

AU Yousif, FB, Mitchell, JBA, Rogelstad, M, Le Padellec, A, Canosa, A, Chibisov, MI  
TI Dissociative Recombination OF HeH<sup>+</sup> - A Reexamination

SO PHYSICAL REVIEW A

LA English

DT Article

ID ION BEAM EXPERIMENTS; CONFIGURATION INTERACTION; MOLECULAR ION;  
STATES; ENERGY; TRANSITIONS; COLLISIONS

AB A high-energy-resolution study of the dissociative recombination of HeH<sup>+</sup> has been performed. A theoretical analysis has indicated that the recombination at low energy is due to the presence of a metastable triplet-state component of the ion beam.

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NR 26

TC 27

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV A

JI Phys. Rev. A

PD JUN

PY 1994

VL 49

IS 6

BP 4610

EP 4615

PG 6

SC Physics, Atomic, Molecular & Chemical; Optics

GA NT908

UT ISI:A1994NT90800046

AU Le Padellec, A, Sheehan, C, Talbi, D, Mitchell, JBA  
TI A merged-beam study of the dissociative recombination of HCO+  
SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS  
LA English  
DT Article  
ID STORAGE RING; IONS; H-3+; HEH+; COEFFICIENTS; IONIZATION; ELECTRONS;  
APPARATUS; STATE; CROSS  
AB Cross sections for the dissociative recombination of HCO+ ions have been measured in the energy range from 0.01-1.0 eV. The large values measured for low-energy electrons are supported by an earlier extensive quantum mechanical study by Talbi and co-workers which is reviewed. A broad maximum has been found in the region from 0.3-0.8 eV and this is attributed to the opening up of a second product channel leading to CH + O.  
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NR 33  
TC 8  
PU IOP PUBLISHING LTD  
PI BRISTOL  
PA DIRAC HOUSE, TEMPLE BACK, BRISTOL, ENGLAND BS1 6BE  
SN 0953-4075  
J9 J PHYS-B-AT MOL OPT PHYS  
JI J. Phys. B-At. Mol. Opt. Phys.  
PD JAN 28  
PY 1997  
VL 30  
IS 2  
BP 319  
EP 327  
PG 9  
SC Physics, Atomic, Molecular & Chemical; Optics  
GA WJ025  
UT ISI:A1997WJ02500023

AU Le Padellec, A, Laube, S, Sidko, O, Rebrion-Rowe, C, Rowe, BR, Sarpal, B, Mitchell, JBA  
TI The dissociative recombination of KrH<sup>+</sup> and XeH<sup>+</sup>

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID HEH<sup>+</sup>

AB The dissociative recombination of KrH<sup>+</sup> and XeH<sup>+</sup> has been studied using a FALP-MS technique. KrH<sup>+</sup> is found to have a small recombination rate while that of XeH<sup>+</sup> is  $8.3 \times 10^{-8}$  cm<sup>3</sup> s<sup>-1</sup> at 300 K.

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RP Le Padellec, A, UNIV RENNES 1, CNRS, UMR 1203, F-35042 RENNES, FRANCE.

NR 23

TC 4

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SN 0953-4075

J9 J PHYS-B-AT MOL OPT PHYS

J1 J. Phys. B-At. Mol. Opt. Phys.

PD FEB 28

PY 1997

VL 30

IS 4

BP 963

EP 967

PG 5

SC Physics, Atomic, Molecular & Chemical; Optics

GA WM293

UT ISI:A1997WM29300016

AU Larsson, M, Danared, H, Larson, A, Le Padellec, A, Peterson, JR, Rosen, S, Semaniak, J, Stromholm, C

TI Isotope and electric field effects in dissociative recombination of D-3(+)

SO PHYSICAL REVIEW LETTERS

LA English

DT Article

ID INTERSTELLAR CLOUDS; STORAGE-RING; ENERGY; H-3+; HEH+; H-3(+); IONS; CHEMISTRY; H3+

AB The cross section for dissociative recombination of vibrationally cold D-3(+) has been measured at the ion storage ring CRYRING. The rate constant at 300 K,  $\alpha = 2.7 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$ , is a factor of 4.3 smaller than the corresponding value for H-3(+) measured earlier in CRYRING. An electric field of 30 V/cm was introduced in the electron-ion interaction region. This had no measurable effect on the dissociative recombination cross section. This suggests that the cross sections measured in storage rings for H-3(+) and its isotopic variants can be directly compared with theoretical results once such results become available.

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NR 45

TC 15

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J9 PHYS REV LETT

JI Phys. Rev. Lett.

PD JUL 21

PY 1997

VL 79

IS 3

BP 395

EP 398

PG 4

SC Physics, Multidisciplinary

GA XL549

UT ISI:A1997XL54900016

AU Al-Khalili, A, Danared, H, Larsson, M, Le Padellec, A, Peverall, R, Rosen, S, Semaniak, J, af Ugglas, M, Vikor, L, van der Zande, PJ

TI Dissociative recombination of (HeH<sup>+</sup>)-He-3: comparison of spectra obtained with 100, 10 and 1 meV temperature electron beams

SO HYPERFINE INTERACTIONS

LA English

DT Article

ID HEH+; EXCITATION

AB The heavy-ion storage ring CRYRING at the Manne Siegbahn Laboratory at Stockholm University has been used for the study of dissociative recombination of (HeH<sup>+</sup>)-He-3. The new adiabatically expanded electron beam at CRYRING, which is achieved by means of a superconducting magnet, was used. The electron-beam expansion factor of 100 gave a transverse electron temperature of about 1 meV. This allowed the observation of several new resonances in the recombination cross-section.

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NR 17

TC 5

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J9 HYPERFINE INTERACTIONS

JI Hyperfine Interact.

PY 1998

VL 114

IS 1-4

BP 281

EP 287

PG 7

SC Physics, Atomic, Molecular & Chemical; Physics, Condensed Matter; Physics, Nuclear

GA 144JY

UT ISI:000077312400034

AU Le Padellec, A, Larsson, M, Danared, H, Larson, A, Peterson, JR, Rosen, S, Semaniak, J, Stromholm, C

TI A storage ring study of dissociative excitation and recombination of D-3(+)

SO PHYSICA SCRIPTA

LA English

DT Article

ID PRODUCT-STATE DISTRIBUTIONS; DIELECTRONIC RECOMBINATION; CROSS-SECTIONS; H-3(+); H-3+; ION; (HEH+)-HE-4; BEAM; H3+

AB Dissociative recombination and excitation of D-3(+) have been studied in CRYRING, a heavy-ion storage ring at the Manne Siegbahn Laboratory at Stockholm University. The measured cross section for dissociative recombination was used to deduce a 300 K rate constant of  $2.7 \times 10^{-8}$  cm<sup>3</sup> s<sup>-1</sup>. This is a factor of four smaller than the corresponding value for H-3(+) measured earlier in CRYRING. Dissociative excitation into both the D and 2D channels (D + D or D-2) were studied. The 2D channel occurs at energies below threshold for the ion's dissociative states, which indicates that resonant enhanced dissociative excitation via autoionizing resonances takes place. No measurable effect could be observed for the dissociative recombination cross sections when an electric field of 30 V/cm was applied to the electron-ion interaction region.

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NR 49

TC 6

PU ROYAL SWEDISH ACAD SCIENCES

PI STOCKHOLM

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J9 PHYS SCR

JI Phys. Scr.

PD FEB

PY 1998

VL 57

IS 2

BP 215

EP 221

PG 7

SC Physics, Multidisciplinary

GA YW677

UT ISI:000071961500010

AU Peterson, JR, Le Padellec, A, Danared, H, Dunn, GH, Larsson, M, Larson, A, Peverall, R, Stromholm, C, Rosen, S, af Ugglas, M, van der Zande, WJ

TI Dissociative recombination and excitation of N-2(+): Cross sections and product branching ratios

SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID STATE DISTRIBUTIONS; RATE COEFFICIENT; MOLECULAR-IONS; (HEH+)-HE-4; MECHANISMS; ELECTRONS; NITROGEN; ESCAPE; VENUS; MARS

AB The absolute dissociative recombination and absolute dissociative excitation rate coefficients and cross sections have been determined for N-2(+) and electrons for collision energies between 10 meV and 30 eV. The ion storage ring CRYRING has been used in combination with an imaging technique with a position-and-time-sensitive detector. Information is retrieved on the ion beam vibrational state populations and on the product branching in the dissociative recombination process at 0 eV collisions. A hollow cathode ion source has been used to lower the vibrational excitation in the ion beam; a more traditional hot-cathode ion source was used as well. The most important findings are the following. The rate coefficient for an N-2(+) ion beam (46%,  $\nu = 0$ , 27%  $\nu = 1$ ) versus electron temperature (K) is  $\alpha(T-e) = 1.75(+/-0.09) \times 10^{-7}(T-e/300)^{-0.30} \text{ cm}^3 \text{ s}^{-1}$ . The dissociative recombination rate is found to be weakly dependent on the N-2(+) vibrational level. At 0 eV collision energy, the  $\nu = 0$  product branching is found to be 0.37(8):0.11(6):0.52(4) for N(S-4) + N(D-2):N(P-2) + N(S-4) + N(D-2) + N(D-2) fragments. The dissociative recombination cross section does not have a high-energy peak as was found in a number of lighter molecular systems. The dissociative excitation signal starts only slightly above the energy threshold for dissociation, and peaks near 25 eV. From the dissociative excitation data and literature data, information is retrieved on the dissociative ionization of N-2(+). The comparison of these results with earlier DR measurements is extensively discussed. (C) 1998 American Institute of Physics.

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RP Peterson, JR, SRI Int, Mol Phys Lab, Menlo Park, CA 94025 USA.

NR 61

TC 43

PU AMER INST PHYSICS

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J9 J CHEM PHYS

JI J. Chem. Phys.

PD FEB 1

PY 1998

VL 108

IS 5

BP 1978

EP 1988

PG 11

SC Physics, Atomic, Molecular & Chemical

GA YU725  
UT ISI:000071748000028



AU Le Padellec, A, Sheehan, C, Mitchell, JBA

TI The dissociative recombination of  $CN^+$

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID BEAM EXPERIMENTS; ION; STATES

AB The dissociative recombination of  $CN^+$  has been measured using a single-pass merged-beam apparatus. It is found that the cross section displays resonant structure and falls-off abruptly above 0.3 eV.

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NR 18

TC 4

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J9 J PHYS-B-AT MOL OPT PHYS

JI J. Phys. B-At. Mol. Opt. Phys.

PD APR 28

PY 1998

VL 31

IS 8

BP 1725

EP 1728

PG 4

SC Physics, Atomic, Molecular & Chemical; Optics

GA ZM801

UT ISI:000073577200021

AU Semaniak, J, Larson, A, Le Padellec, A, Stromholm, C, Larsson, M, Rosen, S, Peverall, R, Danared, H, Djuric, N, Dunn, GH, Datz, S

TI Dissociative recombination and excitation of CH<sub>5</sub><sup>+</sup>: Absolute cross sections and branching fractions

SO ASTROPHYSICAL JOURNAL

LA English

DT Article

DE ISM, clouds; ISM, molecules; methods, laboratory; molecular processes

ID HIGH-RESOLUTION MEASUREMENT; POLYATOMIC IONS; DIELECTRONIC RECOMBINATION; IONOSPHERE; ELECTRONS; MOLECULES; PRODUCTS; H-3(+); H-3+; BEAM

AB The heavy-ion storage ring CRYRING was used to measure the absolute dissociative recombination and dissociative excitation cross sections for collision energies below 50 eV. Deduced thermal rates coefficients are consistent with previous beams data but are lower by a factor of 3 than the rates measured by means of the flowing afterglow Langmuir probe technique. A resonant structure in dissociative recombination cross section was found at 9 eV. We have determined the branching fractions in DR of CH<sub>5</sub><sup>+</sup> below 0.2 eV. The branching is dominated by three-body CH<sub>3</sub> + H + H and CH<sub>2</sub> + H-2 + H dissociation channels, which occur with branching ratios of approximate to 0.7 and approximate to 0.2, respectively; thus methane is a minor species among dissociation products. Both the measured absolute cross sections and branching in dissociative recombination of CH<sub>5</sub><sup>+</sup> can have important implications for the models of dense interstellar clouds and abundance of CH<sub>2</sub>, CH<sub>3</sub> and CH<sub>4</sub> in these media.

