Crystal growth methods are according to the crystal chemistry and properties of the particular compound. Several examples from our recent research work serve to illustrate this point.

The n,n'-bis(4-nitrophenyl)methanediamines (NMDA) crystal is monoclinic system, space group C2, with a=1.6795 b=0.5233, c=0.9802(nm), and ß =120.6°. In this crystal, a type molecules stack along one direction, which means all the molecular dipoles align along the crystal axis[1]. In this structure show the line structure and strongly bond in the line axis. It has stronger SHG effect. One of the most challenging crystal growth problems we have encountered this crystal. The DSC study show it is with many phase transformations, with different SHG effect. Solutions offer the most suitable means to crystal production. Habits of crystallization are growing along needle-like crystals. We have been using more than thirty organic solvents to growing this monocrystal. The influence of crystal growth are assumed to be different morphologies in the dipole moments between the crystallizing component and the solvent. At a solvent providing poor solubility needle crystals can be expected to growing in the solution. For three month period at a small difference in dipole moments from crystallizing substances and solvent is we were able to grow planer and prismatic, which can performed phase matched in perpendicular to the plane or prismatic.

The organic NLO materials have usually hyperpolar molecule, but most typical organic solvents are a dipole moment less than about 3 Debye. The nonpolar solvents tend to form lowly dimensional crystal, and a polar solvents favors formation of bulk crystals.

1 Yamamoto Hironoba, et al., Nippon Kagaku Katshi 1990,(1) 789-96.

PS06.00.37 A STUDY OF THE ELECTROSTATIC POTENTIAL IN 8-HYDROXY-4-METHOXY-1-NAPHTHALDE-HYDE BENZOATE

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Experimental and theoretical electrostatic potentials in the molecule $C_{19}H_{14}O_4$, 8-hydroxy-4-methoxy- 1-naphthaldehyde,benzoate were determined from x-ray diffraction experiments and *ab initio* SCF molecular orbital calculations. A multipole model upto hexadecapoles was used to fit the x-ray data collected at 110K using Mo Ka radiation. The electrostatic potential thus determined was compared to the electrostatic potential calculated from a single point density matrix determined at the Hartree Fock 6-31G* level. Surface plots of electrostatic potential plotted over isosurfaces of electron density aid in the study of the leaning effect observed in 1,8 disubstituted naphthalenes. This study demonstrates the effects of intramolecular interactions on the overall reactivity of the molecule.

PS06.00.38 CRYSTAL STRUCTURE OF LONG CHAIN COMPOUND, 1,13-TRIDECANEDIOL.

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Crystal structures of normal long chain compounds are quite similar to that of liquid crystals. For example, normal paraffins show smectic A or smectic C like structure. And some of them exhibit high temperature phase in which molecules rotate around its long axes. The crystal structure of 1,13-tridecanediol was analyzed as one of the model compounds of liquid crystals. A selected thin plate crystal having approximate dimensions of 0.50 x 0.30 x 0.10 mm was used. The intensity data from a single crystal were collected by RIGAKU AFC5R diffractometer with graphite monochromated CuKα radiation. The data were collected at a room temperature of 296±1K using ω-2Θ scan technique to a maximum 2Θ value of 120.0°. The intensities of three representative reflections were measured after every 150 reflections. An empirical absorption correction based on azimuthal scans of several reflections was applied. The data were corrected for Lorentz and polarization effects. The structure was solved by direct methods with SIR88 and expanded using Fourier with DIRDIF92. The final cycle of full-matrix least-squares refinement was based on observed reflections [I>5.0σ(I)] and 137 variable parameters, $\Sigma w(|Fo|-|Fc|)^2$ minimized, R=0.079, wR=0.108. Crystal data obtained are as follows, C13H28O2=216.36, a=7.143(2), b=37.541(7), c=5.111(1)Å, α=90.00, β=90.00, γ=90.00, P212121, Z=4. One of the most interesting feature of this molecule is that one of the two terminal hydroxyl groups shows gauche conformation, whereas the another one shows trans conformation.

Lipids

PS06.02.01 STRUCTURAL STUDIES ON PHOSPHOLIPID BILAYERS.

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Phospholipids are large natural amphipathic molecules that have long hydrophobic hydrocarbon chains, saturated and/or unsaturated, and polar zwitterionic polar headgroups. In contact with water phospholipids spontaneously assemble into higher molecular aggregates. However, the most relevant phase is the bilayer for its relation to the structure, properties and functions of cell membranes. These are very complex entities. They are not only constituted by an extremely large number of different molecules but they show a very low degree of periodical order. This has led to the proposal of several different models of which that of Singer and Nicolson has been widely accepted. Therefore, given the complexity of cell membranes, simpler models based on phospholipid bilayers are widely used.

We have determined the structure of lecithin and cephaline multilayers. These are types of phospholipids that are respectively located in the outer and inner monolayers of most biomembranes. Besides, we have studied the perturbing effect of water upon their structures. Since then, we have been using lecithin and cephalin bilayers as models to study the way different chemicals interact with cell membranes. This is achieved by making them to interact under a wide range of concentrations in hydrophobic and aqueous media at a constant temperature. The structure perturbation induced to the phospholipid bilayers is followed by X-ray techniques. The results we have obtained in these models have allowed us to interpret the effects these compounds have produced to cell membranes, both in vivo and in vitro. In fact, human erythrocytes, myelin from rat sciatic nerve and neuroskin tissue from toad have been respectively studied by scanning electron microscopy, X-ray fiber diffraction and electrophysiological measurements. It has been found a good correlation between the results observed in the models and the biological systems. The compounds we have analyzed so far are mainly antibiotics, tranquilizers, antiarrhythmic drugs, pesticides and metallic ions.