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On the reaction path concept of Olender and Elber. (English summary)

J. Math. Chem. **28** (2000), *no. 1-3,* 241–246.

Summary: "The Olender-Elber (OE) reaction path concept [R. Olender and R. Elber, J. Mol. Struct.: THEOCHEM **398/399** (1997), 63–71] is shown to be unrelated in general to a true steepest descent path (SDP) in the mathematical sense, yet the solutions of such a variational problem may even replace the old reaction path (RP) concept if the RP passes through several critical points of the potential energy surface. We have found a chemically interesting and sufficient condition for the coincidence of OE's 'SDP' and the IRC of Fukui. The OE concept has been discussed here in a rather straightforward manner, giving it an exact mathematical description."