The Reaction Force

Peter Politzer\textsuperscript{1,2}

\textsuperscript{1}Department of Chemistry, Cleveland State University, Cleveland, OH 44115, USA,  
\textsuperscript{2}Department of Chemistry, University of New Orleans, New Orleans, LA 70148 USA

The reaction force $F(R)$ is the negative gradient of the potential energy $V(R)$ of a chemical process along its intrinsic reaction coordinate \( R \). $F(R)$ normally has one or more maxima and/or minima which represent a natural division of the process into regions. Some of these are dominated by structural changes in the reacting system, while others feature electronic as well as structural factors.\textsuperscript{1} Since activation barriers include contributions from both types of regions, it is possible to determine whether the effects of catalysts, solvents, etc. are primarily structural or electronic.\textsuperscript{1,2} $F(R)$ defines a “transition-to-products” region, which is characterized by the reaction force constant [the second derivative of $V(R)$] being negative throughout its entirety, not just at the maximum of $V(R)$.\textsuperscript{3} This is consistent with the concept of a continuum of transient states that comes out of transition state spectroscopy.\textsuperscript{4}