

III. PRODUCTION SCIENTIFIQUE

Publications

107 publications parues ou acceptées dont 92 dans des revues internationales à comité de lecture, 2 chapitres de livres, 6 articles de revue, 7 comptes-rendus de conférences internationales (autres que résumés).

Édition d'un livre.

Publications dans des revues internationales à comité de lecture

1 - Time-resolved study of intramolecular vibrational redistribution in p-difluorobenzene,

N. Halberstadt et A. Tramer, J. Chem. Phys. **73**, 6343 (1980).

2 - Photodissociation of Van der Waals molecules: adiabatic treatment,

N. Halberstadt et J.A. Beswick, Faraday Discuss. Chem. Soc. **73**, 357 (1982).

3 - Vibrational predissociation decay channels for glyoxal complexes,

N. Halberstadt et B. Soep, Chem. Phys. Lett. **87**, 109 (1982).

4 - Isotope effect in the vibrational predissociation of Van der Waals molecules: complexes of glyoxal with H₂ and D₂,

J.A. Beswick, N. Halberstadt, C. Jouvet et B. Soep, Laser Chem. **1**, 77 (1982).

5 - From selective to non-selective vibrational predissociation in glyoxal Van der Waals complexes,

N. Halberstadt et B. Soep, Laser Chem. **2**, 115 (1983).

6 - Vibrational predissociation in Van der Waals complexes of glyoxal with Ar and Kr,

N. Halberstadt et B. Soep, J. Chem. Phys. **80**, 2340 (1984).

7 - Infrared absorption and predissociation of NO dimer,

Ph. Bréchignac, S. De Benedictis, N. Halberstadt, B. J. Whitaker et S. Avrillie, J. Chem. Phys. **83**, 2064 (1985).

8 - Theory of mode specific vibrational predissociation: the HF dimer,

N. Halberstadt, Ph. Bréchignac, J.A. Beswick et M. Shapiro, J. Chem. Phys. **84**, 170 (1986).

9 - Performances of a pulsed tunable infrared Raman laser for spectroscopy,

Ph. Bréchignac, N. Halberstadt, S. De Benedictis et Nguyen Dai Hung, Revue de Physique Appliquée, **21**, 735 (1986).

10 - Three-dimensional quantum mechanical study of Ne...Cl₂ vibrational predissociation

N. Halberstadt, J.A. Beswick et K.C. Janda, J. Chem. Phys. **87**, 3966 (1987).

11 - Infrared predissociation of (NO)₂: Rotational distribution of the fragments,

Ph. Bréchignac, N. Halberstadt, B. J. Whitaker et B. Coutant, Chem. Phys. Letters **142**, 125 (1987).

12 - Vibrational and Rotational Wave Functions for the Triatomic Van der Waals Molecules HeCl₂, NeCl₂, and ArCl₂,

