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ROTOR-STATOR COCRYSTALS OF FULLERENES WITH CUBIC AND OCTAHEDRAL MOLECULES

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Fullerenes form cocrystals with a great variety of organic molecules. The majority of these materials belongs to various host-guest systems, depending on the shape and size of the counter molecules. Fullerene-cubane cocrystals represent a special family: none of the components form a host framework, they rather form separated sublattices[1]. The major stabilizing factor of such structures is the almost perfect mach of the molecular surfaces of convex fullerenes and concave cubanes. The expanded fullerene sublattice confines cubanes in static positions. On the other hand, the atomic arrangement of the fullerene surface is incommensurate with that of cubane, therefore, the rotation of fullerenes has no influence on the match. Thus, cubanes behave as a molecular bearing for the freely rotating fullerene, resulting in unusual dynamics. The alternating array of static and rotating components distincts this family of rotor-stator phases from both the orientationally ordered and plastic crystals. Rotor-stator properties slightly depend on the size and symmetry of the fullerenes and the substituents of cubane, but the major properties are characteristic of the whole family. We present here a new member of this family, the rotor-stator cocrystal of the endohedral $Sc_3N@C_{80}$ with cubane. In this material the rotor-stator properties of the molecules are extended to the rotation of the endohedral Sc_3N units. Besides the cubic shaped cubane, octahedral and other high-symmetry molecules may form similar cocrystals with fullerenes. In the absence of octahedral molecules of suitable size, we studied the fullerene cocrystals with the distorted octahedral pairs of mesitylene. We compare the influences of the cubic and octahedral shapes on the structures and properties.

References:

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INVESTIGATION OF THE SOL-GEL CHEMISTRY FOR THE PREPARATION OF TIO_2-ZRO_2 AND PURE TIO_2 NANOSTRUCTURED POWDERS

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Nanostructured titania materials can be used in a wide field of applications. The most popular application is maybe the use of TiO_2 nanoparticles as photocatalyst. For this application, it is important to have a look on the materials characteristics, which were found to influence the catalytic activity in a sensitive way. Desired characteristics for good catalysts are a small particle size and a large specific surface area, a high crystallinity and the anatase TiO_2 polymorph. To prepare nanostructured materials with tailored characteristics, the sol-gel process is very popular. It has been found by different research groups that the preparation of TiO_2-ZrO_2 composite nanopowders is very interesting due to the stabilization of the crystallite size and phase and an enhanced photocatalytic activity.

Different possibilities are known to influence the sol-gel chemistry and by doing so the structure of the reaction products. Nevertheless, there are to our best knowledge no systematical investigations of the influence of sol-gel chemistry on the reaction products of TiO_2-ZrO_2 composite samples, in contrast to the case of pure TiO_2 samples.

We studied the influence of the zirconia concentration on the composite powder structure and conducted further experiments concerning the influence of the chemical reaction path. The powders were prepared from titanium isopropoxide and zirconium n-propoxide precursors. Powder characterization was made with x-ray diffraction to determine the crystallite structure and size and x-ray absorption spectroscopy, which provides information about the crystallinity and the atomic environment of the absorbing species.

We found that the possibility of crystallization of the titania to anatase particles is only given for small zirconia concentrations. The crystallite size stayed nearly constant in the composite samples with increasing annealing temperature and phase transformations can substantially/successfully be suppressed, which could be derived from comparison with pure titania powders.

Keywords: *Sol-gel processes; Nanoparticles; X-ray absorption spectroscopy; X-ray diffraction;*