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Loading Dependent Diffusion Studies on Aromatic Hydrocarbons Adsorbed in MOF-5 via PFG NMR

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1. Introduction

This study focuses on one of the promising metal-organic frameworks, the MOF-5 (*also abbreviated:* IRMOF-1), which is builT of zinc oxide clusters as metal coordination centers and terephtalic acid as organic linkers [1]. For realization of the prospective applications, knowledge about mobility of aromatic hydrocarbons adsorbed in MOF-5 is necessary. For this reason the self-diffusion coefficients of aromatic hydrocarbons in MOF-5 are studied via pulseD field gradient (PFG) NMR and compared with molecular dynamic simulations.

2. Sample and Results

MOF-5 crystals were synthesized and loaded with benzene and toluene from Saeed Amirjalayer, under completely hermetically sealed conditions. We measured three different loadings (20%, 32% and 56% of the fully filled pore volume) for each guest molecule.

The self-diffusion of benzene adsorbed in MOF-5 were investigated using proton (^{1}H) pulsed field gradient (PFG) NMR [2]. The measurements carried out in a temperature range of 233 K to 328 K, yielded activation energies of self-diffusion of 11.2 kJ/mol. This result agrees very well with the simulated activation energy for a flexible framework of Amirjalayer et al., who found a value of 13.6 kJ/mol [3]. For a temperature of 273 K the experimentally determined self-diffusion coefficients are in the range of $2.6 \cdot 10^{-10}$ m^2/s (56% benzene) to $3.2 \cdot 10^{-10}$ m^2/s (20% benzene). This trend of slower diffusivity for higher loading is also shown by the simulations.

Measurements of toluene adsorbed in MOF-5 are currently under process.

3. Conclusion

This work shows the temperature and loading dependence of self-diffusion of aromatic hydrocarbons adsorbed in MOF-5. The good agreement of the experimental values for the activation energy of self-diffusion with the simulated values confirms the assumption of a flexible MOF-5 lattice.

References

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