B. P. Reid, K.C. Janda et N. Halberstadt, J. Phys. Chem. **92**, 587 (1988).

- 13 - State-to-State Vibrational Predissociation Dynamics and Spectroscopy of He...Cl₂: Experiment and Theory,**
J.I. Cline, B.P. Reid, D.D. Evard, N. Sivakumar, N. Halberstadt et K.C. Janda, *J. Chem. Phys.* **89**, 3535 (1988).
- 14 - Decay of Vibrationally Excited States of the Ne...Cl₂ Complex,**
N. Halberstadt, O. Roncero et J.A. Beswick, *Chem. Phys.* **129**, 83 (1989).
- 15 - A theoretical study of the Ar₂HCl Van der Waals cluster,**
J.M. Hutson, N. Halberstadt et J.A. Beswick, *J. Chem. Phys.* **90**, 1337 (1989).
- 16 - Product State Distributions for the Vibrational Predissociation of Ne-Cl₂**
J.I. Cline, N. Sivakumar, D.D. Evard, C.R. Bieler, N. Halberstadt, B.P. Reid, S. Hair et K.C. Janda, *J. Chem. Phys.* **90**, 2605 (1989).
- 17 - Photofragmentation of the Ne...ICl complex: A three-dimensional quantum mechanical study**
O. Roncero, J.A. Beswick, N. Halberstadt, P. Villarreal et G. Delgado-Barrio, *J. Chem. Phys.* **92**, 3348 (1990).
- 18 - Quantum dynamical calculations for the vibrational predissociation of the He...ICl complex: Product rotational distribution**
R.L. Waterland, M.I. Lester et N. Halberstadt, *J. Chem. Phys.* **92**, 4261 (1990).
- 19 - A wave packet Golden Rule treatment of vibrational predissociation**
P. Villarreal, S. Miret-Artés, O. Roncero, G. Delgado-Barrio, J.A. Beswick, N. Halberstadt et R.D. Coalson, *J. Chem. Phys.* **94**, 4230 (1991).
- 20 - Intramolecular vibrational relaxation in a triatomic Van der Waals molecule: Ar...Cl₂**
N. Halberstadt, J.A. Beswick, O. Roncero et K.C. Janda, *J. Chem. Phys.* **96**, 2404 (1992).
- 21 - Consequences of electronic-state mixing on the dynamics of photodissociation of H₂ by barrier tunneling**
L.D.A. Siebbeles, J.M. Schins, W.J. van der Zande, J.A. Beswick et N. Halberstadt, *Phys. Rev. A* **45**, 4481 (1992).
- 22 - Vibrational predissociation of Ar...Cl₂ complex: the small molecule limit for intramolecular vibrational relaxation**
N. Halberstadt, S. Serna, O. Roncero et K.C. Janda, *J. Chem. Phys.* **97**, 341 (1992).
- 23 - A theoretical study of the HgAr₂ (³P₁ ← ¹S₀) vibronic spectrum**
J. Zúñiga, A. Bastida, A. Requena, N. Halberstadt et J.A. Beswick, *J. Chem. Phys.* **98**, 1007 (1993).
- 24 - Quantum calculation of vibrational states in the aniline-argon Van der Waals cluster**
P. Parneix, N. Halberstadt, Ph. Bréchignac, F. G. Amar, A. van der Avoird et J. W. I. van Bladel, *J. Chem. Phys.* **98**, 2709 (1993).
- 25 - Coherence effects between intramolecular vibrational relaxation and dissociation in triatomic van der Waals systems**
O. Roncero, P. Villarreal, G. Delgado-Barrio, N. Halberstadt et K.C. Janda, *J. Chem. Phys.* **99**, 1035 (1993).
- 26 - Vector correlations in the photo-predissociation of van der Waals molecules**
O. Roncero, P. Villarreal, G. Delgado-Barrio, N. Halberstadt et J.A. Beswick, *J. Phys. Chem.* **98**, 3307 (1994).
- 27 - Calculated rotational spectrum of Ar...CO from an ab initio potential energy**

surface: A very floppy Van der Waals molecule

V. Castells, N. Halberstadt, S. K. Shin, R. A. Beaudet, et C. Wittig, J. Chem. Phys. **101**, 1006 (1994).

28 - Calculation of the rovibrational $B \leftarrow X$ excitation spectrum of the He_2Cl_2 cluster

M. I. Hernández et N. Halberstadt, J. Chem. Phys. **100**, 7828 (1994) .

29 - Excited state dynamics in Hg-Ar_2 : Statistical analysis of vibrational state distribution

A. Bastida, J. Zúñiga, A. Requena, N. Halberstadt et J.A. Beswick, Faraday Discuss. **97**, "Structure and Dynamics of Van der Waals Complexes", p. 131, 1994.

30 - One-atom cage effect in $\text{I}_2\text{-Ar}$ complexes: can it be explained by linear ground-state isomers?

M. P. de Miranda, J.A. Beswick et N. Halberstadt, Chem. Phys. **187**, 185 (1994) .

31 - A wavepacket study of $\text{Ar}\cdots\text{I}_2(B) \rightarrow \text{Ar} + \text{I} + \text{I}$ electronic predissociation

O. Roncero, N. Halberstadt et J.A. Beswick, Chem. Phys. Lett. **226**, 82 (1994) .

32 - On the vibronic spectrum of small mercury-argon clusters

A. Bastida, J. Zúñiga, A. Requena, B. Soep, N. Halberstadt et J.A. Beswick, J. Chim. Phys. **92**, 384 (1995).

33 - Angular motion of molecular adsorbates influenced by surface coverage

P. Parneix, M. Büchner, G. Rašev et N. Halberstadt, Chem. Phys. Lett. **233**, 430 (1995).

34 - Fragmentation dynamics of the vibrationally excited ammonia-argon Van der Waals complex

J. Millán, N. Halberstadt, G. C. M. van der Sanden et A. van der Avoird, J. Chem. Phys. **103**, 4138 (1995).

35 - The He-Cl_2 potential: Atom-atom and *ab initio* compared to experiment

S. S. Huang, C. R. Bieler, K.C. Janda, F. M. Tao, W. Klemperer, P. Casavecchia, G. G. Volpi et N. Halberstadt, J. Chem. Phys. **102**, 8846 (1995).

