

AU Diaz-Tendero, S, Sanchez, G, Alcamí, M, Martín, F, Hervieux, PA, Chabot, M, Martinet, G, Desesquelles, P, Mezdari, F, Wohrer-Beroff, K, Della Negra, S, Hamrita, H, Le Padellec, A, Montagnon, L

TI Fragmentation of small neutral carbon clusters

SO INTERNATIONAL JOURNAL OF MASS SPECTROMETRY

LA English

DT Article

DE stability and fragmentation of clusters; carbon clusters; statistical model of fragmentation

ID DISSOCIATION-ENERGIES; ATOMIC CLUSTERS; METAL-CLUSTERS; EXACT EXCHANGE; IONS; PHOTODISSOCIATION; DENSITY; ENERGETICS; PHASE; PHOTOFRAGMENTATION

AB We report on theoretical and experimental efforts designed to understand the fragmentation of small neutral carbon clusters. Theoretically, the dissociation dynamics of C<sub>n</sub> has been investigated using a statistical model based on the microcanonical Metropolis Monte Carlo method. In this model various structural quantities (geometries, dissociation energies, harmonic frequencies...) are required for both the parent cluster and the fragments. They have been obtained from quantum chemistry calculations for C<sub>n</sub>, up to n = 9. Experimentally, a new detection system for high velocity fragments has been recently developed allowing the fragmentation of high velocity clusters to be totally recorded. Results for the branching ratios of deexcitation of C<sub>n</sub> with 5 ≤ n ≤ 9 formed by electron capture in high velocity C<sub>n</sub>(+)-He collisions are presented. In all cases, the agreement between theory and experiment is reasonably good provided that the theoretical branching ratios are convoluted with a C<sub>n</sub> energy distribution centered at around 10 eV (C) 2006 Elsevier B.V All rights reserved.

C1 GONLO, Inst Phys & Chim Mat Strasbourg, F-67034 Strasbourg, France., C9 Univ Autonoma Madrid, Dept Quim, Madrid 28049, Spain., CNRS, IN2P3, Inst Phys Nucl, F-91406 Orsay, France., CNRS, F-91405 Orsay, France., UMR Univ Paris Sud, LCAM, Lab Collis Atom & Mol, F-91405 Orsay, France., Univ Toulouse 3, IRSAMC, F-31062 Toulouse 4, France.

RP Hervieux, PA, GONLO, Inst Phys & Chim Mat Strasbourg, 23 Rue Loess, F-67034 Strasbourg, France.

EM hervieux@ipcms.u-strasbg.fr

NR 34

TC 0

PU ELSEVIER SCIENCE BV

PI AMSTERDAM

PA PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS

SN 1387-3806

J9 INT J MASS SPECTROM

J1 Int. J. Mass Spectrom.

PD MAY 15

PY 2006

VL 252

IS 2

BP 126

EP 132

PG 7

SC Physics, Atomic, Molecular & Chemical; Spectroscopy

GA 045UV

UT ISI:000237768900007