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MD-generated molecular volumes and their mechanistic applications NOHAM WEINBERG, University of the Fraser Valley; Simon Fraser University — Experimentally, the effects of pressure on reaction rates are described by their pressure derivatives, known as volumes of activation. Transition state theory directly links activation volumes to partial molar volumes of reactant and transition states. Traditionally, the experimentally measured effects of pressure on reaction rates are expressed in terms of so-called volumes of activation, which represent the difference in volumes of transition states and reactants. Since the volumes of reactants are readily available experimentally, the volumes of activation provide a direct measure of the transition state volumes. In this context, a reliable technique is required for relating the volume of a microscopic system to its geometrical parameters. Until recently, such a technique did not exist. Over the past five years we developed a precise method based on molecular dynamics simulations and applied it to calculation of molecular volumes and volumes of activation. The results of calculations closely matched the experimental values. We are now extending and refining this method in its application to a wider range of reactions, including biochemical processes and processes at extreme pressures.

Noham Weinberg
University of the Fraser Valley; Simon Fraser University

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