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Study of *tert*-butyl bromide hydrolysis in the 1-propanol/water system using the fundamental thermodynamic equation of chemical reactivity

One of our ongoing research projects is the systematic analysis of solution-phase kinetic data using the fundamental thermodynamic equation of chemical reactivity. This expression contains intrinsic terms that relate the activation free energy to the solvent (state) variables. Each term correlates with a specific component of the activation process. These components include the formation of the transition-state structure, changes in the solvent-solute interactions within the solvation shell, and the bulk solvent electrostatic response. The solvent terms in the fundamental equation are appropriately suited for incorporating theoretical solvent models.

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As featured in:



See Floyd L. Wiseman and Dane W. Scott, *Phys. Chem. Chem. Phys.*, 2026, **28**, 5666.

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