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四氢呋喃与全硅**FER**，**MTN**，**MOR**和**MFI**沸石骨架相互作用的计算机模拟

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摘要 结合分子动力学（MD）方法和能量最小化（EM）方法模拟了四氢呋喃（THF）分子作为模板剂与全硅FER，MTN，MOR和MFI沸石骨架的相互作用，判断其在这些沸石中的最佳结合位置。在FER沸石中，THF优先占扰[8~26~26~45~8]笼。在MIN沸石 中，只能分布在[5~(126~4)]笼中。在MOR沸石中，位于十二元环孔道内时与骨架作 用较强，而在MFI沸石中，处于十元环弯曲孔道中作用较强。相对而言，该分子与 FER，MTN相互作用较强，与MOR，MFI的相互作用较强。根据模拟结果，计算THF分 子中氢、氧原子与骨架氧原子的质心距离，研究了该分子与骨架空腔和孔道的匹配 情况，讨论了THF诱导这些沸石形成的模板作用。

关键词 模板剂 四氢呋喃 沸石 相互作用 硅 计算机模拟

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Simulation Studies on the Interaction of Tetrahydrofuran with the Framework of Siliceous FER, MTN, MOR and MFI Type Zeolite

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Abstract The interaction of tetrahydrofuran (THF), a template, with siliceous FER, MTN, MOR and MFI type zeolite has been studied by molecular simulation. Molecular dynamics (MD) together with energy minimization (EM) methods were employed. The preferred positions for THF molecules within these zeolites were investigated. THF molecules prefer [8~26~26~45~8] cage within FER zeolite and can only occupy the [5~(12)6~4] cage in MTN structure. The interaction of THF with MOR framework in 12 member ring (MR) channel is stronger than that in the side-pocket. The preferred binding site in MFI zeolite is in 10-MR zigzag channel. Relatively, the interaction of the molecules with FER or MTN framework is stronger than that with MOR or MFI framework. The distances between the atoms of THF molecule and oxygen atoms of the zeolite framework were calculated. Then the space fitting situation of THF molecule in the cavities or channels of these zeolites was investigated. The templating effect of THF for forming these zeolite structures was also discussed.

Key words TEMPLATE AGENT TETRAHYDROFURAN ZEOLITE INTERACTIONS SILICON COMPUTERIZED SIMULATION

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