ONLINE ISSN : 1348-2246
PRINT ISSN : 0910-6340

Analytical Sciences
Vol. 26 (2010) , No. 4 p.411

[PDF (1025K)] [References]

Structural Analysis of High-Silica Ferrierite with Different Structure-Directing Agents by Solid-State NMR and *Ab Initio* Calculations

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(Received January 19, 2010)
(Accepted March 9, 2010)

The host-guest interaction in high-silica ferrierite (FER) with different structure-directing agents (SDA), pyridine and piperidine, was analyzed by solid-state ^{29}Si NMR relaxation experiments and molecular-orbital calculations. Qualitative and quantitative knowledge of the SDA structure obtained by these methods provides significant insight for understanding the functions in a template, and the stabilizing role of the SDA. Relaxation experiments show a larger magnetic dipolar interaction between the silicon and hydrogen atoms in piperidine as compared to that in pyridine, and the results correlate with the bonding property in terms of the distance between the zeolite framework and the SDA. The ^{1}H MAS NMR spectrum shows that the pyridine molecules mainly act as pore fillers in the pyridine-FER. In contrast, it was presumed that piperidine, adjacent to the aluminosilicate framework and framework defects, acted as a counter cation to balance the charge in the piperidine-FER. H^{+}-FER synthesized with piperidine shows a lower hydrothermal stability as compared to that synthesized with pyridine. The hydrothermal stability of H^{+}-FER is discussed by considering the contributions of framework defects and the different properties pertaining to the bonding between the zeolite framework and the SDA.

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