Supplementary Material (ESI) for Chemical Communications

Methane and Carbon Dioxide Storage in Nanoporous Dipeptide-based Materials

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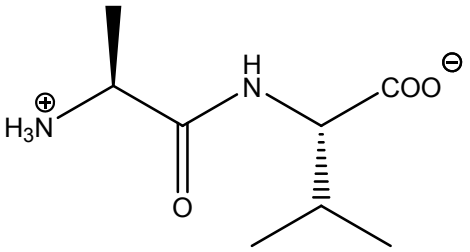
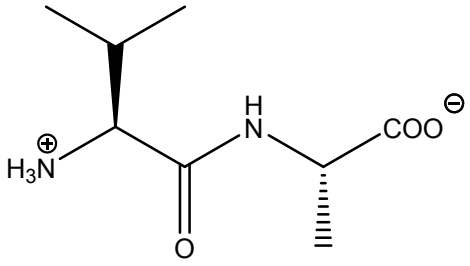
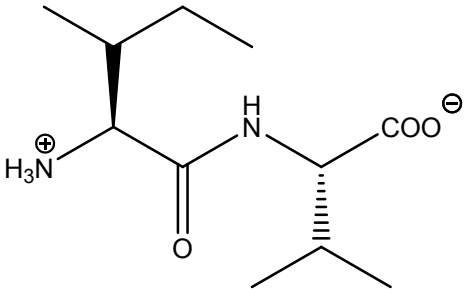


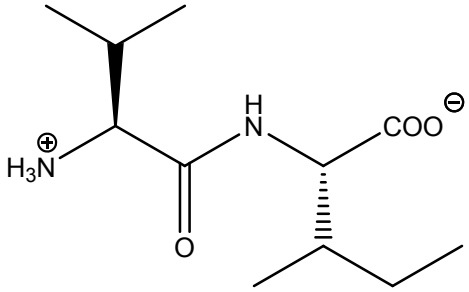
AV



VA



IV



VI

Experimental

Sample Preparation. L-alanyl-L-valine AV, L-valyl-L-alanine VA, L-isoleucyl-L-valine IV and L-valyl-L-isoleucine VI samples were purchased from Bachem company. They were evacuated at 10^{-3} torr and 60°C for several hours. Their purity and the absence of the solvent was checked by ^{1}H MAS NMR (300 MHz and spinning speed of 15 kHz) and ^{13}C CP MAS NMR (75 MHz).

Powder X-ray diffraction analyses. Powder X-ray diffraction experiments were performed using a Bruker D8 diffractromer in the Bragg-Brentano geometry. The radiation wavelength λ of the incident X-rays was 1.54 Å and a 2θ range from 5° to 60° was investigated.

Volumetric Adsorption measurements. Carbon dioxide and methane absorption isotherms were determined by volumetric measurements equipped with precision manometers (±0.5 torr). The measurements were carried out at 298 K and 195 K and in a pressure range up to 1 atm. The adsorption kinetics were followed for each point and the equilibrium value was reported in the isotherms. The isosteric energies were calculated using Clausius-Clapeyron equation. Hydrogen adsorption-desorption isotherms were measured at liquid nitrogen temperature using a Micromeritics ASAP 2050 analyzer operating up to 10 atm. The samples were outgassed overnight at 70°C under vacuum (10^{-3} torr). No hysteresis was apparent throughout the entire pressure range.

Table S1. Room Temperature Crystal Structural data and unit cell parameters refined by non linear least squares analysis of the powder X-ray diffraction patterns.

