

MS31.P34*Acta Cryst.* (2011) **A67**, C437**Synthesis of ytterbium-doped yttrium aluminum garnet nano-powders by carbonate altogether precipitation methods**Zhang Xuejian Zou Guangtian,^a Li Chun Liu Jinghe^a *Jilin University*^b, *Changchun University of Science and Technology Changchun (China)*. E-mail: zxj_0620@163.com

Yb³⁺-co-doped YAG transparent ceramic nano-powders were prepared by carbonate altogether precipitation methods, and their structure, morphology and properties were also analyzed by X-ray diffraction, absorption and fluorescence spectra. The results show Yb³⁺:YAG nano-powders are obtained with higher sintering performance and purity, and the particle shapes are regular with average diameter in the range of 100 nm. The crystalline size grew with the increase of the heat treatment temperature. The size of powder calcined at 1100°C was about 70–150 nm, which is favorable for good sinterability of Yb³⁺:YAG ceramics.

Keywords: Yb:YAG laser materials, transparent ceramics, nano-powder

MS31.P35*Acta Cryst.* (2011) **A67**, C437**Synthesis of Yb:GGG laser ceramic nanopowder**Zhang Xuejian, Liu Jinghe, *Jilin Architectural and civil Engineering institute Changchun (China)*. E-mail: zxj_0620@163.com

The sol-gel combustion method was used to synthesize Yb:GGG laser ceramic nanopowder. The phase structure, thermal stability, particle size and morphology of Yb:GGG powder were studied by means of XRD, TG-DTA, IR and SEM methods. It was found that the as-synthesized powder belongs to GGG phase. The crystalline size grew with the increase of the heat treatment temperature. The size of powder calcined at 900°C was about 40–50 nm, which is favorable for good sinter ability of Yb:GGG ceramics.

Keywords: Yb:GGG, nanopowder, structure and morphology

MS31.P36*Acta Cryst.* (2011) **A67**, C437**Structure and properties of Mo(II) complexes with dinitrogen bidentate ligands**

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Reaction of $[M(\eta^3-C_3H_5)(CO)_2X(NCMe)_2]$ ($M = Mo, W$; $X =$ halide) complexes with bidentate nitrogen ligands leads to substitution of the two nitriles, and two different isomers may be formed. The two carbonyls and the centroid of the allyl group always adopt a facial arrangement in the pseudo octahedral environment around Mo(II), with the halide occupying a position trans (equatorial isomer) or cis (axial isomer) to the allyl. When $C_5H_4NCH=N(CH_2)_2CH_3$ (pyca) is used, the two main isomers have very close energies (DFT calculations) and they coexist in the crystal. With the other ligands, only one isomer is

observed in the solid, though often several are detected in solution, especially when ligands are small, owing to the fluxional behavior of the complexes in solution (NMR).

Some of the complexes display catalytic activity, both in homogeneous and heterogeneous conditions, in olefin oxidation in the presence of t-butylhydroperoxide.[1] and others can act as anti tumor agents.[2] The antitumor properties have been tested in vitro against human cancer cell lines such as cervical carcinoma (HeLa) and breast carcinoma (MCF-7), using the MTT metabolic activity test (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide). 1,10-phenanthroline (phen) seems to be the most effective ligand, with a IC_{50} of 23.7 μM (Mo, Br). The substitution of Br by triflate usually enhances the cytotoxic activity. In $[M(\eta^3-C_3H_5)(CO)_2(CF_3SO_3)(phen)_2]$, for instance, it drops to 2.9 μM . The binding constant of this complex with ct DNA, determined by absorption titration, is $2.08 (\pm 0.98) \times 10^5 M^{-1}$, a value comparable to the one determined for ethidium bromide. This result suggests that the complexes may interact with DNA changing its conformation. The molecular structures may give information about the possibility of complex intercalation in DNA. Crystal structures exhibit different features (inter and intra molecular hydrogen bond, π - π stacking) depending on the functional groups available.

[1] D. Bandarra, M. Lopes, T. Lopes, J. Almeida, M.S. Saraiva, M. Vasconcellos-Dias, C.D. Nunes, V. Félix, P. Brandão, M. Meireles, M.J. Calhorda, *J. Inorg. Biochem.* **2010**, *104*, 1171-1177. [2] J.C. Alonso, P. Neves, M.J. Pires da Silva, S. Quintal, P.D.Vaz, C. Silva, A.A.Valente, P.Ferreira, M.J. Calhorda, V.Félix, M.G.B. Drew *Organometallics* **2007**, *26*, 5548-5556.

Keywords: molybdenum, nitrogen ligand, antitumor

MS31.P37*Acta Cryst.* (2011) **A67**, C437**Crystal structure of bacterial citrate lyase**

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Citrate lyase activity exists in eukaryotes, bacteria, and archaea. This underscores its central importance in energy metabolism and biosynthesis. There are two types of citrate lyases, ATP-dependent and non ATP-dependent. The latter bacterial citrate lyase converts citrate to acetate and oxaloacetate by a two-step reaction for which a complex of α - β - γ -lyase is required. We present the crystal structure of the bacterial citrate lyase complex comprising six copies of α -, β -, and γ -lyase at 4 Å resolution. The structure reveals how the 18-subunit complex is assembled and provides insights into citrate catalysis.

Keywords: structure, citrate, lyase

MS32.P01*Acta Cryst.* (2011) **A67**, C437-C438**Microstructure of synthetic Mg-Co cordierite studied by X-ray diffraction methods**

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