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Mathematical foundation of a global strategy for searching reaction paths. (English summary)

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For the determination paths and critical points on the potential energy hypersurface of chemical reactions, a rigorous mathematical background for the theory of a global searching procedure based on the catchment regions of the gradient field is given. The basic idea lies in the concept of the exponential of analytical vector fields. Having a curve c and a potential function f , a sufficient condition is that $\exp(t \operatorname{grad} f)c$ converges uniformly to the intrinsic reaction coordinate if $t \rightarrow \infty$. However, in concrete cases the conditions formulated are difficult to verify.

Reviewed by *V. I. Bykov*

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