36 - Electron impact ionization of small argon clusters

A. Bastida, N. Halberstadt, J.A. Beswick, F. X. Gadéa, U. Buck, R. Galonska et C. Lauenstein, Chem. Phys. Lett. **249**, 1 (1996).

37 - A 3-dimensional wavepacket study of $\text{Ar}\cdots\text{I}_2(B) \rightarrow \text{Ar} + \text{I} + \text{I}$ electronic predissociation

O. Roncero, N. Halberstadt et J.A. Beswick, J. Chem. Phys. **104**, 7554 (1996).

38 - Modeling the production and fragmentation of Ar_3^+ after threshold photon impact ionization of Ar_3

A. Bastida, N. Halberstadt, J.A. Beswick et F. X. Gadéa, J. Chem. Phys. **104**, 6907 (1996).

39 - High resolution spectroscopy of the $\text{He}^{79}\text{Br}_2$ Van der Waals molecule: An experimental and theoretical study

D. G. Jahn, W. S. Barney, J. Cabalo, S. G. Clement, A. Rohrbacher, T. J. Slotterback, J. Williams, K.C. Janda et N. Halberstadt, J. Chem. Phys. **104**, 3501 (1996).

40 - Vibrational predissociation of ArCl_2 : Toward the determination of the potential energy surface of the B state

K.C. Janda, O. Roncero et N. Halberstadt, J. Chem. Phys. **105**, 5830 (1996).

41 - *Ab initio* calculations of the interaction of He with the $B^3\Pi_{0u+}$ state of Cl_2 as a function of the Cl_2 internuclear separation

A. Rohrbacher, J. Williams, K.C. Janda, S. M. Cybulski, R. Burcl, M. M. Szczęśniak, G. Chałasinski

et N. Halberstadt, J. Chem. Phys. **106**, 2685 (1997).

42 - Vibrational predissociation of the ND₃-Ar Van der Waals complex: Comparison with NH₃-Ar

J. Millán, N. Halberstadt, G. C. M. van der Sanden et A. van der Avoird, J. Chem. Phys. **106**, 9141 (1997); *erratum*: J. Chem. Phys. **114**, 6487 (2001)

43 - From the sparse to the statistical limit of intramolecular vibrational redistribution in vibrational predissociation: ArCl₂ as an example

O. Roncero, D. Caloto, K.C. Janda et N. Halberstadt, J. Chem. Phys. **107**, 1406 (1997).

44 - Are rare-gas Cl₂ Van der Waals molecules linear or T-shaped?

J. Williams, A. Rohrbacher, D. Djahandideh, K.C. Janda, A. Jamka, F.-M. Tao et N. Halberstadt, Mol. Phys. **91**, 573 (1997).

45 - Application of Trajectory Surface Hopping to vibrational predissociation

A. Bastida, J. Zúñiga, A. Requena, I. Sola, N. Halberstadt et J.A. Beswick, Chem. Phys. Lett. **280**, 185 (1997).

46 - The resonant charge hopping rate in positively charged Helium clusters

N. Halberstadt et K.C. Janda, Chem. Phys. Lett. **282**, 409 (1998).

47 - Capture and ionization of argon within liquid helium droplets

B.E. Callicoat, K. Förde, T. Ruchti, L. Jung, K.C. Janda et N. Halberstadt, J. Chem. Phys. **108**, 9371 (1998).

48 - A hybrid classical/quantum approach to cluster fragmentation dynamics: Application to the vibrational predissociation of He₂Cl₂

M.I. Hernández, A. García-Vela, C. García-Rizo, N. Halberstadt, P. Villarreal et G. Delgado-Barrio, J. Chem. Phys. **108**, 1989 (1998).

