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Comment on the reply to the paper “On the Elber-Karplus reaction path-following method and related procedures”. (English)

J. Math. Chem. 29, No. 3, 169-175 (2001).

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<http://www.springerlink.com/openurl.asp?genre=journal&issn=0259-9791>

Summary: The flaws in the Reply [Chem. Phys. Lett. 311, 335 (1999)] to our paper [Chem. Phys. Lett. 311, 328 (1999)] have been pointed out. Elber and Karplus (EK) have not disproved our irrefutable global statement that the energy average cannot be minimized which rebuts the theoretical background of EK-type calculations. Another statement of ours has shown that even a curve for which the average energy is locally minimal for all directional perturbations in the sense of classical variational calculus cannot be identical with the reaction path (RP) defined as a steepest descent path (SDP). EK found an error in the early preprint of our theoretical paper [J. Math. Chem. 26, No. 1-3, 87-94 (1999; Zbl 1048.92503)] and because of this error they qualified our correct variational statement as false for all the SDPs consisting of a straight line each. Mixing global and variational arguments, EK refuted our criticism in a logically incorrect manner.

In this Comment we prove that both of our earlier statements invariably remain in force and the criticism included in those has been as well-established and solid as was before.

Classification :

***92E20** Chemical flows, reactions, etc.