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NR 45

TC 34

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J9 ASTROPHYS J

JI Astrophys. J.

PD MAY 10

PY 1998

VL 498

IS 2

PN Part 1

BP 886

EP 895

PG 10

SC Astronomy & Astrophysics

GA ZN664

UT ISI:000073669300034

AU Laube, S, Le Padellec, A, Sidko, O, Rebrion-Rowe, C, Mitchell, JBA, Rowe, BR  
TI New FALP-MS measurements of H-3(+), D-3(+) and HCO+ dissociative recombination  
SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID STORAGE-RING; H-3+; ENERGY; IONS; H3+; BEAM; COEFFICIENTS; ELECTRONS

AB A series of measurements of the rate coefficient for the dissociative recombination (DR) of H-3(+) has been recorded. A value of  $7.8 \pm 2.3 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$  was found for ions that are vibrationally cold. This is somewhat smaller than that measured previously by this group. The difference is ascribed to aerodynamic effects which affected our earlier measurement that have been eliminated in the present work. Results for D-3(+) and HCO+ DR are also reported.

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NR 38

TC 19

PU IOP PUBLISHING LTD

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J9 J PHYS-B-AT MOL OPT PHYS

J1 J. Phys. B-At. Mol. Opt. Phys.

PD MAY 14

PY 1998

VL 31

IS 9

BP 2111

EP 2128

PG 18

SC Physics, Atomic, Molecular & Chemical; Optics

GA ZQ091

UT ISI:000073820500023

AU Rosen, S, Peverall, R, Larsson, M, Le Padellec, A, Semaniak, J, Larson, A, Stromholm, C, van der Zande, WJ, Danared, H, Dunn, GH

TI Absolute cross sections and final-state distributions for dissociative recombination and excitation of CO<sup>+</sup> (v=O) using an ion storage ring

SO PHYSICAL REVIEW A

LA English

DT Article

ID DIELECTRONIC-RECOMBINATION; TEMPERATURE-DEPENDENCE; RADIATIVE LIFETIMES; CARBON-MONOXIDE; RYDBERG STATES; 115 NM; PHOTODISSOCIATION; COEFFICIENTS; ELECTRONS; FRAGMENT

AB Absolute cross sections and rate coefficients have been determined for dissociative recombination of electrons and CO<sup>+</sup> ions for energies from 1 meV to 54 eV. We found values of  $4 \times 10^{-12}$  cm<sup>2</sup> at 1 meV and  $10^{-15}$  cm<sup>2</sup> at 1 eV, with an essentially 1/E energy dependence. Branching ratios over the final atomic product states have been determined using a position-and time-sensitive imaging system. At zero eV collision energy the predominant yield is to ground-state atomic fragments (76%). At higher collisional energies the branching ratio to the ground-state Limit is reduced. A new limit, O(D-1)+C(D-1), opens up and branching to the O(P-3) +C(D-1) limit increases. Cross sections are also determined for dissociative excitation of CO<sup>+</sup>. Thermal rate coefficients are deduced from the dissociative recombination (DR) data, and compared with measurements in the literature. Consideration of both the theoretical and spectroscopic data in the literature giving information about the potential curves along which DR may take place reveals both a paucity and disparity of the data.

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NR 47

TC 24

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J9 PHYS REV A

JI Phys. Rev. A

PD JUN

PY 1998

VL 57

IS 6

BP 4462

EP 4471

PG 10

SC Physics, Atomic, Molecular & Chemical; Optics

GA ZU090

UT ISI:000074160600053

AU Larson, A, Le Padellec, A, Semaniak, J, Stromholm, C, Larsson, M, Rosen, S, Peverall, R, Danared, H, Djuric, N, Dunn, GH, Datz, S

TI Branching fractions in dissociative recombination of CH<sub>2</sub><sup>+</sup>

SO ASTROPHYSICAL JOURNAL

LA English

DT Article

DE ISM : molecules; methods : laboratory; molecular processes

ID DENSE INTERSTELLAR CLOUDS; CROSS-SECTIONS; MOLECULAR-IONS; EXCITATION; ELECTRONS; ABUNDANCE; MODELS; RATIOS; H<sub>3</sub>O<sup>+</sup>; H<sub>2</sub>D<sup>+</sup>

AB The absolute cross section and branching ratios for dissociative recombination of CH<sub>2</sub><sup>+</sup> with electrons have been measured by means of the heavy-ion storage ring CRYRING. Contrary to what has been previously believed, recombination of CH<sub>2</sub><sup>+</sup> is dominated by the three-body channel C + H + H (63%), whereas breakup into the CH + H and C + H-2 channels occurs with branching ratios of 25% and 12%, respectively. The thermal rate coefficient for dissociative recombination at 300 K is 6.4 x 10<sup>(-7)</sup> cm<sup>(3)</sup> s<sup>(-1)</sup>, which is higher by a factor of 2.5 than the value used in modelling dark molecular clouds. The low CH production and the high production of energetic carbon atoms could be favourable factors for the turbulence model to explain the large abundance of interstellar CH<sup>+</sup>. The cross section for dissociative excitation was also measured and found to be in good agreement with results from a crossed electron-ion beam experiment.

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NR 39

TC 37

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J9 ASTROPHYS J

JI Astrophys. J.

PD SEP 20

PY 1998

VL 505

IS 1

PN Part 1

BP 459

EP 465

PG 7

SC Astronomy & Astrophysics

GA 152LA

UT ISI:000077777900040

AU Le Padellec, A, Mitchell, JBA, Al-Khalili, A, Danared, H, Kallberg, A, Larson, A, Rosen, S, af Ugglas, M, Vikor, L, Larsson, M

TI Storage ring measurements of the dissociative recombination and excitation of the cyanogen ion  $CN+(X-1 \text{ Sigma}(+))$  and a  $(3)Pi, \nu=0$

SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID HIGH-RESOLUTION MEASUREMENT; ABSOLUTE CROSS-SECTIONS; DIELECTRONIC-RECOMBINATION; RADIATIVE LIFETIMES; LYING STATES; ENERGY CO+; CURVES; CLOUDS; ESCAPE

AB Absolute cross sections and rate coefficients were measured for the dissociative recombination of  $CN+(X(1) \text{ Sigma}(+))$  and a  $(3)Pi, \nu=0$  with electrons using the heavy ion storage-ring CRYRING at Stockholm University. The a  $(3)Pi$  State that lies only 0.08 eV above the  $X(1) \text{ Sigma}(+)$  ion ground state is most certainly populated in the ion beam injected into CRYRING, as this is a long-lived excited state. Over the 1 meV-3 eV energy range that was investigated, two energy dependencies were found for the cross sections, namely  $E^{-1.05}$  below 0.1 eV and  $E^{-1.41}$  above 0.4 eV. The energy domain 0.1-0.3 eV exhibits a resonant structure. Branching fractions over the final atomic product states were determined using a position sensitive imaging detector. Thermal rate coefficients are deduced from the measurements and the efficiency displayed by the dissociative recombination mechanism is typical of that of a diatomic ion ( $3.4 \times 10^{-7} \text{ cm}^3 \text{ s}^{-1}$  at room temperature). Cross sections for the dissociative excitation process are also reported and their magnitude at the plateau are unusually large. This may be explained by the number of potential curves which can be populated at moderate collision energy ( $<10 \text{ eV}$ ) for the  $CN+$  ion. (C) 1999 American Institute of Physics. [S0021-9606(99)00201-9].

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NR 56

TC 7

PU AMER INST PHYSICS

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J9 J CHEM PHYS

J1 J. Chem. Phys.

PD JAN 8

PY 1999

VL 110

IS 2

BP 890

EP 901

PG 12

SC Physics, Atomic, Molecular & Chemical

GA 153NT

UT ISI:000077839700021

AU Vikor, L, Al-Khalili, A, Danared, H, Djuric, N, Dunn, GH, Larsson, M, Le Padellec, A, Rosen, S, af Ugglas, M

TI Branching fractions in the dissociative recombination of  $\text{NH}_4^+$  and  $\text{NH}_2^+$  molecular ions

SO ASTRONOMY AND ASTROPHYSICS

LA English

DT Article

DE ISM : molecules; ISM : clouds; molecular processes

ID HIGH-RESOLUTION MEASUREMENT; ABSOLUTE CROSS-SECTIONS;  
DIELECTRONIC RECOMBINATION; INTERSTELLAR CLOUDS; ABUNDANCES;  
EXCITATION; ELECTRONS; GAS

AB Branching fractions in the dissociative recombination of  $\text{NH}_4^+$  and  $\text{NH}_2^+$  molecular ions with electrons were measured using the CRYRING heavy ion storage ring. We have determined complete branching fractions for  $\text{NH}_4^+$  at 0 eV and 2 meV collision energies, and at 0 eV collision energy for  $\text{NH}_2^+$ . We found the dissociative recombination of  $\text{NH}_4^+$  to be dominated by the two body, 'ammonia' channel. The branching fractions we obtained at 0 eV are 0.69 +/- 0.03 for the  $\text{NH}_3 + \text{H}$  channel, and for the breakup into the  $\text{NH}_2 + \text{H}_2$  and  $\text{NH}_2 + 2\text{H}$  channels 0.10 +/- 0.02 and 0.21 +/- 0.03, respectively. The values we obtained for 2 meV are about the same as at 0 eV. For the  $\text{NH}_2^+$  ion we obtained 0.66 +/- 0.01 for the three body  $\text{N} + \text{H} + \text{H}$  channel, 0.34 +/- 0.02 for  $\text{NH} + \text{H}$ , and no breakup into the  $\text{N} + \text{H}_2$  channel. Dissociative recombination of  $\text{NH}_4^+$  and  $\text{NH}_2^+$  is important as a potential source of some neutral molecules found in the interstellar clouds ( $\text{NH}_3$ ,  $\text{NH}_2$ , and  $\text{NH}$ ) and the measured branching fractions have important implications for modelling the chemistry of these clouds. We report also on the relative dissociative recombination cross sections for  $\text{NH}_4^+$  and  $\text{NH}_2^+$  for collision energies below 60 eV.

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NR 27

TC 20

PU SPRINGER VERLAG

PI NEW YORK

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SN 0004-6361

J9 ASTRON ASTROPHYS

JI Astron. Astrophys.

PD APR

PY 1999

VL 344

IS 3

BP 1027

EP 1033

PG 7

SC Astronomy & Astrophysics

GA 191NC

UT ISI:000080027600037

AU Sheehan, C, Le Padellec, A, Lennard, WN, Talbi, D, Mitchell, JBA

TI Merged beam measurement of the dissociative recombination of HCN<sup>+</sup> and HNC<sup>+</sup>

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID STIMULATED RADIATIVE RECOMBINATION; ABSOLUTE CROSS-SECTIONS;  
MOLECULAR-IONS; STORAGE-RING; EXCITATION; HCO<sup>+</sup>; PHOTOELECTRON;  
SPECTRUM; CH<sub>5</sub><sup>+</sup>; BAND

AB Cross sections for the dissociative recombination of isomeric HCN<sup>+</sup>/HNC<sup>+</sup> ions with electrons were measured using the single-pass merged beam experiment located at the University of Western Ontario in Canada. The source conditions were varied so that an HCN<sup>+</sup>/HNC<sup>+</sup> mixture was first studied. The HNC<sup>+</sup> ion was then isolated via the fast ion-molecule reaction HCN<sup>+</sup> + CO<sub>2</sub> --> HNC<sup>+</sup> + CO<sub>2</sub>. The two sets of measurements, which both refer to vibrationally (and electronically) excited states of HCN<sup>+</sup> and HNC<sup>+</sup>, exhibit differences in the magnitudes of the cross sections. Thermal rate coefficients have been calculated for both species. An attempt has been made to identify the valence states involved in the dissociation to the CN + H channel for HCN<sup>+</sup> recombination.

