An enhanced splined saddle method

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We present modifications for the method recently developed by Granot and Baer [J. Chem. Phys. 128, 184111 (2008)]. These modifications significantly enhance the efficiency and reliability of the method. In addition, we discuss some specific features of this method. These features provide important flexibilities which are crucial for a double-ended saddle point search method in order to be applicable to complex reaction mechanisms. Furthermore, it is discussed under what circumstances this methods might fail to find the transition state and remedies to avoid such situations are provided. We demonstrate the performance of the enhanced splined saddle method on several examples with increasing complexity, isomerization of ammonia, ethane and cyclopropane molecules, tautomerization of cytosine, the ring opening of cyclobutene, the Stone-Wales transformation of the C-60 fullerene, and finally rolling a small NaCl cube on NaCl(001) surface. All of these calculations are based on density functional theory. The efficiency of the method is remarkable in regard to the reduction of the total computational time.

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