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AF Beroff, K., Van-Oanh, N. T., Chabot, M., Tuna, T., Pino, T., Martinet, G., Le Padellec, A., Carpentier, Y., Lavergne, L.
TI Fragmentation of multiply charged hydrocarbon molecules C(n)H(q+) (n <=4, q <= 9) produced in high-velocity collisions: Branching ratios and kinetic energy release of the H(+) fragment
SO PHYSICAL REVIEW A
LA English
DT Article
ID COULOMB-EXPLOSION; ION-IMPACT; IONIZATION; STATES; CLUSTERS; SPECTRA; PICTURE; C2+
AB Fragmentation branching ratios for channels involving H(+) emission and associated kinetic energy release of the H(+) fragment [KER(H(+))] have been measured for multicharged C(n)H(q+) molecules produced in high velocity (3.6 a.u.) collisions between C(n)H(+) projectiles and helium atoms. For CH(q+) (q <= 4) molecules, measured KER(H(+)) were found well below predictions of the simple point charge Coulomb model (PCCM) for all q values. Multireference configuration interaction (MRCI) calculations for ground as well as electronic excited states were performed which allowed a perfect interpretation of the CH(q+) experimental results for low charges (q = 2-3) as well as for the highest charge (q = 4). In this last case we could show, on the basis of ionization cross sections calculations and experimental measurements performed on the same systems at slightly higher velocity (4.5 a.u.), the prominent role played by inner-shell ionization followed by Auger relaxation and could extract the lifetime of this Auger relaxation giving rise to the best agreement between the experiment and the calculations. For dissociation of C(2)H(q+) and C(3)H(q+) with the highest charges (q >= 5), inner-shell ionization contributed in a prominent way to the ion production. In these two cases it was shown that measured KER(H(+)) were in good agreement with PCCM predictions when those were corrected for Auger relaxation with the same Auger lifetime value as in CH(3+).
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NR 41
TC 0
Z9 0
PU AMER PHYSICAL SOC
PI COLLEGE PK
PA ONE PHYSICS ELLIPSE, COLLEGE PK, MD 20740-3844 USA
SN 1050-2947
J9 PHYS REV A
JI Phys. Rev. A
PD SEP 6
PY 2011
VL 84
IS 3
AR 032705

DI 10.1103/PhysRevA.84.032705
PG 12
WC Optics; Physics, Atomic, Molecular & Chemical
SC Optics; Physics
GA 815XV
UT WOS:000294564200010