

The relationships between activation energies and reaction energies

Lei Liu¹ and Yanhua Lei^{2,*}

¹School of Mathematics and Information Science, Xiangnan University, Chenzhou, Hunan Province, 423 000, People's Republic of China

²Hunan Provincial Key Laboratory of Xiangnan Rare-Precious Metals Compounds and Applications, School of Chemistry and Environmental Science, Xiangnan University, Chenzhou, Hunan Province, 423 000, People's Republic of China

The relationship between reaction energies and activation energies has been of interest for long in the field of chemistry. Two such relationships, Brønsted–Evans–Polanyi principle and Marcus equation, are well-known and widely used. Here we derived an extended Marcus equation with reaction distance. From this equation, the parabolic curve of activation energy–reaction energy can be both upward and downward. We also predict the existence of the reverse BEP relationship in which the activation energy decreases with the increase of reaction endothermicity in a certain range.