

Dissociative recombination of NS^+ in collision with low-energy electrons

Riyad Hassaine

Laboratoire Ondes et Milieux Complexes (LOMC), UMR CNRS 6294, Université Le Havre Normandie (ULHN)

in collaboration with:

Ioan F. Schneider (ULHN-LOMC/LAC, Le Havre/Paris, France),

Janos Z. Mezei (HUN-REN ATOMKI, Debrecen, Hungary),

F. Gauchet (ULHN-LOMC, Le Havre, France),

F. Iacob (Physics Faculty, Timisoara, Romania),

E. Roueff (LERMA-Observatoire de Paris, Meudon, France),

J. Tennyson (University College London, UK)

PCMI 2024 - Bordeaux - 30/10/2024



- 1) Introduction
- 2) Theory & Results
- 3) Conclusions
- 4) Perspectives

1) Introduction

2) Theory & Results

3) Conclusions

4) Perspectives

Introduction

- Discovery of nitrogen sulfide (NS) in the early years of radio-astronomy in molecular interstellar clouds, dense cores, comets (Gotlieb *et al*, 1975), (McGonagle *et al*, 1997), (Hily-Blant, Pineau Des Forêts, Faure, Lique, 2022), (Irvine *et al*, 2000).

Introduction

- Discovery of nitrogen sulfide (NS) in the early years of radio-astronomy in molecular interstellar clouds, dense cores, comets (Gotlieb *et al*, 1975), (McGonagle *et al*, 1997), (Hily-Blant, Pineau Des Forêts, Faure, Lique, 2022), (Irvine *et al*, 2000).
- Recent discovery of the nitrogen sulfide cation (NS^+) thanks to laboratory spectroscopy (Cernicharo, Roueff *et al*, 2018) → ubiquitous from molecular and pre-stellar cores to photon dominated regions (Rivière-Marichalar, Pety, Gratier, Roueff, Loison, Wakelam, Gérin *et al*, 2019).

Introduction

- Discovery of nitrogen sulfide (NS) in the early years of radio-astronomy in **molecular interstellar clouds, dense cores, comets** (Gotlieb *et al*, 1975), (McGonagle *et al*, 1997), (Hily-Blant, Pineau Des Forêts, Faure, Lique, 2022), (Irvine *et al*, 2000).
- Recent discovery of the nitrogen sulfide cation (NS^+) thanks to laboratory spectroscopy (Cernicharo, Roueff *et al*, 2018) \rightarrow **ubiquitous from molecular and pre-stellar cores to photon dominated regions** (Rivière-Marichalar, Pety, Gratier, Roueff, Loison, Wakelam, Gérin *et al*, 2019).
- **Dissociative Recombination (DR)** \rightarrow likely the most important pathway for the destruction of NS^+ : $e^- + \text{NS}^+ (v_i^+) \rightarrow \text{N} + \text{S}^*$

Introduction

- Discovery of nitrogen sulfide (NS) in the early years of radio-astronomy in **molecular interstellar clouds, dense cores, comets** (Gotlieb *et al*, 1975), (McGonagle *et al*, 1997), (Hily-Blant, Pineau Des Forêts, Faure, Lique, 2022), (Irvine *et al*, 2000).
- Recent discovery of the nitrogen sulfide cation (NS^+) thanks to laboratory spectroscopy (Cernicharo, Roueff *et al*, 2018) \rightarrow **ubiquitous from molecular and pre-stellar cores to photon dominated regions** (Rivière-Marichalar, Pety, Gratier, Roueff, Loison, Wakelam, Gérin *et al*, 2019).
- **Dissociative Recombination (DR)** \rightarrow likely the most important pathway for the destruction of NS^+ : $e^- + \text{NS}^+ (v_i^+) \rightarrow \text{N} + \text{S}^*$
- Need for **cross sections (XS) and rate coefficients (RC)** for the **dissociative recombination of NS^+** to describe aforementioned media.

