MS39-P2 **Nanostructured metal-polymeric catalysts**
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Nanometer-sized particles of metals and their compounds being stabilized in organic, inorganic and hybrid matrice are widely used for creation of functional (magnetic, semiconductor and catalytic) materials. The dependence of properties of nanoparticles and derived materials on a number of parameters (form, size, chemical composition, crystal structure, surrounding media etc.) motivates the development of specific synthesis technologies providing outcome of nanoparticles of the required composition and size and thus of operational characteristics. A complex of modern structural techniques has to be used for permanent control. Samples of Ru/super cross-linked polystyrene granules containing 5% Ru have been synthesized in this study. The samples were prepared by wetting granules with a salt solution $Ru(OH)CI_3$. After wetting and preliminary drying, granules were treated in NaOH and H_2O_2 solutions followed by the secondary drying. Samples were reduced in hydrogen flow at 300°C, then they were cooled to room temperature in nitrogen atmosphere. Scanning electron microscopy was used for observation of the form and size of polystyrene granules, which was determined as 350-550 μ. A 2 μ surface layer of one of the granules was sputtered by a focused ion beam directly in the scanning microscope that made it possible to observe the internal porous structure of the granules. Energy dispersive X-ray spectra showed the presence of Ru nanoparticles in the samples. Transmission electron microscopy studies showed that Ru nanoparticles on granules surface are 1.5-4 nm in size. They assemble into agglomerates of the chain form with length of 60-80 nm. Phase composition of the samples was investigated by electron diffraction technique. The samples were found to be single phase with a cubic face centered lattice (ICSD Ru ą 41515, space group Fm-3m, a=3.83 Å). This study was performed on equipment of the multiple-access center at the Institute of Crystallography and supported by the Presidential grant MK_3695.2011.3.

Keywords: nanoparticles; metal-polymeric catalysts; structure

MS41-P1 **Symmetry analysis of IR, Raman and high-order Raman scattering phenomena on the Bilbao Crystallographic Server.**
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The *Bilbao Crystallographic Server* (http://www.cryst.ehu.es) [1] is a web site offering online crystallographic tools and databases. The programs and databases do not need a local installation; an internet connection and a web browser are sufficient. The server is freely available on the web since 1997 and since then, it is being further developed and improved. The purpose of the present contribution is to report on a new shell of the *Bilbao Crystallographic Server* with computer tools for the symmetry analysis of infrared (IR), Raman and high-order Raman scattering phenomena (second-order Raman and hyper-Raman scattering). The program SAM, which was already available for the analysis of IR and Raman activity of symmetry adapted modes at the Brillouin-zone centre [2], has been extended to include the calculation of selection rules for hyper-Raman and second-order IR and Raman processes. The database with polarizability Raman tensors has been updated and expanded to include the data of the hyper-Raman tensors. Switching between different orientations of Raman and hyper-Raman tensors can be achieved by the program TENSOR TRANSFORM. The orientation domains (twins) occurring during a phase transition and the corresponding Raman and hyper-Raman tensors are calculated by the program TWINS TENSORS. The program POLARIZATION SELECTION RULES is designed to help in the choice of the best geometrical configuration for scattering experiment; the program calculates polarization selection rules in different orientations and indicates the active modes allowed to be observed on different configurations. The available data on group-subgroup relations between point groups and the corresponding correlations between their irreducible representations permit the analysis of the behaviour of the phonon modes during a symmetry break (CORRELATIONS POINTS). The behaviour of the modes can also be studied when an external field is applied by the program MORPHIC EFFECTS. Similar studies for group-subgroup related space groups are carried out by the program RAMAN CORRELATIONS SPACE: given the high- and low-symmetry structures, the program determines the set of active modes in the low-symmetry phase and their correlations to the symmetry modes of the high-symmetry structure which in general, may include modes with wave vectors outside the Brillouin-zone centre. The utility of the developed tools will be demonstrated by the analysis of the vibrational spectra of several compounds.

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Keywords: Bilbao Crystallographic Server; Raman scattering; symmetry analysisdelaflor