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Quasiclassical Trajectory Study of the Kinetics and Dynamics of the O(^{3}P) + HBr Reaction

Bruno E. S. de Freitas, Antonio G. S. de Oliveira Filho

Departamento de Química, Faculdade de Filosofia Ciências e Letras, Universidade de São Paulo, Ribeirão Preto, SP, Brasil

Abstract: Reactions between atoms and diatomic molecules can be investigated to high degrees of detail and precision using high-level ab initio potential energy surfaces (PES) and the quasiclassical trajectories (QCT) method. [1, 2] In this work, we use a PES constructed using internally contracted multireference configuration interaction with complete basis set extrapolation (icMRCI+Q/CBS) and the QCT method to calculate the rate constant and product energy distribution of the O(^{3}P) + HBr reaction. [2] The rate constants, in cm^3 $molecule^{-1}$ s^{-1} and at 298 K, for the O + HBr reaction is 2.31 x 10^{-14} for QCT.

Key-words: **Quasiclassical trajectory, rate constant, potential energy surfaces**
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References:

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