

**Quantum chemical calculations for the dissociative recombination of HCN<sup>+</sup> and HNC<sup>+</sup>**  
**TALBI D, LE PADELLEC A, MITCHELL JBA**  
**JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS**  
**33 (18): 3631-3646 SEP 28 2000**

AMITAY Z Dissociative recombination of CH<sup>+</sup>: Cross section and final states PHYSICAL REVIEW A 54 : 4032 1996

ANICICH VG EVALUATED BIMOLECULAR ION-MOLECULE GAS-PHASE KINETICS OF POSITIVE-IONS FOR USE IN MODELING PLANETARY-ATMOSPHERES, COMETARY COMAE, AND INTERSTELLAR CLOUDS JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA 22 : 1469 1993

BACCHUSMONTABON.MC COMPUT PHYS COMMUN 163 : 30 1983

BECKE AD DENSITY-FUNCTIONAL THERMOCHEMISTRY .3. THE ROLE OF EXACT EXCHANGE JOURNAL OF CHEMICAL PHYSICS 98 : 5648 1993

BERKOWITZ J 3 METHODS TO MEASURE RH BOND-ENERGIES JOURNAL OF PHYSICAL CHEMISTRY 98 : 2744 1994

DEFREES DJ THE ROTATIONAL SPECTRA OF HCNH<sup>+</sup> AND COH<sup>+</sup> FROM QUANTUM-MECHANICAL CALCULATIONS ASTROPHYSICAL JOURNAL 257 : 376 1982

DUNNING TH MODERN THEORETICAL C 3 : 1 1977

FRISCH MJ GAUSSIAN 92 REVISION : 1994

HANSEL A Energy dependence of the isomerization of HCN<sup>+</sup> to HNC<sup>+</sup> via ion molecule reactions JOURNAL OF CHEMICAL PHYSICS 109 : 1743 1998

HANSEL A J CHEM PHYS 109 : 1749 1998

HERZBERG G ELECT SPECTRA ELECT : 1966

LAUBE S New FALP-MS measurements of H-3(+), D-3(+) and HCO<sup>+</sup> dissociative recombination JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 31 : 2111 1998

MACLEAN AD ALCHEMY 2 MOTEC 90 : 1990

PETERSON KA CONFIGURATION-INTERACTION SPECTROSCOPIC PROPERTIES OF X-2-SIGMA<sup>+</sup> HNC<sup>+</sup> AND X-2-PI HCN<sup>+</sup> JOURNAL OF CHEMICAL PHYSICS 93 : 4946 1990

PETRIE S THE ION CHEMISTRY OF HNC<sup>+</sup>/HCN<sup>+</sup> ISOMERS - ASTROCHEMICAL IMPLICATIONS MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY 248 : 272 1991

SCHNEIDER IF DISSOCIATIVE RECOMBI 4 : 131 2000

SHEEHAN C Merged beam measurement of the dissociative recombination of HCN<sup>+</sup> and HNC<sup>+</sup> JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 32 : 3347 1999

SUNDSTROM G DESTRUCTION RATE OF H-3<sup>+</sup> BY LOW-ENERGY ELECTRONS MEASURED IN A STORAGE-RING EXPERIMENT SCIENCE 263 : 785 1994

TALBI D POTENTIAL-ENERGY SURFACES FOR DISSOCIATIVE RECOMBINATION REACTIONS OF HCO<sup>+</sup> AND HCS<sup>+</sup> CHEMICAL PHYSICS 126 : 291 1988

TALBI D Potential energy surfaces for the electronic dissociative recombination of HCNH<sup>+</sup>: astrophysical implications on the HCN/HNC abundance ratio CHEMICAL PHYSICS LETTERS 288 : 155 1998

TALBI D Isomerization versus hydrogen exchange reaction in the HNC reversible arrow HCN conversion  
CHEMICAL PHYSICS LETTERS 263 : 385 1996