49 - A theoretical study of photodissociation and geminate recombination of ICN in solid argon

S. Fernández-Alberti, N. Halberstadt, J.A. Beswick et J. Echave, J. Chem. Phys. **109**, 2844 (1998).

50 - Vibrational Predissociation Dynamics of I₂...Ne₂: A Trajectory Surface Hopping Study

A. Bastida, J. Zúñiga, A. Requena, N. Halberstadt et J.A. Beswick, J. Chem. Phys. **109**, 6320 (1998).

51 - Competition between electronic and vibrational predissociation in Ar-I₂(B): A molecular dynamics with quantum jumps calculation

A. Bastida, J. Zúñiga, A. Requena, N. Halberstadt et J.A. Beswick, Chem. Phys. **240**, 229 (1999).

52 - The B ← X spectrum of ArCl₂: Linear and perpendicular isomers

K.C. Janda, D. Djahandideh, O. Roncero et N. Halberstadt, Chem. Phys. **239**, 177 (1998).

53 - Time Dependent Wave Packet Study of the One-Atom Cage Effect in Ar-I₂ van der Waals Complexes

S. Zamith, C. Meier, N. Halberstadt et J.A. Beswick, J. Chem. Phys. **110**, 960 (1999).

54 - Short-time charge motion in He_n⁺ clusters

J. Seong, K.C. Janda, N. Halberstadt et F. Spiegelmann, J. Chem. Phys. **109**, 10873 (1998).

55 - Intramolecular vibrational redistribution and fragmentation dynamics of I₂...Ne_n (n=2-6) clusters

S. Fernández Alberti, N. Halberstadt, J.A. Beswick, A. Bastida, J. Zúñiga et A. Requena, J. Chem. Phys. **111**, 239 (1999).

56 - A three-dimensional potential energy surface for He + Cl₂ (*B* $^3\Pi_{0u+}$): *Ab initio* calculations and a multiproperty fit

J. Williams, A. Rohrbacher, J. Seong, N. Marianayagam, K.C. Janda, R. Burcl, M. M. Szcześniak, G. Chałasinski S. M. Cybulski et N. Halberstadt, *J. Chem. Phys.* **111**, 997 (1999).

57 - Hybrid quantum/classical simulation and kinetic study of the vibrational predissociation of Cl₂...Ne_n (*n* = 2, 3)

A. Bastida, B. Miguel, J. Zúñiga, A. Requena, N. Halberstadt et K.C. Janda, *J. Chem. Phys.* **111**, 4577 (1999).

58 - HeNe⁺: Resolution of an apparent disagreement between experiment and theory

J. Seong, K.C. Janda, M.P. McGrath et N. Halberstadt, *Chem. Phys. Lett.* **314**, 501 (1999).

59 - Quantum calculations on the vibrational predissociation of NeBr₂: Evidence for continuum resonances

T.A. Stephenson et N. Halberstadt, *J. Chem. Phys.* **112**, 2265 (2000).

60 - Mixed Quantum Classical Steps: a DVR hopping method

A. Bastida, J. Zúñiga, A. Requena, N. Halberstadt et J. A. Beswick, *Phys. Chem. Comm.* **7**, (2000).

61 - Hybrid Quantum/Classical Study of ICN in an Ar matrix: Photofragmentation and Cage Exit

S. Fernández-Alberti, J. Echave, N. Halberstadt, J.A. Beswick et V. Engel, *J. Chem. Phys.* **113**, 1027 (2000).

62 - Caging and excited state emission of ICN trapped in cryogenic matrices: experiment and theory

J. Helbing, M. Chergui, S. Fernández-Alberti, J. Echave, N. Halberstadt et J.A. Beswick, *Phys. Chem. Chem. Phys.* **2**, 4131 (2000).

63 - Structure and spectroscopy of the He₂Cl₂ Van der Waals cluster

M.I. Hernández, N. Halberstadt, W.D. Sands et K.C. Janda, *J. Chem. Phys.* **113**, 7252 (2000).

64 - Time evolution of reactants, intermediates, and products in the vibrational predissociation of Br₂...Ne: A theoretical study

B. Miguel, A. Bastida, J. Zúñiga, A. Requena et N. Halberstadt, *J. Chem. Phys.* **113**, 10130 (2000); *erratum*: *J. Chem. Phys.* **114**, 7713 (2001)

65 - Ab initio anharmonic intermolecular potential of the C₂H₂—HCl hydrogen bonded complex

P. Çarçabal, V. Brenner, N. Halberstadt et P. Millié, *Chem. Phys. Lett.* **336**, 335 (2001).

66 - Size evolution of the vibrational predissociation process in Br₂Ne_n clusters: Simulation and kinetic study

