PS06.00.32 STRUCTURES OF TWO 6-SUBSTITUTED [II] CYCLOHEXYL & [II] 4-CHLOROPHENOXOY [2,10-DICHLORO-12H-DIBENZO [d,g] [1,3,2] DIOXAPHOSPHOCIN 6-OXIDES-CONFORMATION OF 8MEMBERED HETERO CYCLOG RING. M. Krishnaiah, C. Devendranath Reddy, Departments of Physics & Chemistry, Sri Venkateswara University, Tirupati-517 502, India

Organophosphorus heterocycles containing phosphoryl unit reacts rapidly with proteins and nucleic acids in the cell to alkylation carboxyl sulphydryl and amino groups. These molecules are often important in terms of multiple applications as insecticides, bactericides, fungicides and lubricants etc. A few members of this family were evaluated for toxicity in the insect P americana (C. D. Reddy et al., 1991).

Structure analysis of the title compounds has been carried out as part of a series on 8-membered dioxaphosphochinen derivatives to understand the effect of the substituents on the molecular geometry and conformation of hetero ring. Both compounds are cristallized from 1-butanol.

Crystal data: (I):C_{19}H_{19}P_{0}Cl_{2}, monoclinic, P_{2}1/c with a = 11.394 (1) b = 24.254(2), c = 13.576(1) Å, β = 91.94(1)°, v = 3749.6(5) Å³, z = 8, ρ_{c} = 1.407g/cm³, μ(CuKα) = 1.233cm⁻¹, F(000) = 1645, R = 0.058 and Rw = 0.073 for 5687 significant reflections [2θ30(1)]. (II):C_{19}H_{19}P_{0}Cl_{2}, Mon = 44634, triclinic, P-1 with a = 11.392(1), b = 15.936(1), c = 10.617(1) Å, α = 93.14(1), β = 101.10(1), γ = 86.27 (1)°, ρ_{c} = 1.8856.3(3) Å, ρ_{e} = 1.556, ρ_{m} = 1.550g/cm³, μ(CuKα) = 55.24 cm⁻¹, F(000) = 896. R = 0.0895 and Rw = 0.1108 for 5774 significant reflections [1 ≥ 2σ(I)].

Both structures were solved by direct methods and refined by full matrix leastsquares method using SHELX–76. The dioxaphosphochinen ring shows a boat-chair conformation in both structures. The chair form of cyclohexane moieties of both molecules are oriented at 75.8 and 47.6° in the former, where as the phenyl rings are oriented at 22.6 and 46.6° with their hetero planes of the asymmetric unit.

PS06.00.33 CRYSTAL STRUCTURE OF 4,4'-DICHLORO-2,2' IMINODIBENZOIC ACID. Ramón Pomés Hernández*, Héctor Novea de Armas1, Julio Duque Rodriguez, Raúl Alfredo Toscano2, National Center for Scientific Research, P. O. Box 6990, Havana, Cuba, 1 Center of Pharmaceutical Chemistry, P. O. Box 16042, Havana, Cuba, 2 Institute of Chemistry, UNAM, México, D. F.

In the title compound, C_{14}H_{10}Cl_{2}NO_{4}, although the pharmacological activity has not been tested, the substituents bounds to diphenylamine skeleton causes this compound to be an analogue of Lobenzarit acid. Lobenzarit acid (4-chloro-2,2'-iminodibenzoic acid) is an intermediary compound in the synthesis of Lobenzarit disodium (CCA, Disodium 4-chloro-2,2'-iminodibenzoate) which is an anti-rheumatic drug.

Aromatic rings in the title compound are planar and the dihedral angle between the two planes is 44.8(3)°, the out-of-plane r.m.s. deviation being 0.007Å. An internal N—H...O bifurcated hydrogen bond with the imino N atom as donor and a carbonyl O atom as the acceptor is present [N(1)...H(1) 2.12(6)Å, N(1)—H(1)...O(1) 129.6(6)° and H(1)...O(4) 2.16(6)Å, N(1)—H(1)...O(4) 124.6(6)°]. The imino group is not involved in intermolecular interactions, an common feature of related compounds such as fenamates. Therefore, the carboxyl group is the only common site of specific interaction appearing to be a site for intermolecular interactions. A dimerization occurs through hydrogen bonding of the carboxylic groups [H(3a)...O(3) 1.351(9)Å and H(4)...O(4a) 1.351(9)Å, symmetry: 2-x, y, 0.5-z]. The H atoms of the carboxyl group C(14) O(3) O(4) were tied in special position constrains (for H(3a): x = 1.00, z = 0.25 and s.o.f. = 0.50; for H(4): x = 1.00, z = 0.25 and s.o.f. = 0.50; input constraints retained, at least in part, for xzy, s.o.f. and Uij in both cases. The bonds lengths are in good agreement with the average literature values. Crystals are orthorhombic, Pbcn, Z = 8, a = 8.653(2), b = 20.225(4), c = 14.724(3)Å.

PS06.00.34 A COMPARATIVE STRUCTURAL ANALYSIS OF OXALIC ACID AND ITS SALTS M_{2}(C_{2}O_{4})·nH_{2}O (n=0-3), Dmitry Yu. Naumov1, Nina V. Podbereezkaya1, Alexander V. -Virovets2, 1 Institute of Solid State Chemistry SD RAS, Katalazhezic, 18, Novosibirsk, 128, 630128 Russia and Novosibirsk State University, Pirogova, 2, Novosibirsk, 90, 630090 Rusa; 2 Institute of Inorganic Chemistry SD RAS, Lavrent’eva 3, Novosibirsk, 90, 630090 Russia.