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NR 52

TC 4

PU IOP PUBLISHING LTD

PI BRISTOL

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SN 0953-4075

J9 J PHYS-B-AT MOL OPT PHYS

JI J. Phys. B-At. Mol. Opt. Phys.

PD JUL 28

PY 1999

VL 32

IS 14

BP 3347

EP 3360

PG 14

SC Physics, Atomic, Molecular & Chemical; Optics

GA 225DE

UT ISI:000081941500015



AU Zong, W, Dunn, GH, Djuric, N, Larsson, M, Greene, CH, Al-Khalili, A, Neau, A, Derkatch, AM, Vikor, L, Shi, W, Le Padellec, A, Rosen, S, Danared, H, Ugglas, MA

TI Resonant ion pair formation in electron collisions with ground state molecular ions

SO PHYSICAL REVIEW LETTERS

LA English

DT Article

ID DISSOCIATIVE RECOMBINATION; CROSS-SECTIONS

AB Resonant ion pair formation from collisions of electrons with ground state diatomic molecular ions has been observed and absolute cross sections measured. The cross section for  $\text{HD}^+$  is characterized by an abrupt threshold at 1.9 eV and 14 resolved peaks in the range of energies 0 less than or equal to E less than or equal to 14 eV. The dominant mechanism responsible for the structures appears to be resonant capture and stabilization, modified by two-channel quantum interference. Data on  $\text{HF}^+$  show structure correlated with photoionization of HF and with dissociative recombination of electrons with this ion.

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NR 18

TC 10

PU AMERICAN PHYSICAL SOC

PI COLLEGE PK

PA ONE PHYSICS ELLIPSE, COLLEGE PK, MD 20740-3844 USA

SN 0031-9007

J9 PHYS REV LETT

JI Phys. Rev. Lett.

PD AUG 2

PY 1999

VL 83

IS 5

BP 951

EP 954

PG 4

SC Physics, Multidisciplinary

GA 223BT

UT ISI:000081820400016

AU Rosen, S, Derkatch, A, Semaniak, J, Neau, A, Al-Khalili, A, Le Padellec, A, Vikor, L, Thomas, R, Danared, H, af Ugglas, M, Larsson, M

TI Recombination of simple molecular ions studied in storage ring: dissociative recombination of H<sub>2</sub>O<sup>+</sup>

SO FARADAY DISCUSSIONS

LA English

DT Article

ID ABSOLUTE CROSS-SECTIONS; DIELECTRONIC-RECOMBINATION; BRANCHING FRACTIONS; POLYATOMIC IONS; EXCITATION; ELECTRONS; CHEMISTRY; PRODUCTS; OXYGEN; STATES

AB Dissociative recombination of vibrationally relaxed H<sub>2</sub>O<sup>+</sup> ions with electrons has been studied in the heavy-ion storage ring CRYRING. Absolute cross-sections have been measured for collision energies between 0 eV and 30 eV. The energy dependence of the cross-section below 0.1 eV is found to be much steeper than the E<sup>-1</sup> behaviour associated with the dominance of the direct recombination mechanism. Resonant structures found at 4 eV and 11 eV have been attributed to the electron capture to Rydberg states converging to electronically excited ionic states. Complete branching fractions for all dissociation channels have been measured at a collision energy of 0 eV. The dissociation process is dominated by three-body H + H + O breakup that occurs with a branching ratio of 0.71.

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NR 32

TC 17

PU ROYAL SOC CHEMISTRY

PI CAMBRIDGE

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J9 FARADAY DISCUSS

JI Faraday Discuss.

PY 2000

IS 115

BP 295

EP 302

PG 8

SC Chemistry, Physical

GA 342PQ

UT ISI:000088654700021

AU Neau, A, Al Khalili, A, Rosen, S, Le Padellec, A, Derkatch, AM, Shi, W, Vikor, L, Larsson, M, Semaniak, J, Thomas, R, Nagard, MB, Andersson, K, Danared, H, af Ugglas, M  
TI Dissociative recombination of D3O+ and H3O+: Absolute cross sections and branching ratios  
SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID DIELECTRONIC RECOMBINATION; INTERSTELLAR CLOUDS; IONS; OH

AB Dissociative recombination of the polyatomic ions D3O+ and H3O+ with, electrons have been studied at the heavy-ion storage ring CRYRING (Manne Siegbahn Laboratory, Stockholm University). Absolute cross sections have been determined from 0.001 eV to 0.25 eV center-of-mass energy for D3O+ and from 0.001 eV to 28 eV for H3O+. The cross sections are large ( $7.3 \times 10^{-13}$  cm<sup>2</sup>) for D3O+ and  $3.3 \times 10^{-12}$  cm<sup>2</sup> for H3O+ at 0.001 eV). At low energies, the cross sections for D3O+ are E-1 energy dependent whereas it is slightly steeper for H3O+. A similar E-1 energy dependence was also observed by Mul [J. Phys. B 16, 3099 (1983)] with a merged electron-ion beam technique for both H3O+ and D3O+ and by Vejby-Christensen [Astrophys. J. 483, 531 (1997)] with the ASTRID storage ring in Denmark, who presented relative cross sections for H3O+. A resonance has been observed around 11 eV for H3O+. It reflects an electron capture to Rydberg states converging to an excited ionic core. A similar structure was reported by Vejby-Christensen Our absolute measurements are in fairly good agreement with those from Mul, which were first divided by 2 (Mitchell, 1999, private communication) and from Heppner [Phys. Rev. A 13, 1000 (1976)] for H3O+. Thermal rates were deduced from the measured cross sections for electron temperatures ranging from 50 K to 30 000 K. At 300 K, the thermal rate is equal to  $7.6 \times 10^{-7}$  cm<sup>3</sup> s<sup>-1</sup> for H3O+ and to  $3.5 \times 10^{-7}$  cm<sup>3</sup> s<sup>-1</sup> for D3O+. Complete branching ratios for all the possible product channels have been determined from 0 eV to 0.005 eV center-of-mass energy for D3O+ and at 0 eV for H3O+, using a well-characterized transmission grid in front of an energy-sensitive surface-barrier detector. No isotope effect was observed within the experimental uncertainties. The three-body break-up channel OX+X+X (where X stands for H or D) is found to occur for 67%-70% of the dissociations. Water or heavy water is produced with an 18%-17% probability and the production of oxygen atoms is negligible. These results support the three-body break-up dominance already found by Vejby-Christensen for the DR of H3O+ in a similar heavy-ion storage ring experiment. However, even if the general trend is the same for both storage rings, significant differences have been observed and will be discussed. (C) 2000 American Institute of Physics. [S0021- 9606(00)01229-0].

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NR 28

TC 36

PU AMER INST PHYSICS

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J9 J CHEM PHYS

JI J. Chem. Phys.

PD AUG 1

PY 2000

VL 113

IS 5

BP 1762

EP 1770

PG 9

SC Physics, Atomic, Molecular & Chemical

GA 335XB

UT ISI:000088269400013

AU Talbi, D, Le Padellec, A, Mitchell, JBA

TI Quantum chemical calculations for the dissociative recombination of HCN+ and HNC+

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID ISOMERIZATION; EXCHANGE

AB A theoretical investigation of the dissociative recombination (DR) of HCN+(X (2)Pi), HNC+(X (2)Sigma) and HCN+(A (2)Sigma) has been undertaken in order to complement the recent experimental measurement (Sheehan C, Le Padellec A, Lennard WN, Talbi D and Mitchell J B A 1999 J. Phys. B: At. Mol. Opt. Phys. 32 3347) of the DR of [CHN](+). Using quantum chemical methods, we have shown that the dissociative recombination of HNC+(X (2)Sigma) should involve the indirect mechanism while that of HCN+(X (2)Pi) and HCN+(A (2)Sigma) should be possible through both direct and indirect processes. Our theoretical study therefore suggests that HCN+(X (2)Pi) and HCN+(A (2)Sigma) should recombine much more rapidly than HNC+(X (2)Sigma) explaining the large rate coefficient measured for the DR of HCN+ compared with the HNC+ case.

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NR 21

TC 1

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J9 J PHYS-B-AT MOL OPT PHYS

J1 J. Phys. B-At. Mol. Opt. Phys.

PD SEP 28

PY 2000

VL 33

IS 18

BP 3631

EP 3646

PG 16

SC Physics, Atomic, Molecular & Chemical; Optics

GA 364YX

UT ISI:000089922600014

AU Larson, A, Djuric, N, Zong, W, Greene, CH, Orel, AE, Al-Khalili, A, Derkatch, AM, Le Padellec, A, Neau, A, Rosen, S, Shi, W, Vikor, L, Danared, H, af Ugglas, M, Larsson, M, Dunn, GH

TI Resonant ion-pair formation in electron collisions with HD<sup>+</sup> and OH<sup>+</sup>

SO PHYSICAL REVIEW A

LA English

DT Article

ID DISSOCIATIVE RECOMBINATION; CROSS-SECTIONS; DIELECTRONIC RECOMBINATION; RYDBERG STATES

AB Resonant ion-pair formation from collisions of electrons with, electronic and vibronic ground-state diatomic molecular ions has been, studied in the present work for HD<sup>+</sup> and OH<sup>+</sup>. The cross section for HD<sup>+</sup> has a magnitude of the order of  $3 \times 10^{-19}$  cm<sup>2</sup> and is characterized by an energy threshold and 14 resolved peaks in the energy range up to 16 eV. A theoretical study confirms that the structures derive primarily from quantum interference of the multiple dissociation pathways. Measurements for OH<sup>+</sup> reveal that the cross section for H<sup>+</sup> and O<sup>-</sup> formation is lower than  $10^{-21}$  cm<sup>2</sup> at energies of 6 and 12 eV.

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NR 29

TC 7

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV A

JI Phys. Rev. A

PD OCT

PY 2000

VL 6204

IS 4

AR 042707

DI ARTN 042707

PG 8

SC Physics, Atomic, Molecular & Chemical; Optics

GA 360VU

UT ISI:000089688700046

AU Andersson, K, Hanstorp, D, Neau, A, Rosen, S, Schmidt, HT, Thomas, R, Larsson, M, Semaniak, J, Osterdahl, F, Danared, H, Kallberg, A, Le Padellec, A

TI Electron impact single detachment on the F- ions using the heavy ion storage ring CRYRING: Cross-section determination

SO EUROPEAN PHYSICAL JOURNAL D

LA English

DT Article

ID DISSOCIATIVE RECOMBINATION; NONEXISTENCE; RESONANCES; STATE

AB Electron Impact Single Detachment (EISD) of F- has been studied using the heavy ion storage ring CRYRING at the Manne Siegbahn Laboratory, Stockholm, Sweden. F- ions stored in the ring were merged with an electron beam in one of the ring sections. Neutral F atoms produced in the EISD process were detected in the zero-degree direction using a surface barrier detector. The threshold for the detachment process was found to be around 7.6 eV, thus more than twice the binding energy of F-. The cross-sections increased smoothly up to 55 eV where it reached a maximum of  $1.9 \times 10^{-16}$  cm<sup>2</sup>. At higher energies slow decrease of the cross-section was observed. which follows the energy dependence predicted by the Bethe-Born approximation. The experiment showed that CRYRING can be used favourably for studies of anions, and several experiments are forthcoming.

