



Microscale Diffusion in Mixed Linker Zeolitic Imidazolate Framework

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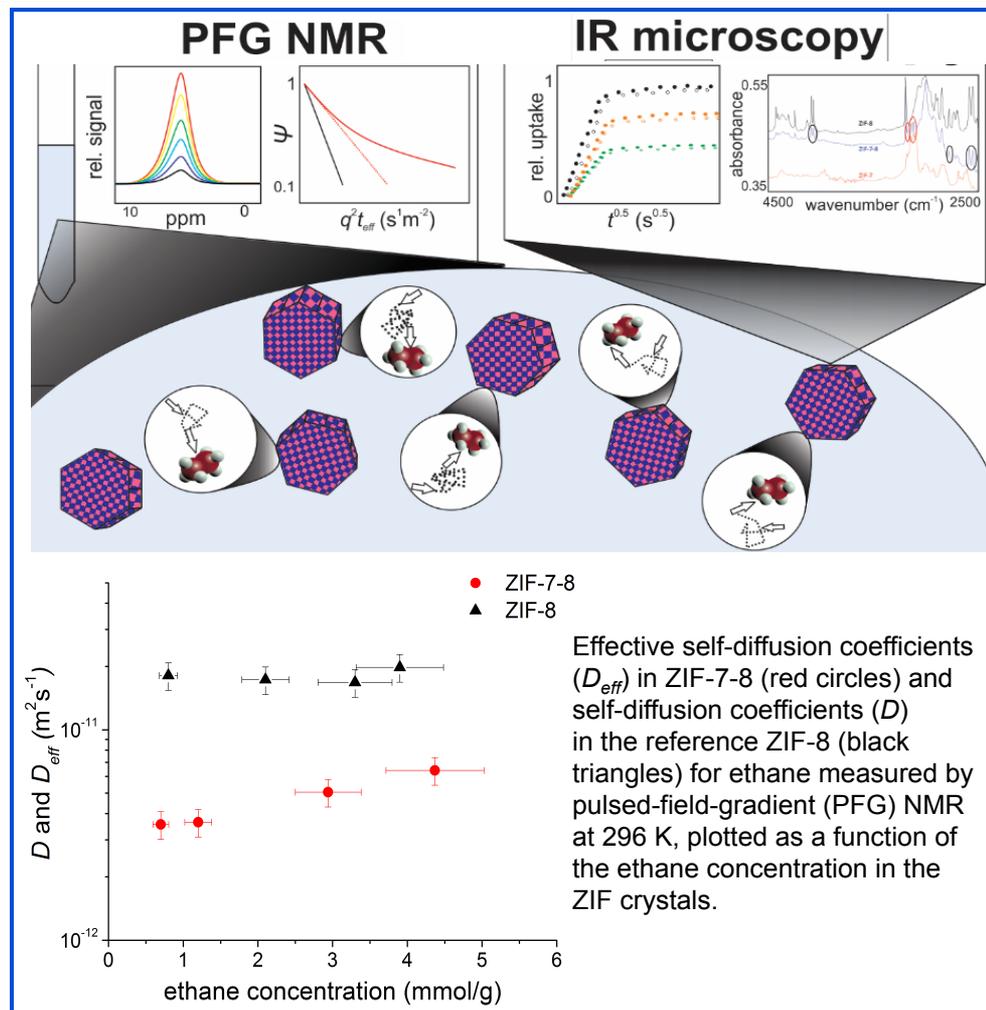


Funding Grants: G.S. Boebinger (NSF DMR-1157490, NSF DMR-1644779); H.-K. Jeong (NSF CMMI-1561897); S. Vasenkov (NSF CMMI-1561347)

Zeolitic imidazolate frameworks (ZIFs) are formed by organic linkers, which are bound to metal centers. ZIFs are porous materials that show promise for gas separation applications. Recently interest has been generated around mixed linker ZIFs owing to the potential of fine-tuning material properties by mixing different linkers in the same material.

Pulsed-field-gradient (PFG) NMR was used in combination with single crystal infrared microscopy (IRM) to study diffusion of ethane inside crystals of a mixed linker ZIF of the type ZIF-7-8. Multinuclear (¹³C and ¹H) PFG NMR diffusion studies of ethane reported here were performed at high magnetic fields (14T and 17.6T) and large magnetic field gradients up to 25 T/m.

PFG NMR in combination with IRM was successfully applied to quantify microscopic gas diffusion in a mixed linker ZIF for the first time. A distribution over ethane diffusivities in ZIF-7-8 was observed and attributed to a difference in the fraction of ZIF-8 and ZIF-7 linkers in different single crystals of ZIF-7-8. In agreement with the expectation of smaller aperture sizes in ZIF-7-8 than in a reference ZIF-8, the average ethane self-diffusivities in ZIF-7-8 were found to be significantly lower than those in ZIF-8. Fundamental understanding of transport properties of ZIFs will enable rational design of ZIF-based gas separations.



Facilities used: AMRIS (Avance III HD 750 MHz and Avance III 600 MHz)

Citation: S. Berens, C. Chmelik, F. Hillman, J. Karger, H.K. Jeong, S. Vasenkov,

Ethane diffusion in mixed linker zeolitic imidazolate framework-7-8 by pulsed field gradient NMR in combination with single crystal IR microscopy, Phys. Chem. Chem. Phys., **20** (37), 23967-23975 (2018), DOI: 10.1039/c8cp04889d