Metal oxalates and metal oxalate crystal hydrates find various practical applications and have been used for studies of various aspects of solid state reactivity. At the same time, their crystal structures were not adequately analysed. The present contribution reviews the structural data on various metal oxalates from a unifying point of view.

The comparative analysis was based on the assumption that optimum packing of oxalate ions determines the crystal structures of metal oxalates. The gravity centres of the oxalate-ions were shown to lie in close packed planes, forming regular triangular loops with angles 60° and edges 5.6 Å. Distortion of the close packed oxalate-net results from the interactions of the anions with metal cations or/and water molecules forming hydrogen-bonds networks. The close packed planes are parallel either to the coordination planes of the lattice or to the diagonal ones. A comparison of the size of the oxalate-ion with the lattice parameters suggests the possible orientation of the close packed plane.

The packing sequence depends on the orientation of the oxalate-ions. The number of water molecules in the structures of crystal hydrates of the salts of the same cation was shown to affect the orientation of the oxalate-ions with respect to each other. The polymorphism of metal oxalates is discussed in relation to the variations in the mutual orientation of the oxalate-ions and in the types of anion packings.

PS06.00.35 CRYSTAL STRUCTURE AND POLYMORPHIES OF THE 4METHOXY-4'-NITRO-DIPHENYL-ACETYLENE (MONA). Chaoguo Wang, College of Chemical Engineering and Materials Science, Beijing Institute of Technology, Beijing 100081.

A Novel tolane 4-methoxy-4'-nitro-diphenyl-acetylene (MONA) has been prepared quantitatively by reacting Cuprous methoxy phenyl-acetylene with piidonitrobenzene. A single crystal of the MONA was grown by solution growth method. The crystal was characterized by X-ray diffraction structure analysis and second-harmonic generation (SHG) investigation. We found polymorphies of the MONA form grown from different solvents and they have different nonlinear optical properties depending on the different crystal structures[1]. Crystals of the MONA for structure studies were grown from ethyl acetate at room temperature yielding a stable form -MONA with yellow color (melting point = 122 °C). The structure was solved by direct method (MULTAN 82) from data collected at room temperature on an Enral-Nonius CAD4 diffractometer and refined by least
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, α=1.9123(2), b=1.2110(3), c=1.48184(8)nm,
α=99.53(2), β=113.02(2), γ=92.81(2). v=1.9276nm^3,
M=253.26, Z=1, Dx=1.31 g/cm^3, β=0.87 cm^-1, F(000)=792. The
relationship between the crystal growth and crystal structure is discussed.

and secondorder nonlinear optical properties of Dossor-Acceptor acrylo-

**PS06.00.36 MORPHOLOGY AND GROWTH OF THE
NMDA IN THE DIFFERENT SOLVENTS.** Li Wang, ChaoGuo
Wang, Beijing Institute of Technology, Beijing, 100081, China

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=5.533,
c=0.9802(nm), and β =120.6°. In this crystal, a type molecules
stack along one direction, which means along the whole molecular
dipoles align along the crystal axis. 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
countered. 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. Habit of crystallization are
slow down needle-like crystals. We have been using more than
thirty organic solvents to growing this monocystal. The
influence of crystal growth are assumed to be different morphologies in the
dipole moments between the crystallizing component and the sol­
vent. 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
perform 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 crys­
tal, and a polar solvents favors formation of bulk crystals.


**PS06.00.37 A STUDY OF THE ELECTROSTATIC POTEN­
TIAL IN 8-HYDROXY-4-METHoxy-1-NAPHTHAL­
EDE BENZOATE C. J. Crasto, E. D. Stevens and P. Politzer
Department of Chemistry, University of New Orleans, New
Orleans, L.A.

Experimental and theoretical electrostatic potentials in the mole­
cule C6H4(O)8-8-hydroxy-4-methoxy-1-napthaldehyde.benzoate
were determined from x-ray diffraction experiments and ab initio
SCF molecular orbital calculations. A multiple model upo hexade­
capoles 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 5-31G* 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
COMPONENT, 1,13-TRIDECANEDIOL.** N. Nakamura, Y. Tanaka
and T. Takayama, Department of Chemistry, Ritsumeikan University,
Kusatsu, Shiga 525-77, Japan

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 AFC8 diffractometer with graphite
monochromated Cu Kα radiation. The data were collected at room
temperature of 298±1K using φ-2θ scan technique to a maximum 2θ
value of 120°. The intensities of three representative reflections were
measured after every 150 reflections. An empirical absorption correction
was used 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,
Σw(Fo-Fc)2 minimized, R=0.079, wR=0.108. Crystal data obtained are as follows, C13H2802=216.36, a=7.143(2),
b=37.541(7), c=5.111(1)A., α=90.00,
β=90.00, γ=90.00, μ=0.87 cm^-1, F(000)=296. The crystal structure is triclinic.

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.

**Lipids**

**PS06.02.01 STRUCTURAL STUDIES ON PHOSPHOLIPID BI-
LAYERS.** M. Suwalsky*, F. Villena, B. Ungerer and C.P. Sotomayor,
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Concepcion, Chile

Phospholipids are large natural amphiphatic molecules that have
long hydrophobic hydrocarbon chains, saturated and/or unsaturated,
and polar zwitterionic polar head groups. 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 periodic 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
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 cephaline bilayers at models to study the way different chemicals interact with cell membranes. This is achieved by making them to interact under a wide range of concentra­
tions 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, my­
celium from rat sciatic nerve and neuroskin tissue from tad has been re­
spectively studied by scanning electron microscopy, X-ray fiber diffraction
and electrophysiological measurements. It has been found a good
relationship between the results observed in the models and the biological
systems. The compounds we have analyzed so far are mainly antibiotics,
tranquilizers, antihypertensive drugs, pesticides and metallic ions.

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