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RP Andersson, K, Chalmers Univ Technol Goteborg Unit, Dept Phys, S-41296, Gothenburg, Sweden.

NR 33

TC 5

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J9 EUR PHYS J D

JI Eur. Phys. J. D

PD MAR

PY 2001

VL 13

IS 3

BP 323

EP 328

PG 6

SC Physics, Atomic, Molecular & Chemical

GA 412BA

UT ISI:000167533100004

AU Peverall, R, Rosen, S, Peterson, JR, Larsson, M, Al-Khalili, A, Vikor, L, Semaniak, J, Bobbenkamp, R, Le Padellec, A, Maurellis, AN, van der Zande, WJ

TI Dissociative recombination and excitation of O-2(+): Cross sections, product yields and implications for studies of ionospheric airglows

SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID ION STORAGE-RING; TEMPERATURE-DEPENDENCE; BRANCHING RATIOS; ELECTRON-BEAM; F-REGION; O-2+; O(1S); NO+; O(1D); STATE

AB We present experimental data on the dissociative recombination (DR) and the dissociative excitation (DE) of O-2(+) in its electronic and vibrational ground state using a heavy ion storage ring. The absolute DR cross section has been determined over an electron collision energy range from 1 meV to 3 eV. The thermal DR rate coefficient is derived;  $\alpha(T-e) = 2.4 \times 10^{-7} (300/T-e)^{0.70 \pm 0.01} \text{ cm}^3 \text{ s}^{-1}$ , for  $T > 200 \text{ K}$ . The threshold for DE was observed near its energetic threshold of 6.7 eV. The DE cross section curve has a maximum of  $3 \times 10^{-16} \text{ cm}^2$  near 15 eV. We have determined the branching fractions to the different dissociation limits and present atomic quantum yields for the DR process between 0 to 300 meV collision energy. The quantum yield of O(D-1) is found to be  $1.17 \pm 0.05$ , largely independent of the electron energy. Arguments are presented that the branching fraction to O(P-3)+O(S-1) is negligible. The branching fraction to the O(S-1)+O(D-1) is smaller than 0.06 and varies strongly as a function of collision energy. The O(S-1) quantum yield is a strong function of electron temperature. Hence, the relative strength of the green, O(S-1), and the red, O(D-1), airglows may be used as a measure of the electron temperature of the upper atmosphere. A qualitative explanation is given of the consequences of nonadiabatic interactions in the dissociation step of the DR process. (C) 2001 American Institute of Physics.

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NR 52

TC 21

PU AMER INST PHYSICS

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J9 J CHEM PHYS

J1 J. Chem. Phys.

PD APR 15

PY 2001

VL 114

IS 15

BP 6679

EP 6689

PG 11

SC Physics, Atomic, Molecular & Chemical

GA 418VG

UT ISI:000167914400022



AU Le Padellec, A, Djuric, N, Al-Khalili, A, Danared, H, Derkatch, AM, Neau, A, Popovic, DB, Rosen, S, Semaniak, J, Thomas, R, af Ugglas, M, Zong, W, Larsson, M

TI Resonant ion-pair formation in the recombination of NO<sup>+</sup> with electrons: Cross-section determination

SO PHYSICAL REVIEW A

LA English

DT Article

ID DISSOCIATIVE RECOMBINATION; RADIATIVE LIFETIMES; METASTABLE STATE; BRANCHING RATIOS; COLLISIONS; EXCITATION; IONIZATION; N-2(+)

AB Resonant ion-pair formation from the collisions of NO<sup>+</sup> ions with electrons was studied using the heavy-ion storage ring CRYRING at the Manne Siegbahn Laboratory of Stockholm University. The total cross section is measured for the formation of N<sup>++</sup>O<sup>-</sup> for electron energies 8-18 eV, and the results are compared with ion-pair formation in photoionization work. A peak in the cross section is observed at 12.5 eV, with a magnitude of  $8.5 \times 10^{-19}$  cm<sup>2</sup>. An attempt to extract the cross section for the reverse process of associative ionization is made.

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NR 33

TC 5

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV A

JI Phys. Rev. A

PD JUL

PY 2001

VL 6401

IS 1

AR 012702

DI ARTN 012702

PG 7

SC Physics, Atomic, Molecular & Chemical; Optics

GA 449XA

UT ISI:000169711400047

AU Djuric, N, Dunn, GH, Al-Khalili, A, Derkatch, AM, Neau, A, Rosen, S, Shi, W, Vikor, L, Zong, W, Larsson, M, Le Padellec, A, Danared, H, af Ugglas, M

TI Resonant ion-pair formation and dissociative recombination in electron collisions with ground-state HF+ ions

SO PHYSICAL REVIEW A

LA English

DT Article

ID HIGH-RESOLUTION MEASUREMENT; ABSOLUTE CROSS-SECTIONS; DIELECTRONIC, RECOMBINATION; STORAGE-RING; EXCITATION; OH+; DF; DISTRIBUTIONS; CH+

AB Rate coefficients and absolute cross sections for center-of-mass energies between 0.0001 and 1 eV are reported for both resonant ion-pair formation and dissociative recombination in electron collisions with HF+ ions. The heavy-ion storage ring CRYRING in Stockholm was used for these measurements. Notable is the fact that the dissociative recombination cross section is substantially smaller than that for most diatomic molecular ions. The recombination seems to have an underlying E-1 energy dependence characteristic of the direct process in dissociative recombination, but both cross sections show structure, which may be attributed to contributions from different indirect processes. The cross sections have no observable energy thresholds. The ratio of the cross section for resonant ion-pair formation to that for dissociative recombination is about 0.25 at 10(-3) eV, with the ratio depending on the interaction energy, so the competition of the ion-pair process is much stronger than for other ions so far studied. The HF+ ion is unique in the fact that the electron affinity of F, the binding energy of HF+, and energy of the atom pair [H(n = 2) + F(P-2(3/2))] are the same within the rotational-energy spread of the HF+ target. The resonant ion-pair formation process,  $e + \text{HF}^+ \rightarrow \text{H}^+ + \text{F}^-$ , has some similarities to the photon process,  $h\nu + \text{HF} \rightarrow \text{H}^+ + \text{F}^-$ , and we discuss comparisons. We deduce thermal rate coefficients from our measurements and discuss them in the context of rate coefficients for other diatomic ions available in the literature.

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NR 38

TC 4

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV A

JI Phys. Rev. A

PD AUG

PY 2001

VL 64

IS 2

AR 022713

DI ARTN 022713

PG 9

SC Physics, Atomic, Molecular & Chemical; Optics

GA 460FJ

UT ISI:000170297300058

AU Le Padellec, A, Andersson, K, Hanstorp, D, Hellberg, F, Larsson, M, Neau, A, Rosen, S, Schmidt, HT, Thomas, R, Semaniak, J, Pegg, DJ, Osterdahl, F, Danared, H, Kallberg, A

TI Electron scattering on CN-

SO PHYSICA SCRIPTA

LA English

DT Article

ID ABSOLUTE CROSS-SECTIONS; DISSOCIATIVE RECOMBINATION; EXCITED-STATES; DYNAMICS; IONS

AB We present the results of an experiment in which electrons have been scattered on CN- ions, over a collision energy range 0-60 eV The experiment was performed at the heavy ion storage ring CRYRING The CN- ions were stored in the ring and merged with a monoenergetic electron beam that was guided in to and out of the ring using strong magnetic fields. Both neutral and positive fragments from the collision process were detected with surface barrier detectors. It was found that pure detachment completely dominates over those channels which involves breaking the molecular bond. The threshold energy for the detachment process was found to be 7 eV The cross section rose from zero to a maximum of about  $5.10(-16)$  cm<sup>2</sup> just below 30 eV, after which it remained essentially constant. The threshold region was carefully investigated in an attempt to find resonance structure arising from the possible existence of the doubly charged ion, CN<sup>2-</sup>. The statistical uncertainty in the data was, however, too large to conclusively prove or disprove the existence of such a resonance.

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NR 34

TC 3

PU ROYAL SWEDISH ACAD SCIENCES

PI STOCKHOLM

PA PUBL DEPT BOX 50005, S-104 05 STOCKHOLM, SWEDEN

SN 0281-1847

J9 PHYS SCR

JI Phys. Scr.

PD NOV

PY 2001

VL 64

IS 5

BP 467

EP 473

PG 7

SC Physics, Multidisciplinary

GA 496EJ

UT ISI:000172383000013

AU Le Padellec, A, Rabilloud, F, Pegg, D, Neau, A, Hellberg, F, Thomas, R, Schmidt, HAT, Larsson, M, Danared, H, Kallberg, A, Andersson, K, Hanstorp, D

TI Electron-impact detachment and dissociation of C-4(-) ions

SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID SMALL CARBON CLUSTERS; DIFFUSE INTERSTELLAR BANDS; ABSOLUTE CROSS-SECTIONS; CHARGED NEGATIVE-IONS; ABSORPTION-SPECTRA; NEON MATRICES; ANIONS; RECOMBINATION; CHAINS; SPECTROSCOPY

AB CRYRING was used to study collision processes between an electron and a negative ion cluster C-4(-). The total detachment cross sections for the production of the neutral 4C, 3C, 2C, and C fragments were measured. The cross sections for pure detachment, and for detachment plus dissociation leading to the production of C-3+C, 2C(2), and C-2+2C were extracted using a grid. It was found that the pure detachment process overwhelmingly dominates all other fragmentation processes. The threshold location for the detachment channel is found to be around 6.0 eV. Although the doubly charged negative ion C-4(2-) has received little previous attention, a defined near-threshold resonance observed in the detachment cross section curve, has been associated with the short-lived state C-4(2-) (0.7 fs lifetime). (C) 2001 American Institute of Physics.

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NR 31

TC 9

PU AMER INST PHYSICS

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J9 J CHEM PHYS

JI J. Chem. Phys.

PD DEC 15

PY 2001

VL 115

IS 23

BP 10671

EP 10677

PG 7

SC Physics, Atomic, Molecular & Chemical

GA 498WF

UT ISI:000172536000011

AU Nzeyimana, T, Naji, EA, Urbain, X, Le Padellec, A  
TI Merged beam study of the associative ionisation (C+, N+ and O+) + O-  
SO EUROPEAN PHYSICAL JOURNAL D

LA English

DT Article

ID ELECTRON-IMPACT; RADIATIVE ASSOCIATION; MUTUAL NEUTRALIZATION;  
CROSS SECTIONS; OXYGEN-ATOMS; RECOMBINATION; IONIZATION; COLLISIONS;  
IONS; DISSOCIATION

AB Total cross-sections have been measured for the associative ionisation of C+ + O-, N+ + O- and O+ + O- by means of a merged-beam set-up operating with keV beams. These original measurements might be relevant to the understanding of some astrophysical objects or laboratory-made plasmas (flames and etching plasmas). The magnitude of these cross-sections is particularly large whatever the associating system, as these are in the range of  $1 \times 10^{-14}$  cm<sup>2</sup> at thermal energies. Their behaviour as a function of energy significantly differs from one system to another, and is characterised by the Wigner law at low energy, and a rapid fall-off at higher energy due to competition with non-associative ionisation processes.

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RP Nzeyimana, T, Univ Catholique Louvain, Dept Phys, Unite FYAM, Chemin Cyclotron 2, B-1348 Louvain, Belgium.

