fluorite $K_2(PtCl_6)$, and NaCl, giving a rough picture. The successive changes from cubic to triclinic symmetry have been observed while preserving the packing rules of complex centers as the most "hard" scattering fragments. It was shown that polyatomic almost linear anions such as NCS^-, N_3^-, ONO a.o. of the complex ions $[MA_6X]$ are oriented in the direction of octahedral cavities of 'closest packing'. To estimate lattice parameters of hexagonal ($a_h=2R_{ef}$) and cubic ($a_c=2\sqrt{2}R_{ef}$) unit cells, R_{ef}, the radius of the basic sphere in the closest packing arrangement has been used. The estimated and observed lattice parameters have been compared and the efficiency of this geometrical approach demonstrated. Estimation of complex ion size permits prediction of cocrystallization and possible isomorphic substitution. It may be used to suggest selective synthesis reactions for complex formation and help to index powder diffraction data.

PS-07.04.38

A STUDY OF REGULARITIES IN LAYER FORMATION OF SOME VOLATILE β-DIKETONATES OF Cu(2+), Y(3+), AND Pb(2+). By S.A. Gromilov, I.A. Baidina*, S.A. Prokhorova, and V.I. Alekseev, Institute of Inorganic Chemistry, Russian Academy of Sciences, Siberian Branch, Novosibirsk, Russia.

Volatile coordination compounds can be used to prepare layers of inorganic substances from the gaseous phase (MO CVD). β-Diketonates of metals are often used as the initial components. It is of interest to study patterns of layer formation on different substrates and to predict their breakdown into metals, oxides, or fluorides under outside influences.

Single crystals, the volatile β-diketonates of Cu(2+), Y(3+), and Pb(2+) have been chosen for X-ray analysis. $Cu(zis1)_2$-*A*, $Cu(zis7)_2$-*B*, $Y(dpm)_3$-*C*, $Y_2(dpm)_6$-*D*, $Pb(gfa)_2$-*E*, $Pb(pta)_2$-*F**. Molecule configurations of these compounds involve a planar (*A,B,E,F*) and an isometric (*C,D*) form. The crystal structures reveal the presence of monomeric (*A,B,C*), dimeric (*D*), and chain (*E,F*) forms.

Powder samples of the compounds and layers prepared by sublimation on substrates of silicon of different orientations and fused quartz have been studied by X-ray diffraction (DRON-UM1, R=192 mm, CuKα-radiation).

In all cases except *A* oriented polycrystal line films have been prepared. The orientation direction is perpendicular to a crystallographic plane with the largest interplane distance regardless of the molecule configurations and crystal structures.

*Hzis1 - pivaloyldimethylmetoxyaceton,
Hzis7 - pivaloylizopropenilaceton,
Hdpm - pivaloylmethan,
Hgfa - hexafluoracetylaceton,
Hpta - pivaloylthrifluoroaceton.

PS-07.04.39

A SUBSTRUCTURE-SUPERSTRUCTURE RELATIONSHIP IN LITHIUM HYDROGEN MALEATE DIHYDRATE $Li(C_4H_2O_4H)\cdot 2H_2O$

Graciela Díaz de Delgado, A.J. Mora, J.M. Delgado
Departamento de Química, Facultad de Ciencias,
Universidad de Los Andes,
Mérida, Venezuela 5101

During the course of our investigations on the crystal chemistry and solid state behavior of metal derivatives of unsaturated mono- and dicarboxylic acids, crystals of lithium, sodium, potassium, magnesium, calcium, strontium, barium, manganese, cobalt, nickel, zinc and cadmium derivatives of maleic acid (*cis*-2-butenedioic acid) have been prepared. To properly follow any structural change that might take place in the maleate crystals upon exposure to UV-, γ- or X-rays or heat, it has been necessary to carry out single crystal x-ray diffraction experiments in the materials before treatment even though the structures of most of these compounds have been reported in the literature. The photographic study of lithium hydrogen maleate crystals, performed on a Buerger precession camera, showed a particularly interesting structural aspect in this material. A set of intense reflections defined a monoclinic subcell with space group $P2_1/m$ and lattice parameters $a = 5.862(1)$ Å, $b = 6.062(1)$ Å, $c = 9.777(2)$ Å, $\beta = 105.99(2)°$ The geometric disposition of the entire diffraction pattern is described by a *pseudo*-B-centered cell with space group $P2_1/n$ and lattice parameters $a = 5.862(1)$ Å, $b = 6.062(1)$ Å, $c = 18.838(3)$ Å, $\beta = 91.34(1)°$ in good agreement with the results previously reported[1]. The unit cell can be derived from the subcell through the transformation matrix $[\mathbf{a},\mathbf{b},\mathbf{c}] = [(1,0,0)\ (0,1,0)\ (1,0,2)]\ [\mathbf{a},\mathbf{b},\mathbf{c}]_{SC}$. The structure refinement of the subcell led to discrepancy factors R(F)=0.0375, R_w(F)=0.0470, *S*=1.02 for the 643 substructure independent reflections while the refinement of the unit cell led to R(F)=0.0585, R_w(F)=0.0528, *S*=1.25 for all 1161 independent reflections. In the subcell, the $C_4H_2O_4H^-$ anion and the water molecules are in special position (mirror plane) while the Li atoms are located in between the sheets, in general positions but with an occupancy factor of ½.

In this contribution, we discuss in detail the interesting substructure-superstructure relation present in $Li(C_4H_2O_4H)\cdot 2H_2O$, a structural feature infrequently found in organic and metal-organic materials.

The purchase of the P3/F Nicolet diffractometer was possible thanks to grants F-74 and TC-19 from CONICIT and CDCHT-ULA, respectively. This work was possible thanks to grant C-435-90 from CDCHT-ULA.

[1] Popelier, P., Lenstra, A.T.H., and Geise, H.J., *Acta Cryst.*, **C45**, 1024-1028 (1989)