VMTS: A transition state search engine based on a vibronic model description of potential energy surface

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Transition states play a vital role in the theory of chemical reaction rates. They help in proposing a mechanism or verifying an experimentally proposed reaction mechanism, and in predicting the thermal or micro-canonical rates. The much celebrated Transition State Theory (TST) is a testament to this fact. The challenging task itself is to locate and characterize these transition structures. While there has been continued developments of theoretical methods to locate transition states, there is no one method that can be called a panacea of finding transition states. In this work, a method based on the vibronic model description of ground state potential energy surface (PES) has been developed. Vibronic model description of the PES, though approximate, provides gradient and Hessian at an extremely cheap cost. Fast availability of these quantities, in particular the Hessian, are crucial to an efficient search algorithm. The proposed methodology has been applied to a test set of Unimolecular reactions and comparisons have been made with the popular QST2/QST3 methodology of the Gaussian quantum chemistry program suite.