NR 32

TC 2

PU SPRINGER-VERLAG

PI NEW YORK

PA 175 FIFTH AVE, NEW YORK, NY 10010 USA

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J9 EUR PHYS J D

JI Eur. Phys. J. D

PD JUN

PY 2002

VL 19

IS 3

BP 315

EP 325

PG 11

SC Physics, Atomic, Molecular & Chemical

GA 566CP

UT ISI:000176409500004

AU Rayane, D, Compagnon, I, Antoine, R, Broyer, M, Dugourd, P, Labastie, P, L'Hermite, JM, Le Padellec, A, Durand, G, Calvo, F, Spiegelman, F, Allouche, AR

TI Electric dipole moments and polarizabilities of single excess electron sodium fluoride clusters: Experiment and theory

SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID ALKALI-HALIDE CLUSTERS; GROUND-STATE; ABSORPTION-SPECTRA; IONIC-CRYSTALS; AB-INITIO; LOCALIZATION; MOLECULES; C-60; 2-LESS-THAN-OR-EQUAL-TO-N-LESS-THAN-OR-EQUAL-TO-29; NANOCRYSTALS

AB In this article we present the first measurement of the electric dipole susceptibility of one excess electron  $\text{Na}_n\text{F}_{n-1}$  clusters. The static electronic polarizability and the permanent electric dipole of these clusters have been calculated with a one-electron model. Experimental values for the susceptibility are clearly related to the calculated values of the permanent dipole. The size evolution of the dipole moments is interpreted in terms of the interplay between the lattice and electron properties. This study outlines that the response of the cluster to the electric field cannot be fully understood with only equilibrium structure calculations and that the coupling between the permanent dipole and the vibrational motion of the cluster has to be taken into account. (C) 2002 American Institute of Physics.

C1 CNRS, Spectrometrie Ion & Mol Lab, UMR 5579, F-69622 Villeurbanne, France., Univ Lyon 1, F-69622 Villeurbanne, France., CNRS, IRSAMC, Lab Collis Agregats React, UMR 5589, F-31062 Toulouse, France., Univ Toulouse 3, F-31062 Toulouse 4, France., CNRS, IRSAMC, Phys Quant Lab, UMR 5626, F-31062 Toulouse 4, France.

RP Rayane, D, CNRS, Spectrometrie Ion & Mol Lab, UMR 5579, Bat A Kastler, 43 Bd 11 Novembre 1918, F-69622 Villeurbanne, France.

NR 38

TC 3

PU AMER INST PHYSICS

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J9 J CHEM PHYS

JI J. Chem. Phys.

PD JUN 22

PY 2002

VL 116

IS 24

BP 10730

EP 10738

PG 9

SC Physics, Atomic, Molecular & Chemical

GA 560DF

UT ISI:000176066200019

AU Le Padellec, A, Collins, GF, Danared, H, Kallberg, A, Hellberg, F, Neau, A, Fritioff, K, Hanstorp, D, Larsson, M

TI Relative cross sections for the electron impact single detachment on Li-

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID NEGATIVE HYDROGEN ION; PHOTODETACHMENT; RESONANCES; THRESHOLD; STATES; NONEXISTENCE; COLLISIONS; ATOMS; NA; H2

AB The electron impact single detachment process on Li- targets was, studied using the storage ring CRYRING located at the Manne Siegbahn Laboratory in Stockholm, Sweden. The Li- ions, first stored in the storage ring, were merged with a cold, 1.4 cm in diameter, electron beam. The neutral Li atoms, originating from the process under scrutiny, were recorded by an energy-sensitive surface barrier detector in order to measure the relative electron single detachment cross section. The findings are the following. The cross section increases smoothly above the 1.4 eV detachment threshold and reaches a maximum at about 12 eV. At even larger energies a slow decrease, which follows the  $\ln(E)/E$  energy dependence predicted by the Bethe-Born approximation, is observed.

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RP Le Padellec, A, Univ Toulouse 3, LCAR, UMR 5589, 118 Route Narbonne, Bat 3 R1B4, F-31062 Toulouse 4, France.

NR 36

TC 3

PU IOP PUBLISHING LTD

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SN 0953-4075

J9 J PHYS-B-AT MOL OPT PHYS

J1 J. Phys. B-At. Mol. Opt. Phys.

PD SEP

PY 2002

VL 35

IS 17

BP 3669

EP 3676

PG 8

SC Physics, Atomic, Molecular & Chemical; Optics

GA 703XH

UT ISI:000184307300008

AU Naji, EA, Nzeyimana, T, Urbain, X, Le Padellec, A

TI Merged beam study of the associative ionization  $O^- + D^+ / O^{++} D^-$  and  $C^{++} D^-$

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID ELECTRON-IMPACT; STATES; H(1S); DYNAMICS; MOLECULE; IONS

AB Absolute total cross sections have been measured for the associative ionization (AI) reactions  $O^- + D^+ / O^+ + D^-$  and  $C^+ + D^-$  using a merged beam set-up. These original measurements might be relevant to the understanding of several astrophysical objects. The internal excitation of the target ions is discussed, and structures appearing in the different cross section curves are related to the interplay between AI and other non-associative reaction channels, such as detachment and multiple ionization.

C1 Univ Catholique Louvain, Dept Phys, Unite FYAM, B-1348 Louvain, Belgium., Univ Toulouse 3, LCAR UMR 5589, F-31062 Toulouse 4, France.

RP Naji, EA, Univ Catholique Louvain, Dept Phys, Unite FYAM, Chemin Cyclotron 2, B-1348 Louvain, Belgium.

NR 26

TC 1

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J9 J PHYS-B-AT MOL OPT PHYS

J1 J. Phys. B-At. Mol. Opt. Phys.

PD NOV 14

PY 2002

VL 35

IS 21

BP 4325

EP 4334

PG 10

SC Physics, Atomic, Molecular & Chemical; Optics

GA 618VC

UT ISI:000179437100003



AU Fritioff, K, Sandstrom, J, Hanstorp, D, Ehlerding, A, Larsson, M, Collins, GF, Pegg, DJ, Danared, H, Kallberg, A, Le Padellec, A  
TI Electron-impact detachment from Cl-  
SO PHYSICAL REVIEW A

LA English

DT Article

ID BOUND NEGATIVE-IONS; SINGLE DETACHMENT; STORAGE-RING; H IONS;  
THRESHOLD; BEAM

AB Single-, double- and triple-electron-impact detachments from the Cl- ion have been investigated over a collision energy range of 0-95 eV. The experiment was performed at the ion storage ring CRYRING at the Manne Siegbahn Laboratory. The Cl- ions, produced in a sputter ion source, were injected into the ring and accelerated to 2.7 MeV. Thereafter the ions were merged with an electron beam. The electrons served to cool the ion beam. Then they were used as a partner in the electron-ion collisions. The products of the detachment processes, Cl atoms, Cl+, and Cl2+ ions, were detected after the interaction region with surface-barrier detectors. The shapes of the cross sections for the single, double, and triple detachments show striking similarities.

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RP Fritioff, K, Chalmers Univ Technol, Univ Gothenburg, Dept Phys, S-41296, Gothenburg, Sweden.

NR 27

TC 5

PU AMERICAN PHYSICAL SOC

PI COLLEGE PK

PA ONE PHYSICS ELLIPSE, COLLEGE PK, MD 20740-3844 USA

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J9 PHYS REV A

JI Phys. Rev. A

PD JUL

PY 2003

VL 68

IS 1

AR 012712

DI ARTN 012712

PG 8

SC Physics, Atomic, Molecular & Chemical; Optics

GA 708MP

UT ISI:000184571600071

AU A-Khalili, A, Rosen, S, Danared, H, Derkatch, AM, Kallberg, A, Larsson, M, Le Padellec, A, Neau, A, Semaniak, J, Thomas, R, af Ugglas, M, Vikor, L, Zong, W, van der Zande, WJ, Urbain, X, Jensen, MJ, Bilodeau, RC, Heber, O, Pedersen, HB, Andersen, LH, Lange, M, Levin, J, Gwinner, G, Knoll, L, Scheffel, M, Schwalm, D, Wester, R, Zajfman, D, Wolf, A

TI Absolute high-resolution rate coefficients for dissociative recombination of electrons with HD<sup>+</sup>: Comparison of results from three heavy-ion storage rings

SO PHYSICAL REVIEW A

LA English

DT Article

ID DIELECTRONIC RECOMBINATION; VIBRATIONAL-STATES; BRANCHING RATIOS; CROSS-SECTIONS; COLD HD<sup>+</sup>; BEAM; EXCITATION; COOLER; H-2(+); ENERGIES

AB Experimental data are presented from three different heavy-ion storage rings (ASTRID in Aarhus, CRYRING in Stockholm, and TSR in Heidelberg) to assess the reliability of this experimental tool for the extraction of absolute rate coefficients and cross sections for dissociative recombination (DR). The DR reaction between HD<sup>+</sup> and electrons has been studied between 0 and 30 eV on a dense energy grid. HD<sup>+</sup> displays two characteristic local maxima in the DR rate around 9 and 16 eV. These maxima influence the data analysis at smaller collision energies. We conclude that resonant structures in the DR cross sections are reproduced among the experiments within the collision energy resolution. The absolute cross sections agree within the systematic experimental errors of 20% related to the measurement of the ion currents. Absolute thermal rate coefficients for HD<sup>+</sup> ions are given for an electron temperature range of 50-300 K. Results for the DR cross section and the thermal rate coefficients are compared to recent theoretical calculations including rotational effects, finding satisfactory agreement.

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NR 54

TC 0

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV A

JI Phys. Rev. A

PD OCT

PY 2003

VL 68

IS 4

AR 042702

DI ARTN 042702

PG 14

SC Physics, Atomic, Molecular & Chemical; Optics

GA 750PJ

UT ISI:000187004700060

AU L'Hermite, JM, Blanchet, V, Le Padellec, A, Lamory, B, Labastie, P

TI Relaxation of photoexcited Na<sub>3</sub>F

SO EUROPEAN PHYSICAL JOURNAL D

LA English

DT Article

ID ALKALI-HALIDE CLUSTERS; SODIUM-FLUORIDE CLUSTERS; OPTICAL-RESPONSE, PROPERTIES; EXCESS-ELECTRON; AB-INITIO; SPECTRAL SIGNATURE; LITHIUM-HYDRIDE; EXCITED-STATES; PULSES; SPECTROSCOPY

AB This paper describes the spectroscopy of Na<sub>3</sub>F both in the frequency and time domains. The photoionization efficiency curve shows two thresholds, associated to two isomers. The excited electronic states of the C-2v isomer have been probed by photodepletion spectroscopy, and the results are used to analyze a time-resolved study of photoexcited Na<sub>3</sub>F, probed by photoionization. The pump-probe signal clearly shows damped oscillations, the period of which is fitted to 39010 fs, close to twice the previously measured bending mode of Na<sub>2</sub>F [1], while the relaxation time is 127550 fs.

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NR 23

TC 3

PU SPRINGER-VERLAG

PI NEW YORK

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J9 EUR PHYS J D

JI Eur. Phys. J. D

PD MAR

PY 2004

VL 28

IS 3

BP 361

EP 366

PG 6

SC Physics, Atomic, Molecular & Chemical

GA 805PO

UT ISI:000220378400006

AU Fritioff, K, Sandstrom, J, Andersson, P, Hanstorp, D, Hellberg, F, Thomas, R, Larsson, M, Osterdahl, F, Collins, GF, Le Padellec, A, Pegg, DJ, Gibson, ND, Danared, H, Kallberg, A

TI Observation of an excited C-4(2-) ion

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID ELECTRON-IMPACT DETACHMENT; PHASE

AB This paper reports an experimental investigation of the electron impact detachment of C-4(-). We observe structure in the electron impact cross section for detaching a single electron from a C-4(-) cluster anion, which we attribute to the formation and decay of the C-4(2-) dianion. The system is energetically unstable and very rapidly decays via double autodetachment. The energy and width of the resonance were determined to be 8.8(5) eV and 1.4(5) eV, respectively, and the resonance lies 1.5(5) eV above the ground state of the neutral system. The experiment was conducted by merging monoenergetic electron and ion beams in the heavy ion storage ring CRYRING. The detachment channel was monitored by detecting neutral C-4 fragments.

