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ABSTRACT

Polymers of intrinsic microporosity (PIMs) are among the most promising candidates for the development of novel polymeric gas separation membranes for processes such as carbon capture and storage, natural gas treatment and biogas upgrading. As one of the approaches to optimize their performance, PIMs are functionalized by CO_2-philic groups to improve the CO_2 separation by the enhancement of specific noncovalent interactions. In this work, we show the preparation of amine-PIM from the archetypal PIM-1, using borane dimethyl sulphide complexes in order to control the degree of conversion. The PIM-1 to amine-PIM-1 conversion was characterized by ATR-IR and NMR analysis. The influence of the amine moiety on the gas transport behaviour was investigated by two complementary techniques: gas permeation measurements by the time lag method and analysis of the sorption kinetics and the equilibrium sorption isotherms by the gravimetric method. Both techniques show that permeability decreases with increasing degree of conversion. The trends in the indirectly calculated solubility confirm those of direct analysis, although quantitative comparison of the two shows fundamental differences. A pressure and temperature study on a fully converted sample indicates that the solution-diffusion model should be expressed in concentration dependent transport parameters to be correct. The experimental work was supported by quantum mechanics studies and by molecular dynamics simulations to confirm the selective non-covalent interaction of CO_2 with the amino groups.