163-170. [4] Photoinduced Phase Transitions, K. Nasu ed., *World Scientific*, **2004.** [5] S. Iwai et al., *Phys. Rev. Lett.* **2006,** *96,* 057403. [6] L. Guérin et al, *Phys. Rev. Lett* 2010, *105*,246101.

Keywords: Diffuse scattering, Photoinduced Phase Transition, precursor phenomena

MS45.P08

Acta Cryst. (2011) A**67,** C523

Structural and electrochemical study of copper complexes derived from dehydroacetic acid

Amel Djedouani,[a] Chaouche Massika,[b] A.Beghidja,[b] C.Beghidja,[b] [a]*Ecole Nornale Superieure de Constantine 25000 (Algerie).* [b]*Département de Chimie Faculté des Science Université Mentouri Constantine (Algeria).* E-mail: Djed_amelle@yahoo.fr

Dehydroacetic acid or [DHA = 3-acetyl-6-methyl-2H-pyran-2,4(3H)-dione], Is an industrially product used as a fungicide, a bactericide and also as an important intermediate in organic synthesis. usually obtained through the auto-condensation of ethyl acetoacetate [1]. However, little is known on ils metal complexes. The Cu and Zn complexes have been reported to be, respectively, a fungicide [2]. and a heat stabilizer for vinyl chloride resins[3]. There are some other reports in the patent literature [3] and also the stability constantes of some complexes have been measured [4].

This has motivated our study of the structural characterization of complexes of dehydroacetic acid. We present here the crystal structures determination of the complexes, [Cu(DHA)$_2$.2DMF], [Cu(DHA)$_2$.2DMSO].

[Cu(DHA)$_2$. 2DMF], has the following structural properties : triclinic, P-1, a = 7.689(5), b = 8.541(5), c = 9.386(5) Å, α = 84.870(5)°, β = 86.964(5)°, γ = 78.852(5)°, V = 601.9(6) Å^3 and Z = 1; for [Cu(DHA)$_2$. 2DMSO] : Monoclinic P2$_1$/n a = 11.580(5) b = 6.320 (5) c = 16.4024 (5) Å; β = 92.269(5); V = 1201.1(11) Å^3 and Z = 2.

The metal atoms are, located on an inversion centre, are surrounded by two DHA ligands occupying the equatorial plane. The two axial positions are occupied by O atoms of two solvant molecules. The structures is stabilized by intermolecular C-H….O hydrogen bonds.

An electrochemical study (cyclic voltammetry) indicates that the reduction of the two complexes, two steps are indicated out : the first as attributed to the reduction of the metal and the seconde to the reduction of the coordinated ligands.

[1] M.E.Smith, R.A.J.Andersen, *Am. Chem. Soc.* **1996,** *118,* 11119–11128. [2] D.S. Rao, M.C. Ganorkar, D.L.S. Rao, V.T. John, *Natl. Acad.Sci. Lett.* **1978,** *1,* 402.. [3] F. Arndt, B. Eistert, H. Scholz, E. Aron, *Berichte Teil B,* **1936,** *69*, 2373-2380. [4] J. Casabo, J. Marquet, M. Moreno-manas, M. Prior, Teixidor, *Polyhedron*, **1987,** 1235–1238.

Keywords: structural study-1, complexe-2, dha-3.

MS45.P09

Acta Cryst. (2011) A**67,** C523

Humidity-induced phase transition of xylose isomerase

Yoko Sugawara,[a] Masanori Ootaki,[a,†] Shigefumi Yamamura,[a] Shigeru Endo,[a] and Masayoshi Nakasako[b] [a]*School of Science, Kitasato University, Kitasato, Minami-ku, Sagamihara, 252-0373,* [b]*Faculty of Science and Technology, Keio University, Hiyoshi, Kohoku-ku, Yokohama, 223-8522, (Japan)* E-mail: sugawara@sci.kitasato-u.ac.jp

We have been examining humidity-induced phase transitions of nucleotide and protein crystals. The dehydration accompanies not only shrinkage of the unit cell volume but also transformation of crystal symmetry and/or conformational changes of biomolecules. Such a phenomenon helps our understanding of the role of hydration which influences the biological function. The role of hydration water is also argued on electronic properties of hydrates of molecular conductors and ferroelectrics.

Xylose isomerase is one of the protein crystals, where the humidity -induced phase transition occurs. An as-grown crystal (the space group $I222$) changes to the dry form (the space group $P2_12_12$) at approximately 84 % relative humidity [1,2]. The intermediate stage was determined crystographically, and the scheme of the phase transition will be discussed paying attention to the hydration networks.

[†] Present adress: Institute of Radioisotope Research, St, Marianna Univ.

[1] M. Ootaki et al., *Joint Conference of AsCA '06 and CrSJ*, Tsukuba, Japan, **2006**, P21-217. [2] C. Besnard et al., *Acta Cryst. A*, **2008**, *64*, C372.

Keywords: phase transition, protein, hydration

MS46.P01

Acta Cryst. (2011) A**67,** C523

X-ray diffraction study of some natural resins

Irma Araceli Belío-Reyes,[a] Lauro Bucio,[b] [a]*Facultad de Odontología, Univer-sidad Autónoma de Sinaloa, 80010 Culiacan, Sinaloa, (Mexico).* [b]*Instituto de Física, Universidad Nacional Autónoma de México 04510 Mexico DF, (Mexico).* E-mail: irmaracelib@yahoo.com

Most copal incense in Mesoamerica is traceable to several species in the family Burseraceae, usually of the genus Bursera. Additionally the genus Hymenaea of the family Leguminosae has been said to be represented among the bearers of incense resin. In the Maya region of southern Mexico and Central Mexico, resin from *Bursera bipinnata* is among the most frequently employed of the copal incenses today and apparently also in former times.

Bursera species were used in diverse medical practices among mesoamericans. Leaves frequently spray a mist of volatile oils when broken. These gums and oils were applied directly to induced wounds before the ceremony so that a direct connection with the circulatory system of the blood might be established. In contemporary Mexico some species of Bursera (especially *B. penicillata*) are used to allay pain in instances of toothache.

The important uses attributed to resin from this particular species are concerned to its adhesive and medicinal properties. It was used as a paint binder in Mesoamerican murals that have long been wrongly called frescoes; and also for dental incrustations of precious stones in dental apatite from the X to VI centuries B.C. [1-3]. In a previous work [4] we have reported the presence of a crystalline phase in a copal resin form a Texcoco market which now, we have identified as α-amyrin. This crystalline phase was also identified to be present in a sample of copal from the archaeological site of Templo Mayor located in Mexico City and also in the species *B. laxiflora* and *B. excelsa*.

[1] S. Fastlicht. *Revista de la Asociación Dental Mexicana y del Colegio de Cirujanos Dentistas*, Mexico City, **1971**, 39-59. [2] J.A. Pompa y Padilla. *Arqueología Mexicana*, **1995**, *3*, 62-65. [3] F. Martínez Cortes, *SEP-Setentas* Mexico City **1974,** *124*, 134-136. [4] L. Bucio, I.A. Belío-Reyes, J.A. Rodríguez, M.N. Orta, J. Arenas-Alatorre, C. Magaña, R. Velázquez, *Zeit. Krist. Suppl.* **2006,** *23*, 569-574.

Keywords: triterpenoid, X-ray, powder