KiSThelP: un programme pour la prédiction de propriétés thermodynamiques et le calcul de constantes de vitesse à partir de résultats de chimie quantique

Sébastien Canneaux[1], Frédéric Bohr[2], and Eric Hénon*†[3]

[1]Laboratoire d'Ingénierie et Sciences des Matériaux (LISM) – Ministère de l'Enseignement Supérieur et de la Recherche Scientifique – Moulin de la Housse - Bat. 6 51687 Reims cedex 2, BP 39, France
[2]Laboratoire d'Ingénierie et Sciences des Matériaux (LISM) – Ministère de l'Enseignement Supérieur et de la Recherche Scientifique – Moulin de la Housse 51687 Reims cedex 2 , BP 39, France
[3]Institut de Chimie Moléculaire de Reims (ICMR) – CNRS : UMR7312, Ministère de l'Enseignement Supérieur et de la Recherche Scientifique – Moulin de la Housse - Bat. 18 51687 Reims Cedex 2 BP 39, France

Résumé

Kinetic and **S**tatistical **The**rmodynamica**l** **P**ackage (KiSThelP) is a cross-platform free open-source program developed to estimate molecular and reaction properties from electronic structure data. To date, three computational chemistry software formats are supported (Gaussian, GAMESS, and NWChem). KiSThelP is intended as a working tool both for the general public and also for more expert users. It provides graphical front-end capabilities designed to facilitate calculations and interpreting results.
Some key features are: gas-phase molecular thermodynamic properties (offering hindered rotor treatment), thermal equilibrium constants, TST rate coefficients (TST, VTST) including 1D tunnelling effects, RRKM rate constants, for elementary reactions with well-defined barriers.
These features make this program also well-suited to support and enhance students learning and can serve as a very attractive courseware, taking the teaching content directly from results in molecular and kinetic modelling.

Mots-Clés: quantum chemistry, statistical mechanics, thermochemistry, rate constant, transition state theory, RRKM

*Intervenant
†Auteur correspondant: eric.henon@univ-reims.fr