

Fig. 1. Reaction energy profile for a one-step chemical transformation.

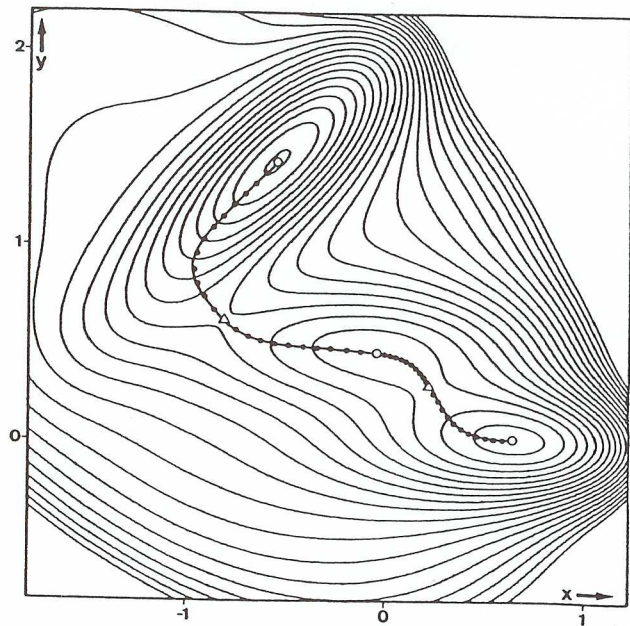


Fig. 15. Approximate minimum-energy reaction path for the two-parametric model potential by means of descending path points.