Compound	**AV**	**VA**	**IV**	**VI**
Empirical formula	$C_8H_{16}N_2O_3$	$C_8H_{16}N_2O_3$	$C_{11}H_{22}N_2O_3$	$C_{11}H_{22}N_2O_3$
Molecular mass	188.2 g/mol^{-1}	188.2 g/mol^{-1}	230.3 g/mol^{-1}	230.3 g/mol^{-1}
Crystal system	Hexagonal	Hexagonal	Hexagonal	Hexagonal
space group	$P6_1$	$P6_1$	$P6_1$	$P6_1$
a, Å	14.478(3)	14.474(3)	14.901(3)	14.828(4)
c, Å	10.036(5)	10.090(5)	10.323(4)	10.323(7)
V, Å^3	1821.832	1830.623	1984.987	1965.599
Z	6	6	6	6

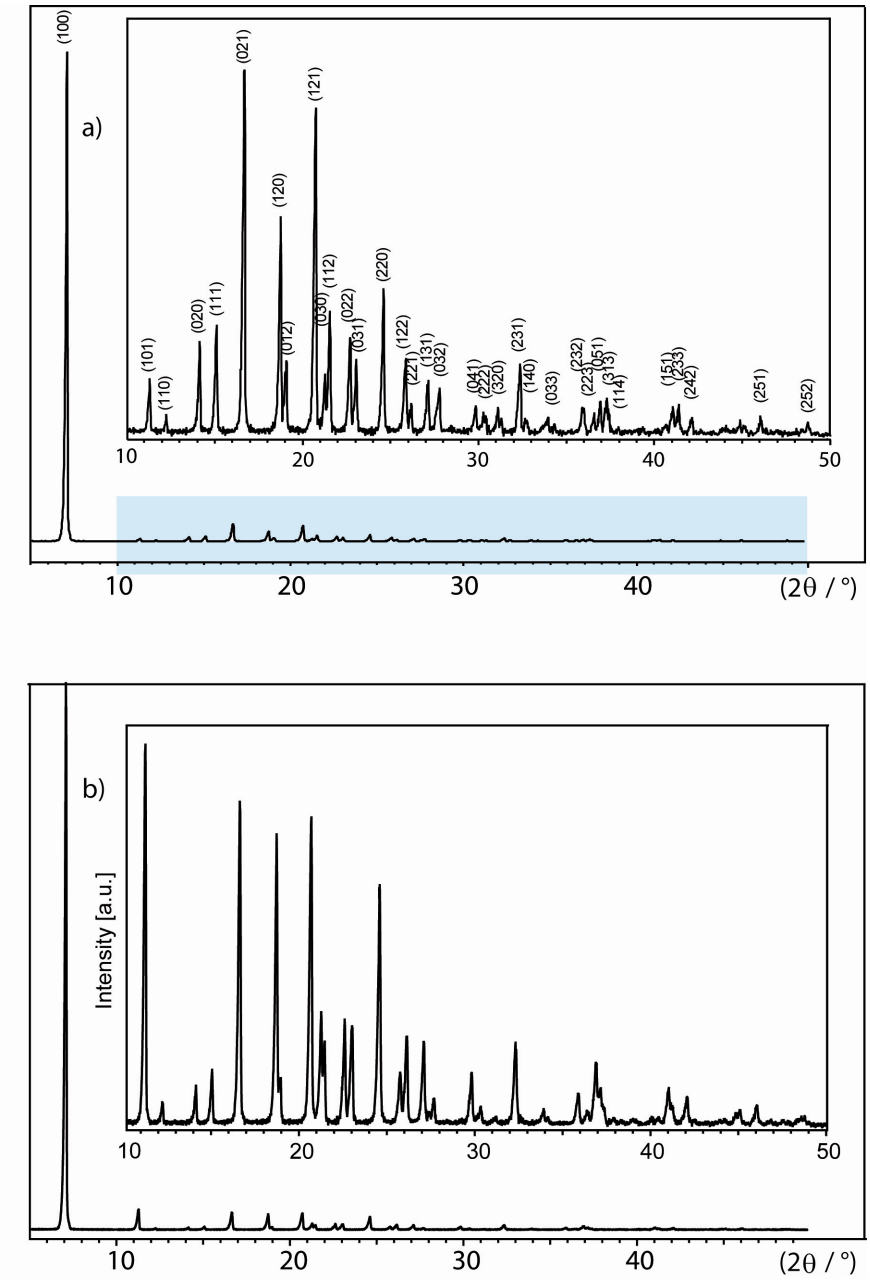


Figure S1. Powder X-ray diffraction patterns of a) AV and b) VA samples.

