structures of square-planar transition-metal complexes. The data in the crystal structures from CSD show mutual slipped-parallel (*offset face-to-face*) orientation between chelate and C_6-aryl rings similar to the slipped-parallel orientation of two benzene rings.

Based on the fact that chelate rings with delocalized π-bonds can form stacking with C_6-aryl rings, one can anticipate that two chelate rings could form mutual stacking interaction. The evidence of chelate-chelate stacking interactions was obtained by analyzing crystal structures of square-planar transition-metal complexes from CSD [3]. The analysis showed that chelate-chelate stacking interactions occur in a large number of the crystal structures of neutral square-planar complexes.

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Keywords: intermolecular interactions, crystal structures, aromatic

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Formation and structure of fullerene and cubane based cocrystals

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Fullerenes form a large variety of high symmetry molecular crystals with cubane molecules [1]. The basic material, $C_{60}C_8H_8$ has a face centered cubic crystal structure at ambient condition, with significantly expanded lattice, related to the parent fullerene structure. This cocrystal consists of separated sublattices of rotating and static components. The stabilizing factor is the strong fullerene-cubane attraction, which we explain as a molecular recognition between the convex C_{60} and concave cubane surfaces. Although this strong shape and size recognition of the constituents allows the rotation of fullerenes, it keeps cubane in the equilibrium position and orientation. This unusual structure gives rise to a complex dynamics, called rotor-stator feature, that is different from both the orientationally ordered and the plastic crystals. As a result of this effect, the orientational ordering phase transition of fullerene-cubane takes place at the lowest temperature in all fullerene-based materials [2].

We prepared several member of this new family of heteromolecular crystals: C_{70}, C_{76}, C_{78}, C_{84} [3] and some endohedral fullerenes also form rotor-stator phases with cubane. C_{60} also forms cocrystals with 1,4-disubstituted cubanes. The ball-shaped fullerenes has an fcc structure with cubane, the elongated molecules compose less symmetrical structures. The different size and symmetry of the components slightly modified the rotor-stator properties. The lattice parameter depends on the sizes of fullerenes and cubane and can be predicted accurately.

The materials have rich phase diagrams and unconventional topochemistry. At elevated temperature the unimolecular isomerization of cubane results in a single phase topochemical reaction with the surrounding fullerenes. The product is a random copolymer that is stable up to high temperature.

Here we present the formation and crystal structure of the recently synthethized members of the fullerene-cubane cocrystals and discuss the effect of the molecular geometry on the crystal structure and the rotor-stator dynamics.

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Automating mail-in data collection at 11-BM at the APS

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The 11-BM powder diffractometer [1] at the Argonne Advanced Photon Source is a high-resolution instrument ($\Delta Q/Q \approx 2\times10^{-4}$) with 12 independent analyzers [2] where a typical dataset is collected in an hour. The beamline is equipped with a robot and cryostream device, allowing completely automated data collection with temperatures of ±200C. The highest priority for the instrument deployment was to offer user access where samples are mailed to the beamline. This was selected, as this service was not widely available and offered the greatest availability to the potential user community.

To allow the high-throughput of the instrument to be accessed by a large number of users with mail-in access, it was necessary to automate not only the operation of the instrument, but all other aspects of the workflow, including: requests for sample mounting kits; filing of safety review forms; programming of the data collection parameters; acknowledging sample receipt; post-collection data reduction; sample storage; dissemination of data to users; sample disposal/return; and query of users for publication information [3]. This is accomplished primarily via web interfaces that offer users additional features, such as tables summarizing samples and datasets. Care is taken to provide privacy for experimental information without demanding user login with password protection. A crucial component of mail-in operation has been adoption of sample bases that regularize sample mounting and where each base has a unique barcode that can be read by the robot.

The sample management system has been sufficiently popular that when on-site data collection software was later deployed, it was requested that on-site users have the option to include their work in this database.

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Automation and efficiency in the powder structure solution by EXPO package

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