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NR 13

TC 1

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J9 J PHYS-B-AT MOL OPT PHYS

JI J. Phys. B-At. Mol. Opt. Phys.

PD JUN 14

PY 2004

VL 37

IS 11

BP 2241

EP 2246

PG 6

SC Physics, Atomic, Molecular & Chemical; Optics

GA 853DZ

UT ISI:000223808000005

AU Martinet, G, Diaz-Tendero, S, Chabot, M, Wohrer, K, Della Negra, S, Mezdari, F, Hamrita, H, Desesquelles, P, Le Padellec, A, Gardes, D, Lavergne, L, Lalu, G, Grave, X, Clavelin, JF, Hervieux, PA, Alcami, M, Martin, F

TI Fragmentation of highly excited small neutral carbon clusters

SO PHYSICAL REVIEW LETTERS

LA English

DT Article

ID MULTIREFERENCE CONFIGURATION-INTERACTION; MOLECULAR-STRUCTURE; COUPLED-CLUSTER; ELECTRON-CAPTURE; CROSS-SECTIONS; COLLISIONS; DENSITY; ENERGY; EXCITATION; IONS

AB We present a combined experimental and theoretical study of fragmentation of small C-n clusters (n=5,7,9) produced in charge transfer collisions of fast (v=2.6 a.u.) singly charged C-n(+) clusters with He. Branching ratios for all possible fragmentation channels have been measured. Comparison with microcanonical Metropolis Monte Carlo simulations based on quantum chemistry calculations allows us to determine the energy distribution of the excited clusters just after the collision.

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NR 34

TC 6

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV LETT

JI Phys. Rev. Lett.

PD AUG 6

PY 2004

VL 93

IS 6

AR 063401

DI ARTN 063401

PG 4

SC Physics, Multidisciplinary

GA 844DS

UT ISI:000223138200016

AU Staicu-Casagrande, EM, Nzeyimana, T, Naji, EA, de Ruelle, N, Fabre, B, Le Padellec, A, Urbain, X

TI Abstraction and insertion mechanisms in reactive collisions of H-2(+) and D-2(+) with O-  
SO EUROPEAN PHYSICAL JOURNAL D

LA English

DT Article

ID EXCITED-STATES; DISSOCIATIVE RECOMBINATION; ULTRAVIOLET EMISSION;  
QUANTUM DYNAMICS; GASEOUS IONS; MERGED BEAM; H2O+; LIFETIMES; ENERGY;  
SCATTERING

AB Integral cross-sections were measured for the associative ionisation and reactive ionisation in collisions of H-2(+) and D-2(+) with O- by means of a merged-beam set-up operating with keV beams. The magnitude of the reactive cross-sections is quite large (10(-14) cm(2) at 10 meV), and surpasses the associative ionisation by an order of magnitude. The observed ratio is discussed in terms of insertion and abstraction mechanisms that prevail in the case of atom-diatom inelastic collisions. These measurements may be relevant to the understanding of some astrophysical objects such as the comets, where the presence of the water cation was highlighted.

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NR 34

TC 0

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J9 EUR PHYS J D

JI Eur. Phys. J. D

PD DEC

PY 2004

VL 31

IS 3

BP 469

EP 475

PG 7

SC Physics, Atomic, Molecular & Chemical

GA 877YH

UT ISI:000225611500003

AU Le Padellec, A

TI Partial near threshold cross sections for the associative ionization to form CO<sup>+</sup>, NO<sup>+</sup> and O<sup>-2(+)</sup>

SO PHYSICA SCRIPTA

LA English

DT Article

ID DISSOCIATIVE RECOMBINATION; SHOCK WAVES; EXCITATION; CLOUDS; STATES; ATOMS; AIR

AB The paper describes a model based on the detailed balance principle that was further applied to extract the near threshold cross sections for the associative ionization along C + O, N + O and O + O. with reactants in various combinations of electronic excitation. When available, comparison was achieved with theoretical and/or experimental results, and the agreement is found excellent in several cases.

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NR 25

TC 0

PU ROYAL SWEDISH ACAD SCIENCES

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J9 PHYS SCR

JI Phys. Scr.

PD JUN

PY 2005

VL 71

IS 6

BP 621

EP 626

PG 6

SC Physics, Multidisciplinary

GA 939QK

UT ISI:000230087300008

AU Mezdari, F, Wohrer-Beroff, K, Chabot, M, Martinet, G, Della Negra, S, Desesquelles, P, Hamrita, H, Le Padellec, A

TI Ionization cross sections of small cationic carbon clusters in high-energy collisions with helium atoms and stability of multiply charged species

SO PHYSICAL REVIEW A

LA English

DT Article

ID MODEL-CALCULATIONS; ELECTRON-CAPTURE; MOLECULAR-IONS; GAS-PHASE; FRAGMENTATION; IMPACT; C-60; TOOL

AB Single, double, triple, and quadruple ionization cross sections of small cationic carbon clusters  $C_n^{(+)}$  colliding with helium atoms at a fixed velocity (2.6 atomic units) have been measured. The size ranges from  $n=1$  to  $n=10$  for single to triple ionization, from  $n=5$  to  $n=10$  for the quadruple ionization. The dependence of the cross sections with the cluster size is found to be well reproduced by predictions of the independent atom and electron (IAE) collision model. This extends the applicability of this simple model to higher  $n$  values and to a higher ionization degree than previously done [M. Chabot, Eur. Phys. J. D 14, 5 (2001)]. The branching ratios of multiply charged  $C_n^{(q+)}$  clusters remaining intact over a 100 ns time window have been measured ( $n=3-10$ ,  $q=2-3$ ). Branching ratios of nonfragmented doubly charged clusters have been interpreted on the basis of calculated internal energies of  $C_n^{(2+)}$  due to single ionization of  $C_n^{(+)}$  clusters using the IAE model. This allowed estimates of the minimum energies required to fragment these  $C_n^{(2+)}$  species to be derived.

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RP Mezdari, F, Univ Paris 11, LCAM, UMR, Collis Atom & Mol Lab, Batiment 351, F-91405 Orsay, France.

NR 46

TC 0

PU AMERICAN PHYSICAL SOC

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J9 PHYS REV A

JI Phys. Rev. A

PD SEP

PY 2005

VL 72

IS 3

AR 032707

DI ARTN 032707

PG 7

SC Physics, Atomic, Molecular & Chemical; Optics

GA 969IR

UT ISI:000232228300087



AU Le Padellec, A, Staicu-Casagrande, EM, Nzeyimana, T, Naji, EA, Urbain, X

TI Reactive collisions between CH<sup>+</sup> and O<sup>-</sup>

JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID FREQUENCY LASER SPECTROSCOPY; DISSOCIATIVE RECOMBINATION;  
RADIATIVE, LIFETIMES; CHEMI-IONIZATION; MERGED-BEAM; MOLECULAR  
CLOUDS; FUNDAMENTAL-BAND; CROSS-SECTION; STATES; HCO<sup>+</sup>

AB Integral cross sections were measured for two reactions occurring in CH<sup>++</sup>O<sup>-</sup> collisions: the formation of the carbon monoxide cation CO<sup>+</sup> via a reactive ionization process and the formation of the (iso)formyl cation HCO<sup>+</sup> (HOC<sup>+</sup>) via the associative ionization process. Both carbon monoxide and formyl cations are present in the interstellar medium, the latter one being quite abundant in dense clouds. Provided the oxygen anion would also be present in the interstellar environment, the large efficiency of the two reactive processes reported here would justify their inclusion in astrochemical models. The whole set of data was obtained by means of a merged-beam setup operating with keV beams. (c) 2006 American Institute of Physics.

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NR 41

TC 0

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J9 J CHEM PHYS

J1 J. Chem. Phys.

PD APR 21

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VL 124

IS 15

AR 154304

DI ARTN 154304

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SC Physics, Atomic, Molecular & Chemical

GA 034ZN

UT ISI:000236969500013

AU Diaz-Tendero, S, Sanchez, G, Alcami, M, Martin, 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, 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 Q, 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-n with  $5 \leq n \leq 9$  formed by electron capture in high velocity C-n(+)-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, energy distribution centered at around 10 eV (C) 2006 Elsevier B.V All rights reserved.

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NR 34

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J9 INT J MASS SPECTROM

J1 Int. J. Mass Spectrom.

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PY 2006

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IS 2

BP 126

EP 132

PG 7

SC Physics, Atomic, Molecular & Chemical; Spectroscopy

GA 045UV

UT ISI:000237768900007

AU Chabot, M, Martinet, G, Mezdari, F, Diaz-Tendero, S, Beroff-Wohrer, K, Desesquelles, P, Della-Negra, S, Hamrita, H, Le Padellec, A, Tuna, T, Montagnon, L, Barat, M, Simon, M, Ismail, I  
TI Charge transfer in high velocity C-n(+)+He collisions

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID CLUSTER-ATOM COLLISIONS; ELECTRONIC-ABSORPTION-SPECTRA; CARBON CLUSTERS; NEON MATRICES; LINEAR C-6; FRAGMENTATION; CAPTURE; SPECTROSCOPY; CHAINS

AB Dissociative and non-dissociative charge transfer cross sections in high velocity ( $v = 2.6$  au) collisions between ionic carbon clusters C-n(+) ( $n = 2-10$ ) and helium atoms have been measured. The sum of the cross sections has been found to increase significantly with n. Measurements of branching ratios for all fragmentation channels of excited C-n clusters are reported. The summed branching ratios associated with a given number of emitted fragments exhibit odd-even alternations reflecting the higher stability of the species having an odd number of atoms. From an analysis of the summed branching ratios within the statistical microcanonical metropolis Monte Carlo model, and knowing the temperature of the incident clusters, deposited energy distributions due to the charge transfer process are deduced ( $n = 5-9$ ). These distributions, of similar characteristics whatever n, peak around 4-5 eV and exhibit a large percentage of superexcited states situated above the continuum.

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NR 32

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PU IOP PUBLISHING LTD

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J9 J PHYS-B-AT MOL OPT PHYS

J1 J. Phys. B-At. Mol. Opt. Phys.

