

A Direct Dynamics Study of Protonated Alcohol Dehydration and the Diels-Alder Reaction

Marcus V. P. dos Santos, Erico S. Teixeira and Ricardo L. Longo*

Departamento de Química Fundamental, Universidade Federal de Pernambuco, 50740-540 Recife-PE, Brazil

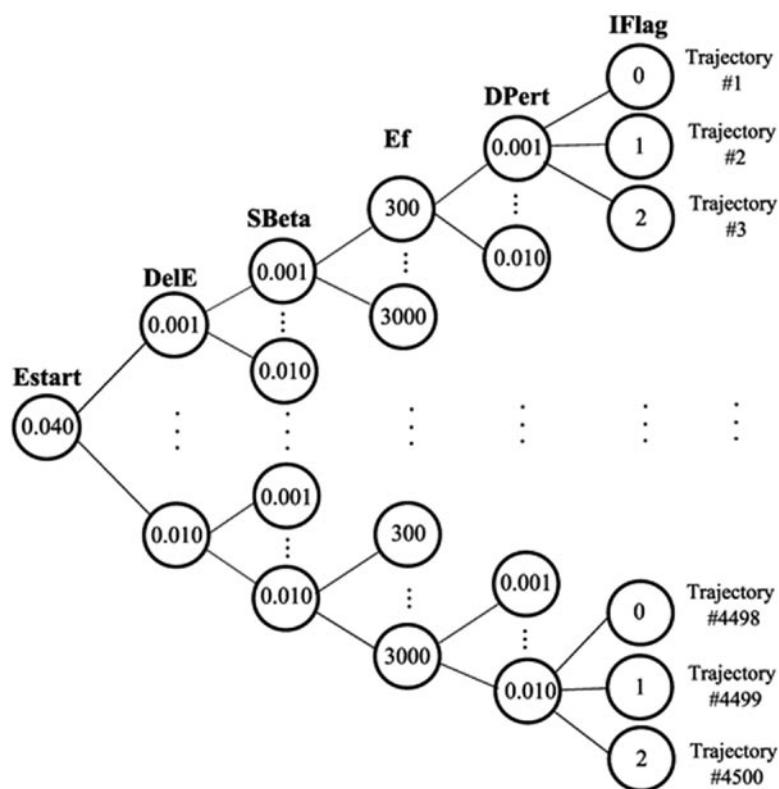


Figure S1. Flow-tree chart for generating the trajectories for the AS/F approach.

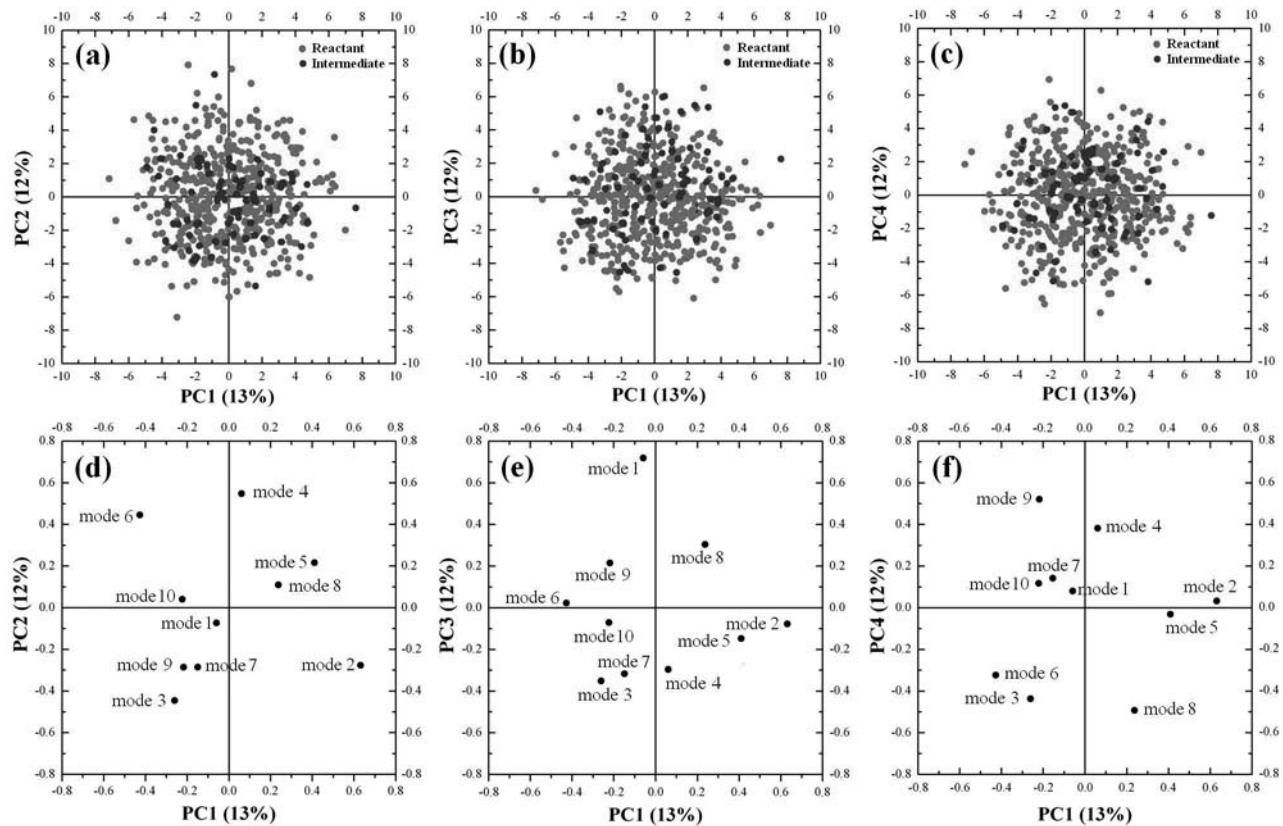


Figure S2. Principal component analysis of the reaction paths and vibrations modes for the dynamics of the protonated alcohol dehydration.