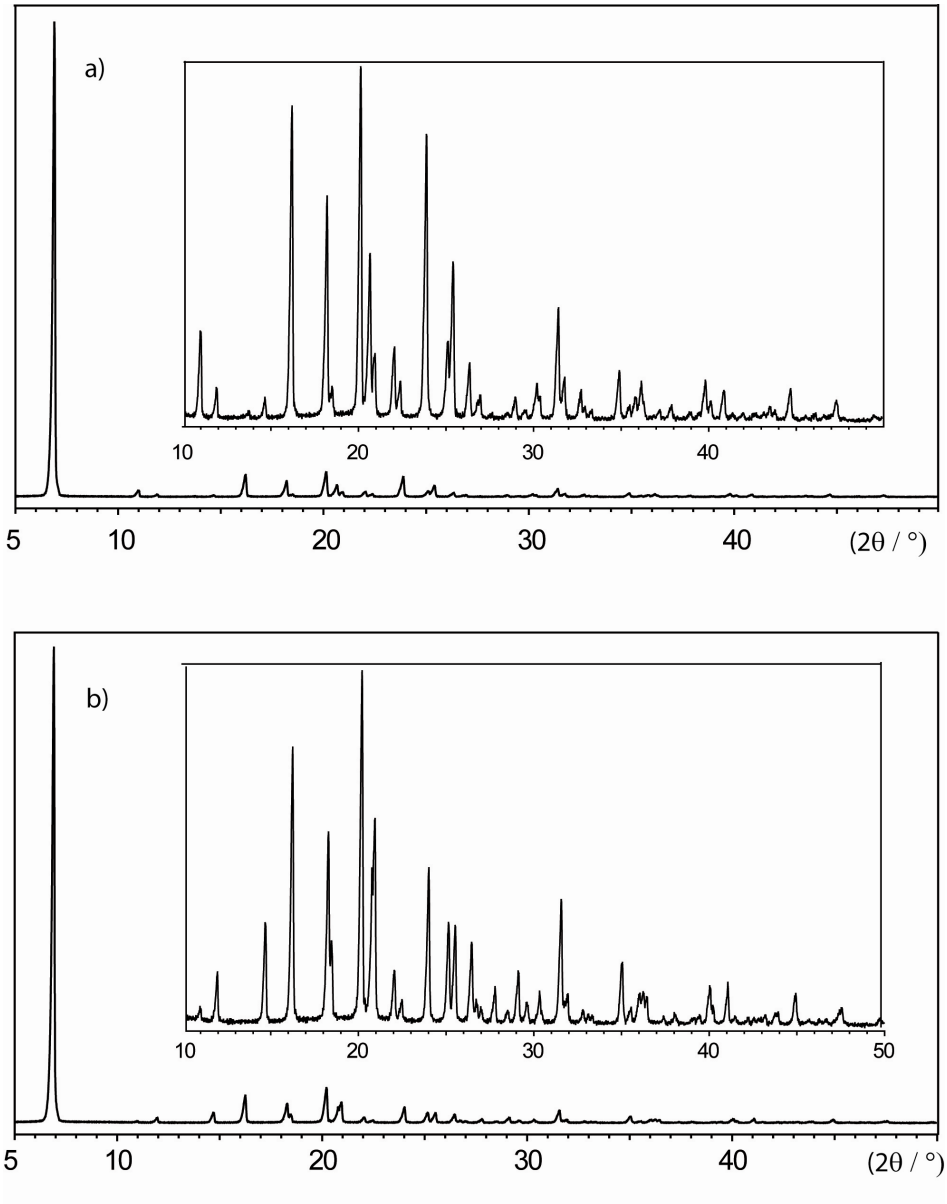


Figure S2. Powder X-ray diffraction patterns of a) IV and b) VI samples.

