


Adsorption equilibrium and kinetics of branched hexane isomers in pellets of BETA zeolite

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Author(s): [Barcia PS](#), [Silva JAC](#), [Rodrigues AE](#) Source: MICROPOROUS AND MESOPOROUS MATERIALS Volume: 79 Issue: 1-3 Pages: 145-163 Published: APR 1 2005 Times Cited: [22](#) References: [36](#)  [Citation](#) [Map](#) Abstract: Sorption equilibrium and kinetics of hexane isomers: n-hexane (nHEX), 3-methylpentane (3MP), 2,3-dimethylbutane (23DMB) and 2,2-dimethylbutane (22DMB) were studied in commercial pellets of zeolite BETA in the form HBEA with a SUM ratio of 150, between temperatures of 423 and 523 K and partial pressures up to 0.3 bar. Four different models were used to interpret the equilibrium data, named: Langmuir, multi-site Langmuir, dual-site Langmuir and Toth. The affinity to the adsorbent measured by the Henry's constants decreases with the degree of branching, with selectivities that can reach a value of 8.8 between nHEX and 22DMB. The heats of adsorption at zero coverage decrease with the degree of branching, being: 63.4 kJ/mol for nHEX, 59.7 kJ/mol for 3MP, 57.1 kJ/mol for 23DMB and 53.6 kJ/mol for 22DMB. However, the isosteric heat of sorption changes with coverage with a different behavior for the three isomers. Sorption kinetics studied by the Zero Length Chromatography (ZLC) technique allowed us to find the nature of controlling the diffusion mechanism (macropore or micropore); for nHEX and 3MP macropore diffusion is controlling with activation energies similar to the heats of sorption at zero coverage. For 23DMB and 22DMB, the controlling mechanism changes, being the system governed apparently by both macropore and micropore diffusion. Data from this work are also compared with those reported in literature for both zeolite BETA and silicalite. (c) 2004 Elsevier Inc. All rights reserved. Document Type: Article Language: English Author Keywords: zeolite BETA; hexane isomers; selectivities; adsorption equilibrium; ZLC KeyWords Plus: LENGTH COLUMN METHOD; N-ALKANES; MOLECULAR SIMULATIONS; HYDROCARBON MIXTURES; 5A ZEOLITE; SILICALITE; DIFFUSION; SEPARATION; MEMBRANES; PARAFFINS Reprint Address: Rodrigues, AE (reprint author), Univ Porto, Fac Engr, Dept Engr Quim, Lab Separat & React Engr, Rua Dr Roberto Frias S-N, P-4200465 Oporto, Portugal Addresses:
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2. Escola Super Tecnol & Gestao, Inst Politecn Braganca, BR-5301857 Braganca Paulista, SP Brazil E-mail Addresses: arodrig@fe.up.pt Publisher: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS Subject Category: Chemistry, Applied; Chemistry, Physical; Nanoscience & Nanotechnology; Materials Science, Multidisciplinary IDS Number: 912VM ISSN: 1387-1811