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A Stochastic Cellular Automata Model of Tautomer Equilibria

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Tautomer equilibria are complex and dynamic, making modeling them a challenge. Cellular automata models are uniquely suited to address this challenge, allowing the equilibria to arise naturally from simple rules. In this study, a stochastic, asynchronous cellular automata model was employed to simulate the tautomer equilibria of 9-anthrone and 9-anthrol in the presence of their common anion. The observed K_E of the 9-anthrone ⇌ 9-anthrol tautomerization along with the measured tautomer pK_a values were used to model the equilibria at pH values 4, 7, and 10. At pH values 4 and 7, the anthrone comprised >99% of the total species population, whereas at pH 10 the anthrone and the anion each represented just under half of the total population. The anthrol population was very small under all conditions.