PD JUN 14

PY 2006

VL 39

IS 11

BP 2593

EP 2603

PG 11

SC Physics, Atomic, Molecular & Chemical; Optics

GA 054LP

UT ISI:000238378500026

AU Moretto-Capelle, P, Le Padellec, A  
AF Moretto-Capelle, Patrick, Le Padellec, Arnaud  
TI Electron spectroscopy in proton collisions with dry gas-phase uracil base  
SO PHYSICAL REVIEW A  
LA English  
DT Article  
ID MONTE-CARLO-SIMULATION; CROSS-SECTIONS; STRAND BREAKS; DNA;  
MOLECULES; RADIATION; PHOTOABSORPTION; IONIZATION; EFFICIENCY;  
ABSOLUTE  
AB We have investigated the electron emission by the RNA uracil base (C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>O<sub>2</sub>) due to collisions with protons in the 25 keV-100 keV energy range. Electron spectroscopy was performed at 35 degrees with respect to the beam direction and absolute values for the double-differential cross section were obtained. Our results show preferential emission of low-energy electrons that are responsible for damage in biological material through dissociative electron attachment [Boudaiffa , Science 287, 1658 (2000)]. Experimental results are compared to calculations that used the classical trajectory Monte Carlo method, and a reasonable agreement is obtained.  
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NR 31  
TC 0  
PU AMERICAN 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 DEC  
PY 2006  
VL 74  
IS 6  
AR 062705  
DI ARTN 062705  
PG 5  
SC Optics; Physics, Atomic, Molecular & Chemical  
GA 121OK  
UT ISI:000243166700073

AU Moretto-Capelle, P, Le Padellec, A, Briere, G, Massou, S, Franceries, F  
AF Moretto-Capelle, Patrick, Le Padellec, Arnaud, Briere, Guillaume, Massou, Sophie, Franceries, Frederic

TI Energetics and metastability of the adenine dication observed in proton-adenine collisions  
SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID ELECTRONIC-STRUCTURE; CROSS-SECTIONS; FRAGMENTATION; IONS; C-60; MOLECULES; THERAPY; SPACE

AB We present here a study that deals with the correlated fragmentation of a doubly charged adenine molecular target induced by a 100 keV proton beam. We have elucidated part of the dissociation dynamics for several channels and have obtained the corresponding kinetic energy released values. We have extracted activation energies by combining our experimental data with computations using the ab initio GAMESS code. We have observed metastability patterns against fragmentation, for which we have extracted the temporal mechanism (one or two steps). Subsequently, we have obtained lifetimes in the 100-200 ns range. In the simplest case of two-body fragmentation with the emission of mass 28, the determination of transition states and reaction paths has showed that emission of the H-C-N-H fragment is preferred to that of C-N-H-2. From the calculated activation barriers and lifetimes, we have deduced an equivalent temperature of the dication that we have compared with the existing models. (c) 2007 American Institute of Physics.

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TC 0

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J9 J CHEM PHYS

JI J. Chem. Phys.

PD DEC 21

PY 2007

VL 127

IS 23

AR 234311

DI ARTN 234311

PG 7

SC Physics, Atomic, Molecular & Chemical

GA 245BD

UT ISI:000251908500019

AU Tuna, T, Chabot, M, Pino, T, Desesquelles, P, Le Padellec, A, Martinet, G, Barat, M, Lucas, B, Mezdari, F, Montagnon, L, Van-Oanh, NT, Lavergne, L, Lachaize, A, Carpentier, Y, Beroff, K  
AF Tuna, T., Chabot, M., Pino, T., Desesquelles, P., Le Padellec, A., Martinet, G., Barat, M., Lucas, B., Mezdari, F., Montagnon, L., Van-Oanh, N. T., Lavergne, L., Lachaize, A., Carpentier, Y., Beroff, K.

TI Fragmentation branching ratios of highly excited hydrocarbon molecules C<sub>n</sub>H and their cations C<sub>n</sub>H<sup>+</sup> (n ≤ 4)

SO JOURNAL OF CHEMICAL PHYSICS

LA English

DT Article

ID SMALL CARBON CLUSTERS; DISSOCIATIVE RECOMBINATION; CROSS-SECTIONS; AB-INITIO; ASTRONOMICAL IDENTIFICATION; ELECTRONIC-SPECTRA; MODEL-CALCULATIONS; ATOM COLLISIONS; LYING STATES; IONIZATION

AB We have measured fragmentation branching ratios of neutral C<sub>n</sub>H and C<sub>n</sub>H<sup>+</sup> cations produced in high velocity (4.5 a.u) collisions between incident C<sub>n</sub>H<sup>+</sup> cations and helium atoms. Electron capture gives rise to excited neutral species C<sub>n</sub>H and electronic excitation to excited cations C<sub>n</sub>H<sup>+</sup>. Thanks to a dedicated setup, based on coincident detection of all fragments, the dissociations of the neutral and cationic parents were recorded separately and in a complete way. For the fragmentation of C<sub>n</sub>H, the H-loss channel is found to be dominant, as already observed by other authors. By contrast, the H-loss and C-loss channels equally dominate the two-fragment break up of C<sub>n</sub>H<sup>+</sup> species. For these cations, we provide the first fragmentation data (n > 2). Results are also discussed in the context of astrochemistry. (c) 2008 American Institute of Physics.

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NR 78

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J9 J CHEM PHYS

JI J. Chem. Phys.

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SC Physics, Atomic, Molecular & Chemical

GA 281ZK

UT ISI:000254537200025

AU Le Padellec, A, Lievin, J, Staicu-Casagrande, EM, Nzeyimana, T, Naji, EA, Urbain, X  
AF Le Padellec, A., Lievin, J., Staicu-Casagrande, E. M., Nzeyimana, T., Naji, E. A., Urbain, X.  
TI Competitive processes in the associative ionization of C<sup>-</sup> with C<sup>+</sup>, N<sup>+</sup>, and O<sup>+</sup>  
SO PHYSICAL REVIEW A

LA English

DT Article

DE ab initio calculations; associative ionisation; atom-ion reactions; carbon; negative ions; nitrogen; oxygen; positive ions; potential energy surfaces; reaction rate constants

ID ELECTRON-IMPACT; TRANSITION-PROBABILITIES; EXCITED-STATES; MERGED BEAM; BASIS-SETS; AB-INITIO; ION; C-2; SPECTROSCOPY; SPECTRUM

AB Absolute integral cross sections have been measured for associative ionization reactions involving the C<sup>-</sup> and C<sup>+</sup>, N<sup>+</sup>, and O<sup>+</sup> reactants. These measurements, obtained using a merged-beam setup in the keV range, provide us with useful experimental information on the efficiency and mechanisms of molecular ion formation from ionic reactants. The relative magnitudes of the different cross sections are rationalized by considering the spin multiplicities of initial and final states, and the exothermicities of the detachment and transfer ionization channels. The very different production efficiencies of CO<sup>+</sup> ions via the O<sup>-</sup>+C<sup>+</sup> and C<sup>-</sup>+O<sup>+</sup> channels are explained by statistical and energetic considerations. The potential energy curves of CO and CO<sup>+</sup> have been calculated by quantum ab initio methods in order to characterize the reactive pathways leading to autoionization. Thermal rate coefficients are derived to serve the plasma physics community.

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FU Belgian National Fund for Scientific Research ; Euratom-Belgian state association ; Action de Recherches Concertees de la Communauté

FX This work was funded by the Belgian National Fund for Scientific Research (F.R.S.-FNRS) and the Euratom-Belgian state association. J. L. thanks the " Action de Recherches Concertees de la Communaut fran aise de Belgique" for financial support. The authors would also like to thank Professon Colin Marsden for valuable comments on the manuscript.

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J9 PHYS REV A

JI Phys. Rev. A

PD DEC

PY 2008

VL 78

IS 6

PN Part A

AR 062705

DI 10.1103/PhysRevA.78.062705

PG 7

SC Optics; Physics, Atomic, Molecular & Chemical

GA 391OK  
UT ISI:000262242400096



AU Pellion, D, Jradi, K, Le Padellec, A, Rennane, A, Moutier, F, Borrel, V, Esteve, D, Magenc, C, Bazer-Bachi, AR

AF Pellion, D., Jradi, K., Le Padellec, A., Rennane, A., Moutier, F., Borrel, V., Esteve, D., Magenc, C., Bazer-Bachi, A. R.

TI Geiger avalanche photodiodes as tentative light detectors for VHE gamma ray astronomy  
SO EXPERIMENTAL ASTRONOMY

LA English

DT Article

DE SiPM; Cerenkov astronomy

ID TELESCOPE OBSERVATIONS; CERENKOV TELESCOPE; CRAB-NEBULA; FLUX

AB Due to its sensitivity and speed, the detector still widely used in Cerenkov astrophysics experiments remains the PhotoMultiplier Tube (PMT). For instance, recent pathbreaking experiments in Very High Energy astrophysics (VHE), such as MAGIC and HESS, have used mainstream PMT technology [Aharonian, F. et al *Astron. Astrophys.* 492(1):L25-L28 (2008)]. Moreover the Cerenkov Telescope Array (CTA) which is now in its design phase, is also planned to be based on PMT's. However, there are some disadvantages to the PMT technology: the rather poor quantum efficiency, the use of high voltages, the high cost when used in large number in a matrix arrangement and the large weight. Hence, we have investigated the possibility to design future Cerenkov telescopes based on solid state technology, specifically Geiger avalanche photodiodes. In a preliminary development test, we placed HAMAMATSU avalanche photodiodes at the focal plane of a 60 cm diameter telescope at the Pic du Midi in the French Pyr,n,es, in order to record incident cosmic rays. In this paper, we describe not only the experimental setup but we also put special emphasis to the reduction of the semi-conductor noise. We also show first data that were recorded during two runs in the fall of 2006, and conclude by the presentation of the design of an "integrated, low-cost solid state photodiode arrangement" which might be an alternative to PMT's for future VHE telescopes.

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J9 EXP ASTRON

JI Exp. Astron.

PD MAR

PY 2010

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PG 9  
SC Astronomy & Astrophysics  
GA 553RX  
UT ISI:000274385600004

AU Chabot, M, Tuna, T, Beroff, K, Pino, T, Le Padellec, A, Desequelles, P, Martinet, G, Nguyen-Thi, VO, Carpentier, Y, Le Petit, F, Roueff, E, Wakelam, V

AF Chabot, M., Tuna, T., Beroff, K., Pino, T., Le Padellec, A., Desequelles, P., Martinet, G., Nguyen-Thi, V.O., Carpentier, Y., Le Petit, F., Roueff, E., Wakelam, V.

TI Statistical universal branching ratios for cosmic ray dissociation, photodissociation, and dissociative recombination of the C<sub>n</sub>=2-10, C<sub>n</sub>=2-4H and C<sub>3</sub>H<sub>2</sub> neutral and cationic species

SO ASTRONOMY & ASTROPHYSICS

LA English

DT Article

DE astrochemistry; molecular data; ISM: clouds; photon-dominated region (PDR)

ID DENSE INTERSTELLAR CLOUDS; CARBON-CHAIN MOLECULES; GAS-PHASE PRODUCTION; COMPLEX HYDROCARBONS; CHEMICAL-MODELS; CROSS SECTIONS; ZETA-OPHIUCHI; CLUSTER IONS; CHEMISTRY; C-3

AB Context. Fragmentation-branching ratios of electronically excited molecular species are of first importance for the modeling of gas phase interstellar chemistry. Despite experimental and theoretical efforts that have been done during the last two decades there is still a strong lack of detailed information on those quantities for many molecules such as C-*n*, C<sub>*n*</sub>H or C<sub>3</sub>H<sub>2</sub>. Aims. Our aim is to provide astrochemical databases with more realistic branching ratios for C-*n* (*n* = 2 to 10), C<sub>*n*</sub>H (*n* = 2 to 4), and C<sub>3</sub>H<sub>2</sub> molecules that are electronically excited either by dissociative recombination, photodissociation, or cosmic ray processes, when no

detailed calculations or measurements exist in literature. Methods. High velocity collision in an inverse kinematics scheme was used to measure the complete fragmentation pattern of electronically excited C-*n* (*n* = 2 to 10), C<sub>*n*</sub>H (*n* = 2 to 4), and C<sub>3</sub>H<sub>2</sub> molecules. Branching ratios of dissociation were deduced from those experiments. The full set of branching ratios was used as a new input in chemical models and branching ratio modification effects observed in astrochemical networks that describe the dense cold Taurus Molecular Cloud-1 and the photon dominated Horse Head region. Results. The comparison between the branching ratios obtained in this work and other types of experiments showed a good agreement. It was interpreted as the signature of a statistical behavior of the fragmentation. The branching ratios we obtained lead to an increase of the C-3 production together with a larger dispersion of the daughter fragments. The introduction of these new values in the photon dominated region model of the Horse Head nebula increases the abundance of C-3 and C<sub>3</sub>H, but reduces the abundances of the larger C-*n* and hydrocarbons at a visual extinction *A<sub>V</sub>* smaller than 4. Conclusions. We recommend astrochemists to use these new branching ratios. The data published here have been added to the online database KIDA (KInetic Database for Astrochemistry, <http://kida.obs.u-bordeaux1.fr>).

