Cheap HEAT protocol: CHEAT1

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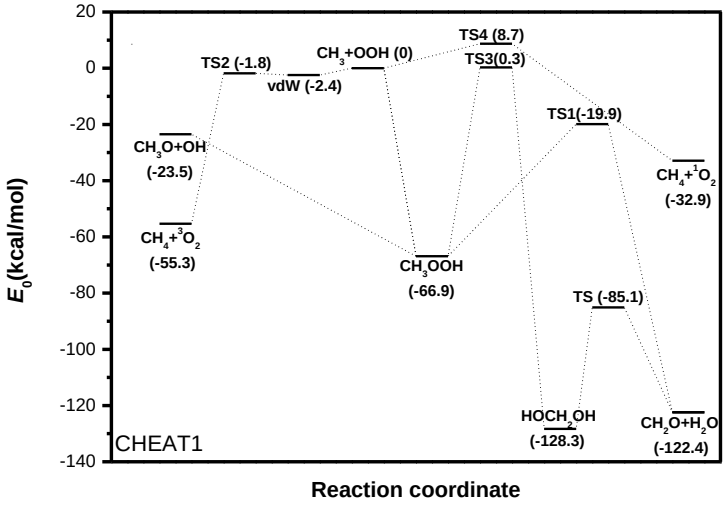
An effective simplification of the HEAT protocol [1], CHEAT1 is to provide accurate potential energy surface for relevant combustion or atmospheric reactions. The performance of CHEAT1 protocol is demonstrated to provide a comprehensive, robust and highly accurate single reference based description of the system. At high T_1 diagnostic values, multi-reference treatment for species in reaction system is often recommended. However, accurate single reference solution to the problem can also be applied involving higher excitation terms. In the case of the CH_3+HO_2 reaction system, the performance of the CHEAT1 is demonstrated within an absolute deviation (AD) from literature values of <0.6 kcal/mol. Such results infer the proposed method to be appropriate for accurate theoretical kinetic calculations. Furthermore, it has found that energetics of the system studied could not be reproduced accurately using any popular standard composite methods due to their inability to provide transition state structures (e.g. CBS-QB3, G3MP2B3, G4, W1U and W1BD) or the finding that the accuracy of the calculated activation energy was too small for CBS-4M and G2 (AD=29.0 and 10.0 kcal/mol, respectively).



[1] Tajti, A.; Szalay, P. G.; Császár, A. G.; Kállay, M.; Gauss, J.; Valeev, E. F.; Flowers, B. A.; Vazquez, J.; Stanton, J. F., *J. Chem. Phys.*, 121:11599-11613, 2004.