# Ethane Diffusion in Mixed Linker Zeolitic Imidazolate Framework-7-8 by Pulsed Field Gradient NMR in Combination with Single Crystal IR Microscopy

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## Introduction

Zeolitic imidazolate frameworks (ZIFs) represent a type of metal organic framework (MOF) that are structurally and topologically similar to zeolites. ZIFs are formed by organic linkers, which are bound to metal centers. Recently, significant interest has been generated around mixed linker ZIFs and MOFs owing to the potential of fine-tuning material properties by mixing different linkers in the same material. An interesting example of a mixed linker ZIF is ZIF-7-8, which is composed of $Zn^{+2}$ ions tetrahedrally coordinated to 2-methylimidazolate (ZIF-8 linker) and benzimidazolate (ZIF-7 linker).

## Experimental

$^{13}C$ PFG NMR at 17.6 and 14 T was used to study self-diffusion of ethane in ZIF-7-8 and ZIF-8 reference at 296 K. Complementary diffusion studies by single crystal IR microscopy (IRM) were also performed under the same experimental conditions.

## Results and Discussion

Measured PFG NMR data provide evidence for a distribution over ethane self-diffusivities in the studied ZIF-7-8 sample, i.e. ethane self-diffusivities are different in different ZIF-7-8 crystals. These data were confirmed by IRM measurements of transport diffusivities of ethane in different crystals of ZIF-7-8. The average ethane self-diffusivities obtained by PFG NMR were found to be in a good agreement with the corresponding corrected diffusivities calculated based on the IRM data (Fig. 1) [1]. Furthermore, the estimates of the distribution width of the ethane diffusivities measured by PFG NMR and IRM yield data that are in a good agreement [1]. Average ethane self-diffusivities were found to be lower in ZIF-7-8 than in ZIF-8 (Fig. 2). This result is in agreement with the expectation that the average aperture size is lower in the former than in the latter ZIF.

## Conclusions

PFG NMR in combination with IRM was successfully applied to quantify microscopic gas diffusion in a mixed linker ZIF for the first time.

## Acknowledgements

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## References

[1] Berens, S., *et al.*, Physical Chemistry Chemical Physics, **20**, 23967-23975 (2018).

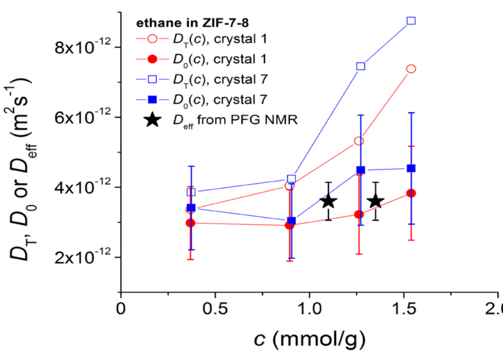


**Fig.1** Comparison of corrected diffusivities, $D_0$, from IRM with the effective self-diffusivities, $D_{eff}$, from PFG NMR of ethane in ZIF-7-8 at different ethane concentrations. $D_0$ was calculated from the transport diffusivities, $D_T$, which are also shown in the figure.

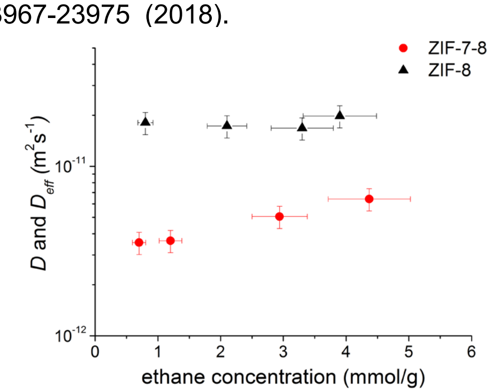


**Fig.2** Effective self-diffusion coefficients ($D_{eff}$) in ZIF-7-8 (red circles) and self-diffusion coefficients ($D$) in ZIF-8 (black triangles) for ethane measured by PFG NMR as a function of the ethane concentration in the ZIF crystals.