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PPF Matière Carbonée of the University Paris Sud 11 are acknowledged for their financial  
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PU EDP SCIENCES S A

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J9 ASTRON ASTROPHYS

JI Astron. Astrophys.

PD DEC

PY 2010

VL 524

AR A39

DI 10.1051/0004-6361/201015010

PG 9

SC Astronomy & Astrophysics

GA 685JP

UT ISI:000284625300052

AU Jradi, K, Pellion, D, Esteve, D, Boizard, JL, Le Padellec, A, Bazer-Bachi, AR  
AF Jradi, K., Pellion, D., Esteve, D., Boizard, J. -L., Le Padellec, A., Bazer-Bachi, A.R.  
TI Computer-aided design (CAD) model for silicon avalanche Geiger mode systems design:  
Application to high sensitivity imaging systems

SO NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-  
ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT

LA English

DT Article

DE APD-Geiger; Noise; VHDL-AMS; Modeling

ID SIPM

AB Our consortium CESR-LAAS in Toulouse has developed generic technology for Geiger-APD and SiPM. The main feature of these devices is the high homogeneity in breakdown voltage. The work presented here describes the model that has been used to design these devices. This also includes the integration into micro-systems, with the ambition in the long term, to develop multiple applications in astrophysics, biology, optical sensing, and above all, imaging systems. The paper is divided as follows: 1. An introduction presents the main issues in the physics of silicon avalanche Geiger mode systems. 2. A section (Geiger mode) divided into two parts. The first part is devoted to the electrical model of the basic device, which provides the response of the Geiger-APD to an incident photon: gain, current, and voltage. The second part presents the production of the model using Simplorer simulation software under VHDL-AMS (VHSIC-Very High Speed Integrated Circuit-Hardware Description Language Analog and Mixed Signal) [1]. 3. A comparison between our model and that used by Otono et al. [5] followed by a discussion with a special emphasis on presenting the noise model based on the real component made and tested by our consortium. 4. A conclusion. (C) 2010 Elsevier B.V. All rights reserved.

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TI Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase

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ID DENSITY-FUNCTIONAL THEORY; BIOLOGICALLY RELEVANT MOLECULES; IONIZATION; COLLISIONS; PROTONS

AB A combination of time-dependent density functional theory and Born-Oppenheimer molecular dynamics methods is used to investigate fragmentation of doubly charged gas-phase uracil in collisions with 100 keV protons. The results are in good agreement with ion-ion coincidence measurements. Orbitals of similar energy and/or localized in similar bonds lead to very different fragmentation patterns, thus showing the importance of intramolecular chemical environment. In general, the observed fragments do not correspond to the energetically most favorable dissociation path, which is due to dynamical effects occurring in the first few femtoseconds after electron removal.

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CA CTA Consortium

TI Design concepts for the Cherenkov Telescope Array CTA: an advanced facility for ground-based high-energy gamma-ray astronomy

SO EXPERIMENTAL ASTRONOMY

LA English

DT Article

DE Ground based gamma ray astronomy; Next generation Cherenkov telescopes; Design concepts

# ID INDUCED AIR-SHOWERS; MAGIC TELESCOPE; COSMIC-RAYS; OPTICAL-SYSTEM; 1ST DETECTION; RADIATION; TEV; BURSTS; SIMULATION; PARTICLES

AB Ground-based gamma-ray astronomy has had a major breakthrough with the impressive results obtained using systems of imaging atmospheric Cherenkov telescopes. Ground-based gamma-ray astronomy has a huge potential in astrophysics, particle physics and cosmology. CTA is an international initiative to build the next generation instrument, with a factor of 5-10 improvement in sensitivity in the 100 GeV-10 TeV range and the extension to energies well below 100 GeV and above 100 TeV. CTA will consist of two arrays (one in the north, one in the south) for full sky coverage and will be operated as open observatory. The design of CTA is based on currently available technology. This document reports on the status and presents the major design concepts of CTA.

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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  $C(n)H(q+)$  ( $n \leq 4$ ,  $q \leq 9$ ) 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  $CH(q+)$  ( $q \leq 4$ ) 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 ( $q \geq 5$ ), 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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AU Cadu, A, Le Padellec, A, Jradi, K, Pellion, D, Bazer-Bachi, AR  
AF Cadu, A., Le Padellec, A., Jradi, K., Pellion, D., Bazer-Bachi, A. R.  
TI The use of silicon photomultipliers for very high energy gamma ray astronomy: the optical issues

SO EXPERIMENTAL ASTRONOMY

LA English

DT Article

DE G-APD; Optics; Microlenses; Cerenkov effect; VHE astronomy

ID ATMOSPHERIC CHERENKOV TELESCOPES; SYSTEM; TUBES

AB Due to its sensitivity and speed, the detector still widely used in Cerenkov astrophysics experiments remains the Photo-Multiplier Tube(PMT). However, there are some disadvantages to the PMT technology: the rather poor quantum efficiency, the use of high voltages, the high cost when used in large number in a matrix arrangement and a subsequent large weight. Hence, we have investigated the possibility to design future Cerenkov telescope cameras based on solid state technology, specifically Geiger Avalanche PhotoDiodes (G-APD's). This paper describes our extensive simulations to design the optical setup to be employed with G APD's. We also discuss the reflector configurations, pixel layouts, light concentrators, microlens arrays and spectral efficiencies to optimize light collection. The electronic aspects of our work were presented in a recent companion paper (Pellion et al., *Exp. Astron.* 27(3):187, 2010).

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TI Anion production in high-velocity cluster-atom collisions; the electron capture process revisited

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

ID HYDROGEN-ATOMS; CROSS-SECTIONS; FRAGMENTATION; EMISSION; GASES; IONS; HE

AB Anion production cross sections in collisions between C-n(+), C<sub>n</sub> carbon clusters (n ≤ 5) and helium atoms have been measured in high-velocity collisions (v = 2.25 and 2.6 au). This paper focuses on two of the three processes responsible for the C-n(-) production, namely double electron capture (DEC) onto C-n(+) cations and single electron capture onto neutral (SECN) C-n. They were experimentally distinguished from a gaseous thickness dependence study. Dissociative and non-dissociative cross sections were measured and, in the case of DEC, all dissociative branching ratios measured; for these small systems, the C-2(-) fragment was found magical. Data concerning electron capture in neutral-neutral collisions are extremely rare, especially at high velocity. Introduction of this measured process in the independent atom and electron (IAE) model allowed us to revisit and satisfactorily reproduce the so-far unexplained size evolution of single electron capture (SEC) cross sections in 2.6 au C-n(+)-He (n ≤ 10) collisions (Chabot et al 2006 J. Phys. B: At. Mol. Opt. Phys. 39 2593-603). IAE calculations for DEC cross sections and their comparison with experiment suggest a loss of electron in anionic C-n(-) species after the collision, competing with fragmentation and depending on the size.

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CA CTA Consortium

TI Introducing the CTA concept

SO ASTROPARTICLE PHYSICS

LA English

DT Editorial Material

DE TeV gamma-ray astronomy; Air showers; Cherenkov Telescopes

ID SUPERNOVA REMNANT W44; TELESCOPE; ASTRONOMY; EMISSION; MISSION; HESS

AB The Cherenkov Telescope Array (CTA) is a new observatory for very high-energy (VHE) gamma rays. CTA has ambitious science goals, for which it is necessary to achieve full-sky coverage, to improve the sensitivity by about an order of magnitude, to span about four decades of energy, from a few tens of GeV to above 100 TeV with enhanced angular and energy resolutions over existing VHE gamma-ray observatories. An international collaboration has formed with more than 1000 members from 27 countries in Europe, Asia, Africa and North and South America. In 2010 the CTA Consortium completed a Design Study and started a three-year Preparatory Phase which leads to production readiness of CTA in 2014. In this paper we introduce the science goals and the concept of CTA, and provide an overview of the project. (C) 2013 Elsevier B.V. All rights reserved.

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TI Time-dependent density functional theory molecular dynamics simulation of doubly charged uracil in gas phase

SO CENTRAL EUROPEAN JOURNAL OF PHYSICS

LA English

DT Article

DE uracil; proton collision; nonadiabatic dynamics; biological damage

ID BIOLOGICALLY RELEVANT MOLECULES; ELECTRONIC-STRUCTURE; AQUEOUS-SOLUTION; LIQUID WATER; FRAGMENTATION; MECHANISMS; COLLISIONS; RADIATION; RADICALS; DAMAGE

AB We use time-dependent density functional theory and Born-Oppenheimer molecular dynamics methods to investigate the fragmentation of doubly ionized uracil in gas phase. Different initial electronic excited states of the dication are obtained by removing electrons from different inner-shell orbitals of the neutral species. We show that shape-equivalent orbitals lead to very different fragmentation patterns revealing the importance of the intramolecular chemical environment. The results are in good agreement with ion-ion coincidence measurements of uracil collision with 100 keV protons.

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TI Ion-pair dissociation of highly excited carbon clusters: Size and charge effects

SO PHYSICAL REVIEW A

LA English

DT Article

ID POLYATOMIC-MOLECULES; ENERGY-DISTRIBUTION; FRAGMENTATION; COLLISIONS; SPECTROSCOPY; IONIZATION; EXCITATION; STABILITY; DYNAMICS

AB We present measurements of ion-pair dissociation (IPD) of highly excited neutral and ionized carbon clusters  $C_{n=2-5}(q=0-3)^+$ . The tool for producing these species was a high-velocity collision between  $C_{n(+)}$  projectiles ( $v = 2.25$  a. u.) and helium atoms. The setup allowed us to detect in coincidence anionic and cationic fragments, event by event, leading to a direct and unambiguous identification of the IPD process. Compared with dissociation without anion emission, we found typical  $10^{-4}$  IPD rates, not depending much on the size and charge of the  $(n, q)$  species. Exceptions were observed for  $C_{2(+)}$  and, to a lesser extent,  $C_{4(3+)}$  whose IPDs were notably lower. We tentatively interpret IPDs of  $C_{2(+)}$  and  $C_{3(+)}$  by using a statistical approach based on the counting of final states allowed by energetic criteria. The model is able to furnish the right order of magnitude for the experimental IPD rates and to provide a qualitative explanation of the lower IPD rate observed in  $C_{2(+)}$ .

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TI Investigation of critical parameters controlling the efficiency of associative ionization

SO JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS

LA English

DT Article

DE ion-ion collisions; associative ionization; astrochemistry

ID MERGED-BEAM MEASUREMENTS; H+-H-COLLISIONS; MUTUAL NEUTRALIZATION; DISSOCIATIVE RECOMBINATION; CROSS-SECTIONS; REACTIVE COLLISIONS; MOLECULAR-HYDROGEN; CHEMI-IONIZATION; SLOW COLLISIONS; LOW-ENERGY

AB This paper compiles our merged-beam experimental findings for the associative ionization (AI) process from charged reactants, with the aim of guiding future investigations with e.g. the double electrostatic ion storage ring DESIREE in Stockholm. A reinvestigation of the isotopic effect in H-(D-) + He+ collisions is presented, along with a review of H-3(+) and NO+ production by AI involving ion pairs or excited neutrals, and put in perspective with the mutual neutralization and radiative association reactions. Critical parameters are identified and evaluated for their systematic role in controlling the magnitude of the cross section: isotopic substitution, exothermicity, electronic state density, and spin statistics.

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