

Jonathan Prince
ICUR Abstract

The purpose of this study is to determine the relative accuracy and computational costs of activation energies derived from the Weizmann-1, Weizmann-2 and W2x methods. An investigation into the accuracy of activation energies derived from these methods is important since current literature focuses on dissociation energies with little work being done on activation energies or other thermochemical properties. If this project is successful, the work will help future theorists make an informed decision on choosing a Weizmann method for their study without having to run a series of expensive calculations, therefore saving the theorist hours of computational time.