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Effects of Rotational Symmetry on the Dynamics of Crystalline Molecular Rotators. Miguel A. Garcia-Garibay, Steven D. Karlen, Dept. of Chemistry and Biochemistry, Univ. of California, Los Angeles, CA 90095.

The potential of controlling rotary dynamics at the molecular level by proper molecular and crystal engineering has been recognized recently. In that context, we have been interested in structures that possess rotating groups held together by a rigid frame that acts as a stator. In this paper, we will describe the solid state rotational dynamics of the phenylene and diamantane rotators of 1,9-Bis(4-[3,3,3-triphenylpropynyl]-phenyl)-diamantane (1). Very thin crystals of 1 with a strong tendency for twinning were obtained from $C_2H_4Cl_2$ -MeCN and the structure was solved in the space group P_{bcn} with half a molecule per asymmetric unit due to coincident molecular and crystallographic inversion centers. The dynamics of phenylene rotation were established by dynamic line shape analysis using ^{13}C CPMAS NMR with the phenylene signals selectively highlighted by deuteration of the aromatic trityls and the use of short contact times for cross polarization. The dynamics of the the diamantane group were established by 1H spin-lattice relaxation under conditions where dipolar relaxation was shown to be the dominant mechanism between 250 and 425 K. A factor of 20,000 between the rates of rotation of the faster diamantane and the slower phenylene at 300 K supports expectations that higher symmetry rotors should have significantly faster dynamics in the solid state.