Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Quantum methyl rotations in zeolitic imidazolate framework-8: Inelastic neutron scattering and first-principles calculations J. J. RUSH, NCNR, NIST and MSE Dept., U. Maryland, W. ZHOU, NCNR, NIST and MSE Dept., U. Penn., H. WU, NCNR, NIST and MSE Dept., U. Maryland, T. J. UDOVIC, NCNR, NIST, T. YILDIRIM, NCNR, NIST and MSE Dept., U. Penn. — Zeolitic imidazolate framework-8 (ZIF8), which consists of ZnN_4 clusters linked by 2-methylimidazole [$H_2C_3N_2$-(CH_3)], is a newly discovered framework compound with interesting hydrogen-adsorption properties. The presence of a single type of methyl group in its crystal structure renders ZIF8 an ideal system for studying quantum methyl rotations. Combining inelastic neutron scattering measurements and first-principles calculations, we studied the quantum rotational tunneling and phonons associated with the ZIF8 methyl groups. The rotational tunnel splitting is an extremely sensitive probe of the local potential. The measured tunnel splitting ($\sim$345 μeV at 1.4 K) indicated a nearly free quantum rotor (*i.e.*, a very low methyl rotational barrier), which is unusual for the solid state. With guest molecules adsorbed inside the framework, the rotational barrier was found to change significantly. Hydrogen adsorption decreased the barrier at low loading, yet increased it at higher loading. Methane adsorption nearly doubled the rotational barrier. These results provided clues for understanding the nature of the ZIF-guest molecule interactions.

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Date submitted: 20 Nov 2006 Electronic form version 1.4