

**minimum-energy reaction path (MERP)**

Path orthogonal to the equipotential contours of a potential energy surface that connects the energy minima through a saddle point (transition state) from which it slopes downwards along the steepest descending lines in  $3N - 6$  configurational space ( $N$  is the number of nuclei in the reacting system).

Note: MERP calculation allows the investigation of detailed changes in molecular structure describing the transformation of reactants to products.

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