B. Miguel, A. Bastida, J. Zúñiga, A. Requena et N. Halberstadt, *Faraday Discuss.* **118**, 257 (2001).

67 - Vibrational predissociation dynamics of methane-Ar: an *ab initio* approach

M. Geleijns, N. Halberstadt, J. Millán, P.E.S. Wormer et A. van der Avoird, *Faraday Discuss.* **118**, 143 (2001).

68 - ArI₂(X) → Ar+I₂(B) photodissociation: Comparison between linear and T-shaped isomers dynamics

O. Roncero, B. Lepetit, J.A. Beswick, N. Halberstadt et A.A. Buchachenko, *J. Chem. Phys.* **115**, 6961 (2001).

69 - Molecular dynamics simulation of the I₂(X)...Ar isomers population in a free-

jet expansion: Thermodynamics versus kinetic control

A. Bastida, J. Zúñiga, A. Requena, B. Miguel, J.A. Beswick, J. Vigué et N. Halberstadt, J. Chem. Phys. **116**, 1944 (2002).

70 - Electronic and vibrational predissociation in ArI₂ photodissociation dynamics

B. Lepetit, O. Roncero, A.A. Buchachenko, et N. Halberstadt, J. Chem. Phys. **116**, 8367 (2002).

71 - Photodissociation of the methane-argon complex: Vibrational predissociation dynamics, spectral line widths and fragment state distributions

M. Geleijns, P.E.S. Wormer, A. van der Avoird et N. Halberstadt, J. Chem. Phys. **117**, 7562 (2002).

72 - Theoretical investigation of the temperature dependence of the O + O₂ exchange reaction

P. Fleurat-Lessard, S.Y. Grebenschchikov, R. Siebert, R. Schinke et N. Halberstadt, J. Chem. Phys. **118**, 610 (2003).

73 - Potential energy surfaces for He_nNe⁺ ions: *ab initio* and diatomics-in-molecules results

J. Seong, A. Rohrbacher, Z. R. Li, K. C. Janda, F. M. Tao, F. Spiegelmann, et N. Halberstadt, J. Chem. Phys. **120**, 7456 (2004).

74 - Fragmentation dynamics of ionized neon trimer inside helium nanodroplets: A theoretical study

D. Bonhommeau, A. Viel, et N. Halberstadt, J. Chem. Phys. **120**, 11359-11362 (2004).

75 - Dissociative ionization of neon clusters Ne_n, n = 3 to 14: A realistic multi-surface dynamical study

D. Bonhommeau, A. Viel, et N. Halberstadt, J. Chem. Phys., **123**, 054316 (2005).

76 - Structure and stability of (NeHe_n)⁺: Experiment and diffusion Quantum Monte Carlo theory with "on the fly" electronic structure

C. A. Brindle, M. R. Prado, Kenneth C. Janda, N. Halberstadt, et M. Lewerenz, J. Chem. Phys. **123**, 064312 (2005).

77 - Fragmentation dynamics of ionized neon clusters (Ne_n, n = 3 to 14) embedded in helium nanodroplets

D. Bonhommeau, A. Viel, et N. Halberstadt, J. Chem. Phys. **124**, 024328 (2006).

78 - Modelization of the Fragmentation dynamics of krypton clusters (Kr_n, n = 2 to 11) after electron-impact ionization

D. Bonhommeau, Th. Bouissou, N. Halberstadt, et A. Viel J. Chem. Phys. **124**, 164308 (2006).

79 - Fragmentation dynamics of argon clusters (Ar_n, n = 2 to 11) after electron-impact ionization Modelization and comparison with experiment

D. Bonhommeau, N. Halberstadt, et A. Viel, J. Chem. Phys. **124**, 184314 (2006).

80 - Modelling the fragmentation dynamics of ionic clusters inside helium nanodroplets: the case of He₁₀₀Ne₄⁺

D. Bonhommeau, P. T. Lake Jr., C. Le Quiniou, M. Lewerenz et N. Halberstadt, J. Chem. Phys. **126**, 051104 (2007).

81 - Two Dimensional H₂O-Cl₂ and H₂O-Br₂ potential surfaces: an ab initio study of ground and valence excited electronic states

R. Hernández-Lamoneda, V.H. Uc Rosas, M.I. Bernal-Uruchurtu, N. Halberstadt et K.C. Janda, J. Phys. Chem. A **112**, 89 (2008).

