

hypereutectic alloys solidify with aluminum-rich dendrites.

In a solidification process, the microstructure depends on the alloy characteristics and is mainly a function of the temperature evolution ahead the solid/liquid interphase [1-3].

Among the several phenomena occurring during solidification, like solute segregation or morphology stability, one of the most important ones is dendritic growth. The most important dendrite parameters are the primary, secondary and tertiary arm spacings due to their influence on mechanical properties.

An efficient method to examine the evolution of the dendrite arms is related to the application of steady-state directional solidification with an imposed growth rate, V , and a thermal gradient, G , at the solid/liquid interphase.

In this work, Zn-Al (wt%) alloys were solidified under unidirectional solidification in a device cooled with water, in a vertical upward direction (0°), inclined at 30° and 45° to the vertical and in a horizontal upward direction (90° to the vertical). We determined the position of the transition from columnar to equiaxed structure (CET) through macro and micro-analysis, and significant thermal parameters by recording temperature-time data. The results show that the direction of dendrite growth is about that of the heat extraction and that the angle of inclination of the columnar grains with the longitudinal axis of the alloy sample coincides approximately with the angle of inclination of the furnace.

The relevance of the problem under study is justified on the basis that the solidification variables, including natural convection, affect the structures of the solid and the formation of defects. The solidification variables are also important for modeling prediction of the structure and property of a given cast piece [3-11]. The results also allow a better understanding of the conditions and mechanisms operating in a solidification with different directions.

[1] L.J. Yang, *Journal of Material Processing Technology* **2003**, *140*, 391-396.

[2] I. Maxwell and A. Hellawell, *Acta Metall.* **1975**, *23*, 229-237. [3] I. Dustin and W. Kurz, *Z. Metallk.*, **1986**, *77*, 265-273.

Keywords: solidification, Zn base alloys, CET

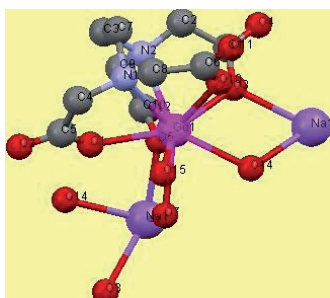
MS24.P85

Acta Cryst. (2011) **A67**, C390

Synthesis, characterization, structural analysis and biological activities of new transition metal complexes

Shahriar Ghammamy,^a Sadjjad Sedaghat,^b Seyed Abolfazl Seyed Sadjadi,^c ^a*Department of Chemistry, Faculty of Science, Imam Khomeini International University, Qazvin, (Iran).* ^b*Department of Chemistry, Faculty of Science, Islamic Azad University, Share Ghods Branch, Share Ghods, (Iran).* ^c*Faculty of Chemistry, Iran University of Science and Technology, Tehran, (Iran).*

In this research, some of the new inorganic complexes of transition metals were synthesized. Complexes were characterized by FT-IR and UV spectra, X-ray diffraction, ¹HNMR, ¹³CNMR, techniques and some physical properties. Different properties of these new compounds such as biological properties including antitumor and antibacterial activities were studied. The antitumor activity of some complexes against a panel of human tumor cell lines were determined by MTT(3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl-tetrazolium bromide) assay. These data suggest that some of these compounds pro-



vide good models for the further design of potent antitumor compounds [1], [2].

[1]. F. Shabani, S. Ghammamy, A. Jahazi, F. Siavoshifar, *Journal of Young Pharmacists*, **2010**, *2*, 399-402. [2]. H. Tavakol, S. Hatami, S. Ghammamy, G.R. Rezaeibehani, F. Shabani, *Heteroatom Chemistry* **2009**, *20*, 398-404.

Keywords: inorganic, complexes, crystals.

MS24.P86

Acta Cryst. (2011) **A67**, C390-C391

Two New Hydroxybenzophenone Complexes of Copper (II)

Iara M. L. Rosa, Antonio C. Doriguetto, *Instituto de Ciências Exatas, Universidade Federal de Alfenas - Unifal-MG, Alfenas-MG, (Brazil).* E-mail: iara_landre@yahoo.com.br

Copper (II) complexes with non-steroidal anti-inflammatory drugs (NSAIDs) shows enhanced anti-inflammatory activity and reduced gastrointestinal toxicity compared with their uncomplexed parent drug [1]. Is known that some hydroxybenzophenones acts as NSAIDs and have antimicrobial activity [2], so is necessary to study the coordination of copper (II) to these molecules and the molecular and supramolecular structure of these complexes since the structure affects directly in these biological activities.

Complexes of bis-2-benzophenonate copper (II) – (B2BC) – and bis-2,2'-hydroxybenzophenonate copper (II) – (B22HBC) – were synthesized from $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$, 2-hydroxybenzophenone and 2,2'-dihydroxybenzophenone reaction with a 2:1 stoichiometry (ligand: metal) and their crystal were obtained from solvent slow evaporation, ethyl acetate/chloroform for B2BC and methanol for B22HBC. These complexes were characterized by single crystal XRD (Gemini, MoK α , 100K, Direct Method and Least square of full matrix) and their molecular structures were analyzed using MOGUL.[3] The main crystallographic parameters of B2BC are C2/c space group, $a = 18,695(1) \text{ \AA}$, $b = 5,7548(3) \text{ \AA}$, $c = 19,920(1) \text{ \AA}$, $\beta = 114,209(7)^\circ$, $R1 = 0,0797$ and $wR2 = 0,2517$, and of B22HBC are P21/n space group, $a = 7,077(5) \text{ \AA}$, $b = 11,037(5) \text{ \AA}$, $c = 13,138(5) \text{ \AA}$, $\beta = 100,643(5)^\circ$, $R1 = 0,0473$ and $wR2 = 0,1677$.

Both complexes have a square planar geometry with the copper atom in the plane of oxygen, since it is present in the structure's inversion center. This coordination is interesting to some biological activities. The presence of the second hydroxyl in ortho position affects the molecular geometry, especially the dihedral angle and the carbonyl bond length. These geometric features can affect the anti-inflammatory and antimicrobial activities, due to changing in the H• donation and, consequently, in the anti-oxidant properties. Many of biological functions have been attributed to free-radical-scavenging and anti-oxidation properties.[4] No intramolecular hydrogen bonding for both complexes.

In terms of supramolecular structure, the crystal packing of B2BC does not show intermolecular hydrogen bond, being stabilized only by weak VDW interactions, while B22HBC is stabilized by one classical intermolecular hydrogen bonding, forming an infinite network along the [010] and [101] directions. $\pi \cdots \pi$ staking interactions help also to stabilize the B22HBC's packing. Structure-activity relationship (SAR) of B2BC and B22HBC is being carried out parallel to the biological activity studies.

Acknowledgements: FAPEMIG, CAPES, FINEP, CNPq, PIBIC-UNIFAL.

[1] J.E. Weder, C.T. Dillon, T.W. Hambley, D.J. Kennedy, P.A. Lay, J.R. Biffin, H.L. Regtop, N.M. Davies, *Coordination Chemistry Reviews* **2002**, *232*, 95-126. [2] A.C. Doriguetto, F.T. Martins, J. Ellena, R. Salloum, M.H. dos Santos, M.E.