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Phase Space and Dynamics in a Caldera-type Hamiltonian system

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We study the phase space transport in a caldera potential energy surface (PES) using techniques from nonlinear dynamics. This potential energy surface is encountered in many organic chemical reactions. The caldera PES is characterized by a flat region or shallow minimum at its center surrounded by potential walls and multiple symmetry-related index one saddle points that allow entrance and exit from this intermediate region. We have discovered four qualitatively distinct cases of the structure of the phase space. These cases are categorized according to the total energy and the stability of the periodic orbits associated with the family of the central minimum, the bifurcations of the same family, and the energetic accessibility of the index one saddles. We have found the mechanisms determined by the invariant manifold structure of the unstable periodic orbits govern the phase space transport and are responsible for the phenomenon of dynamical matching.

References

[1] M. Katsanikas and S. Wiggins "Phase space structure and transport in a caldera potential energy surface", International Journal of Bifurcation and Chaos 28 (13), 1830042 (2018).

[2] M. Katsanikas, V.J. García-Garrido and S. Wiggins, " The dynamical matching mechanism in phase space for caldera-type potential energy surfaces", Chemical Physics Letters 743, 137199 (2020).

[3] M. Katsanikas and S. Wiggins "The nature of reactive and non-reactive trajectories for a three dimensional Caldera potential energy surface " Physica D: Nonlinear Phenomena, 133293 (2022).