82 - Fragmentation of ionized doped helium nanodroplets: Theoretical evidence for a dopant ejection mechanism

D. Bonhommeau, M. Lewerenz et N. Halberstadt, J. Chem. Phys. **128**, 054302 (2008).

83 - Fragmentation of size-selected Xe clusters: Why does the monomer ion channel dominate the Xe_n and Kr_n ionization?

V. Poterya, M. Fárník, U. Buck, D. Bonhommeau et N. Halberstadt, Int. J. Mass Spec. **280**, 78-84 (2009).

84 - An *ab initio* calculation of the valence excitation spectrum of $\text{H}_2\text{O}\cdots\text{Cl}_2$: Comparison to condensed phase spectra

R. Franklin-Mergarejo, J. Rubayo-Soneira, N. Halberstadt, T. Ayed, M.I. Bernal Uruchurtu, R. Hernández-Lamoneda, et K.C. Janda, J. Phys. Chem. A **113**, 7563-7569 (2009).

85 - Vibrational dynamics of the He_2Ne^+ cation

J. Zúñiga, A. Bastida, A. Requena, N. Halberstadt, J.A. Beswick et K.C. Janda, J. Phys. Chem. A **113**, 14896-14903 (2009).

86 - Solvation dynamics through Raman spectroscopy: Hydration of Br_2 and Br_3^- , and solvation of Br_2 in liquid bromine

E. Branigan, N. Halberstadt, et V. Apkarian, J. Chem. Phys. **134**, 174503 (2011).

87 - Large shift and small broadening of Br_2 valence band upon dimer formation with H_2O : An *ab initio* study

R. Franklin-Mergarejo, J. Rubayo-Soneira, N. Halberstadt, T. Ayed, M.I. Bernal Uruchurtu, R. Hernández-Lamoneda, et K.C. Janda, J. Phys. Chem. A, **115**, 5983-5991 (2011).

88 - Exploring the importance of quantum effects in nucleation: the archetypical Ne_n case

W. Unn-Toc, N. Halberstadt, Ch. Meier, and M. Mella, J. Chem. Phys. **137**, 014304 (2012); doi: 10.1063/1.4730033

89 - Quantum dynamics of solid Ne upon photoexcitation of an NO impurity: A Gaussian wave packet approach

W. Unn-Toc, Ll. Uranga-Piña, Ch. Meier, N. Halberstadt, et J. Rubayo-Soneira, J. Chem. Phys. **137**, 054112 (2012); doi: 10.1063/1.4739754

90 - Fluorescence emission of Ca-atom from photodissociated Ca_2 in Ar doped Helium droplets: I- Experiment

A. Masson, M. Briant, A. Hernando, N. Halberstadt, J.-M. Mestdagh et M.-A. Gaveau, J. Chem. Phys. **137**, 184310 (2012); doi: 10.1063/1.4762836

91 - Fluorescence emission of Ca-atom from photodissociated Ca_2 in Ar doped Helium droplets: II- Theoretical

A. Hernando, A. Masson, M. Briant, J.-M. Mestdagh, M.-A. Gaveau et N. Halberstadt, J. Chem. Phys. **137**, 184311 (2012); doi: 10.1063/1.4762837

92 - Angular momentum alignment and fluorescence polarization of alkali atoms photodetached from Helium nanodroplets

A. Hernando, J.A. Beswick et N. Halberstadt, J. Chem. Phys. **139**, 221102 (2013); doi: 10.1063/1.4843235

Chapitres de livres

93 - Caging and nonadiabatic electronic transitions in I_2-M complexes

O. Roncero, N. Halberstadt et J.A. Beswick, in "Reaction Dynamics in Clusters and Condensed Phases", J. Jortner, R. Levine et B. Pullmann Editeurs., Kluwer Academic Press (1993).

94 - Time-resolved studies of the Van der Waals bonds in mercury-rare gas complexes and observation of rotational resonances in mercury-nitrogen

L. Krim, P. Qiu, N. Halberstadt, B. Soep et J. P. Visticot, in "Femtosecond Chemistry", L. Wöste Editeur.

Articles de revue

95 - Theoretical Study of Vibrational Predissociation of Van der Waals Complexes: the Ne...Cl₂ and Ne...ICl Examples

O. Roncero, J.A. Beswick, N. Halberstadt, P. Villarreal et G. Delgado-Barrio, Bulletin de la Société Royale de Sciences de Liège, 58^{eme} année, **3-4**, 227 (1989).

