
A First-Order Markov-Chain Model of Zeolite Crystallization¹

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Abstract: A method using a finite, first-order Markov chain is presented to estimate rate constants for zeolite formation from experimental nuclear magnetic resonance (NMR) data on the abundance of different silica oligomers. An experimental design is suggested by which this method can be implemented. The method uses weighted least squares to estimate transition probabilities from aggregate NMR data. Rate constants, equilibrium constants, and free energies of elementary zeolite-forming reactions can be estimated. Hypothetical zeolite-forming reactions can also be modeled. An example of modeling, using hypothetical data, shows how zeolite formation can result from reactions involving mainly silica cyclic tetramers.

Key Words: Crystallization • Markov-chain model • Rate constants • Silica oligomers • Zeolites

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