Implementation of an algorithm to locate reaction paths using the potential energy as reaction coordinate

Antoni Aguilar Mogas¹

Departament de Química-Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/Martí i Franquès 1, 08028 Barcelona, Spain

A new method to locate reaction paths of the IRC type (Intrinsic Reaction Coordinate) [1] is presented, based on the minimization of the Weierstrass error function associated to an arbitrary curve described on a potential energy surface of a molecular system. Starting from the stationary points character minimum of the potential energy surface corresponding to the geometries of reactants and products, the algorithm displaces the guess curve joining them by using an integration of the Runge-Kutta-Fehlberg type (RKF) [2] in the direction determined by the Weierstrass error function [3] until the guess curve coincides with the IRC. The algorithm uses as reaction coordinate the potential energy of the system [4], which allows to reparametrize the curve in every stage of the iterative process in such a way that the points that compose the curve are equally spaced in energy. The algorithm has been tested in several analytical surfaces and the reaction paths of some simple organic systems have been calculated, as it has been implemented in the GAMESS package.

Figure 1: Depiction of a potential energy surface, with two initial guess curves (with a non-zero value of their respective integrals of the Weierstrass error function), and their IRC converged curves (with zero value of the integral of the Weierstrass error function).

¹Email: toni.aguilar@ub.edu
References