96 - Photofragmentation of weakly bound complexes

O. Roncero, N. Halberstadt et J.A. Beswick, in *Advances in Multiphoton Processes and Spectroscopy*, ed. par S.H. Lin, A. Villaey et Y. Fujimura, Vol XI (1998).

97 - The dynamics of noble gas-halogen molecules and clusters

A. Rohrbacher, N. Halberstadt et K.C. Janda, Ann. Rev. Phys. Chem. **51**, 405 (2000).

98 - Ar...I₂: A model system for complex dynamics

A.A. Buchachenko, N. Halberstadt, B. Lepetit et O. Roncero, Int. Reviews in Phys. Chem. **22**, 153 (2003).

99 - Fragmentation of rare-gas clusters ionised by electron impact: New theoretical developments and comparison to experiments

David Bonhommeau, N. Halberstadt, et U. Buck, Int. Rev. Phys. Chem. **26**, 353 (2007).

100 - Structure and Dynamics of Noble Gas-Halogen and Noble Gas Ionic Clusters: when Theory meets Experiment

J.A. Beswick, N. Halberstadt, et K.C. Janda, Chem. Phys. **399**, 4 (2012). doi=10.1016/j.chemphys.2011.05.026.

Comptes-rendus de conférences internationales

(exceptés les résumés de 4 pages et moins)

101 - A theoretical study of Hg...Ar_n ($n = 1,2,3$) clusters excited in the Hg(³P₁ ← ¹S₀) spectral region

O. Roncero, J.A. Beswick, N. Halberstadt et B. Soep, in “*Dynamics of Polyatomic Van der Waals Complexes*”, NATO ASI Series B Physics, Vol. **227**, édité par N. Halberstadt and K.C. Janda, p 471 (Plenum Press, London, New York, 1990).

102 - Rotational distributions in the vibrational predissociation of weakly bound complexes: Quasi-classical Golden Rule treatment

N. Halberstadt, J.A. Beswick and R. Schinke, in “*Half Collision Resonance Phenomena in Molecules*”, AIP Conference Proceedings Vol. **225**, édité par M. García-Sucre, G. Raşeev et S.C. Ross, pp 211-220, (AIP, New York, 1991).

103 - Photoexcitation and decay of weakly bound complexes: the Ar...Cl₂ case

N. Halberstadt, K.C. Janda et O. Roncero, in “*Laser Techniques for State-Selected and State-to-State Chemistry*”, Cheuk-Yiu Ng Editeur, Proc. SPIE **1858**, 274 (1993).

104 - Energy transfer in Van der Waals complexes as a tool for fitting potential energy surfaces: Examples

N. Halberstadt, in *Fitting Molecular Potential Energy Surfaces*, M.M. Law, J.M. Hutson et A. Ernesti Editeurs, pp 58-64 (CCP6, Daresbury, 1993).

105 - Diffusion Monte Carlo calculations of quasibound states of rare gas-halogen clusters: A diabatic approach

C. García-Rizo, M.I. Hernández, A. García-Vela, N. Halberstadt, P. Villarreal et G. Delgado-Barrio, pp. 91-102 in “*Quantum Systems in Chemistry and Physics, Vol.II: Advanced Problems and Complex Systems*”, A. Hernandez-Lagana, J. Maruani, R. McWeeny et S. Wilson, Eds., Progress in Theoretical Chemistry and Physics, Vol. 3 (Springer, 2002).

106 - Mixed quantum/classical dynamics applied to vibrational energy relaxation in rare gas-halogen clusters

B. Miguel, A. Bastida, S. Fernandez Alberti et N. Halberstadt, in "Time-Dependent Quantum Dynamics", S.C. Althorpe, P. Soldán, et G.G. Balint-Kurti Eds, (Collaborative Computational Project on Molecular Quantum Dynamics -CCP6-, Daresbury, GB, 2001), pp 5-16.

Autres publications

107 - Modelo teórico de potencial para agregados de van der Waals en estados electrónicos excitados.

O. Roncero, J.A. Beswick, N. Halberstadt et B. Soep, Anales de Física **A86**, 177 (1990).

EDITION DE LIVRE

"**Dynamics of Polyatomic Van der Waals Complexes**", NATO ASI Series B Physics, Vol. **227**, N. Halberstadt et K.C. Janda Eds., (Plenum London, New York, 1990).