

Abstract Submitted
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Methyl-Group Rotational Tunneling Perturbations in Zeolitic Imidazolate Framework-8 TERRENCE UDOVIC, NIST Center for Neutron Research, JOHN RUSH, University of Maryland, JASON SIMMONS, TANER YILDIRIM, NIST Center for Neutron Research, WEI ZHOU, HUI WU, University of Maryland, JUSCELINO LEAO, NIST Center for Neutron Research — Using neutron inelastic scattering and diffraction techniques, we have extended our studies of the quantum methyl-group rotations in the metal organic framework: zeolitic imidazolate framework-8 (ZIF-8: $\text{Zn}(\text{MeIM})_2$, MeIM=2-methylimidazolate). The framework-bonded methyl groups are oriented toward the large cavities of the nanoporous ZIF-8 structure and thus exhibit very rapid one-dimensional rotations. Indeed, the rotational potential was previously shown[1] to be primarily 3-fold in character with a very low rotational barrier of ≈ 7 meV and a ground-state tunneling energy of $334 \mu\text{eV}$ at 1.4 K. In this talk, we discuss the observed changes to this potential upon various perturbations to the ZIF-8 system, including Co substitution for Zn; site-specific adsorption of H_2 , D_2 , and CD_4 ; and high-pressure (≤ 10 kbar) He infiltration. Depending on the perturbation, the tunneling energy was found to vary by more than an order of magnitude, with values ranging from $408 \mu\text{eV}$ to $< 30 \mu\text{eV}$. [1] W. Zhou, H. Wu, T. J. Udovic, J. J. Rush, and T. Yildirim, *J. Phys. Chem. A* **112**, 12602 (2008).

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