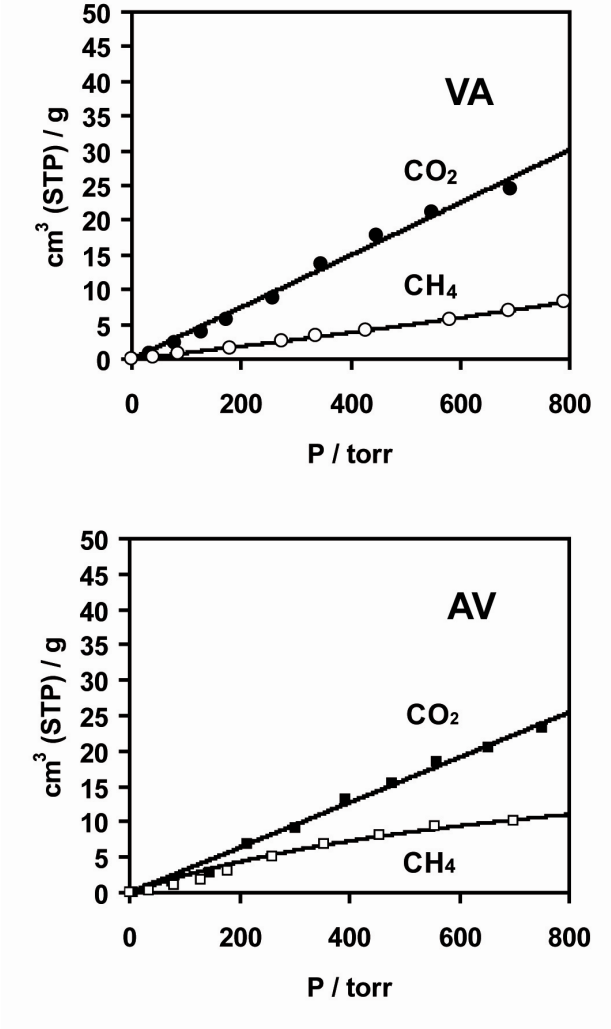


Figure S3. Adsorption isotherms of L-Alanyl-L-Valine (AV) and L-Valyl-L-Alanine (VA) of methane and carbon dioxide under standard conditions of room temperature and up to 1 bar.

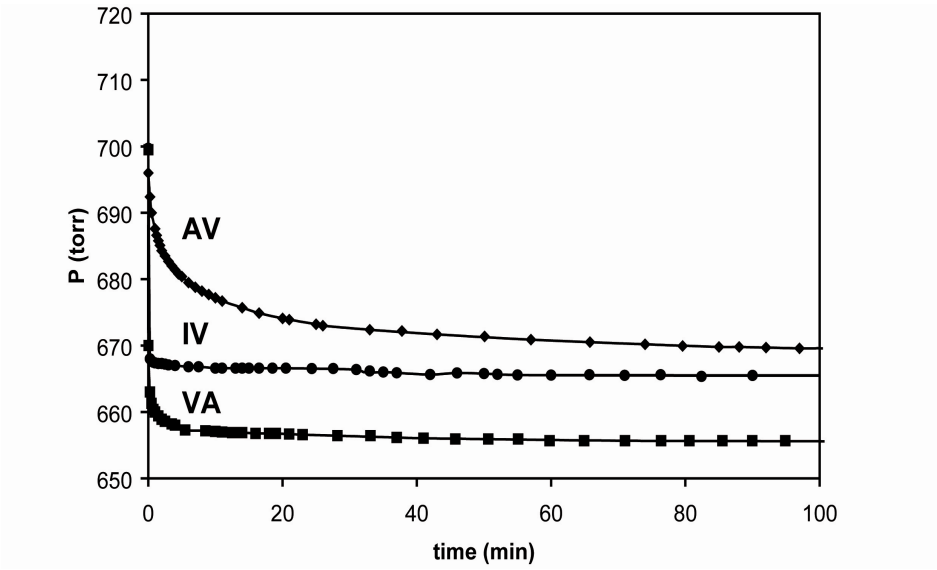


Figure S4. Adsorption kinetics of methane at room temperature for the porous AV, VA and IV samples.