

===== README.TXT =====

ARTICLE INFORMATION

Journal: Physical Chemistry Chemical Physics

Author: Dario De Fazio

Title: The H + HeH+ --> He + H2+ reaction from the ultra-cold regime to the three-body breakup: exact quantum mechanical integral cross sections and rate constants.

DEPOSIT INFORMATION

Description: In the file KN.dat the second column lists rate constants in $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \times 10^{(-11)}$. The first column lists temperatures in K. In the file icsj0.dat the second column lists total integral cross sections in square Angstroms. The first column reports translational collision energies in meV. The third, fourth, fifth and sixth columns are product vibrational resolved integral cross section for $v' = 0, 1, 2$ and 3 respectively. The reactant's rotational state is $j = 0$. The potential energy surface employed is also supplied as a FORTRAN77 subroutine (file PES.f).

Total No. of Files: 4

File Names: README.TXT; KN.dat; icsj0.dat; PES.f;

File Types: txt; dat; FORTRAN77

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