Introduction - Dissociative recombination mechanisms

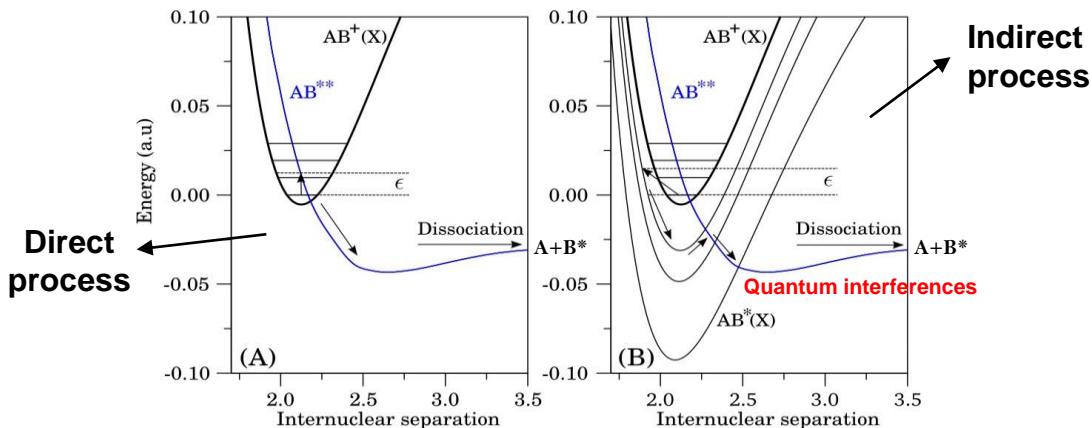


Figure. 1 (from Little, 2015): Mechanisms of DR. (A) the direct mechanism, (B) the indirect mechanism

1) Introduction

2) Theory & Results

3) Conclusions

4) Perspectives

Published paper: Production of structure molecular data

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. **55** (2022) 235202 (9pp)

<https://doi.org/10.1088/1361-6455/ac9cae>

Study of bound and resonant states of NS molecule in the *R*-matrix approach

Felix Iacob¹ , **Thomas Meltzer**², **János Zsolt Mezei**^{3,4} ,
Ioan F Schneider^{4,5}  and **Jonathan Tennyson**^{2,3,4,6,} 

Published in 2022

¹ West University of Timișoara, 300223 Timișoara, Romania

² Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom

³ Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary

⁴ LOMC, CNRS, Université Le Havre Normandie, 76056 Le Havre, France

⁵ LAC, CNRS, Université Paris-Saclay, 91405 Orsay, France

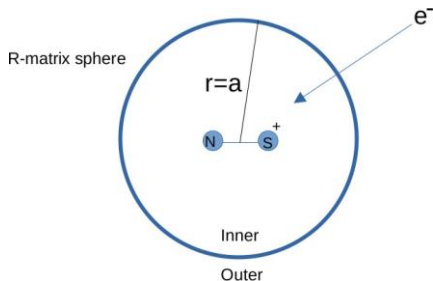
E-mail: j.tennyson@ucl.ac.uk

Theory - Production of molecular structure data through R-matrix theory

1): Solving Schrödinger equation in the **inner region** of R-matrix sphere:

$$\psi_k^\Delta(r_1\sigma_1, \dots, r_N\sigma_N, \underbrace{r_{N+1}\sigma_{N+1}}_{\text{red oval}}, \underbrace{R}_{\text{red circle}}) \leftrightarrow H_{N+1}|\psi\rangle = \underbrace{E}_{\text{red circle}}|\psi\rangle$$

(N+1) electron position and spin **Internuclear distance** **Energy of the target**



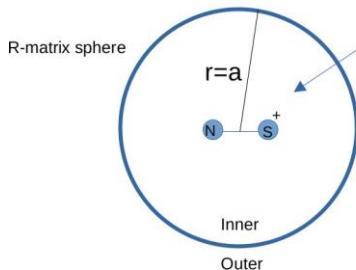
Theory - Production of molecular structure data through R-matrix theory

2) Characterisation of resonant states, i.e. energy + autoionization widths

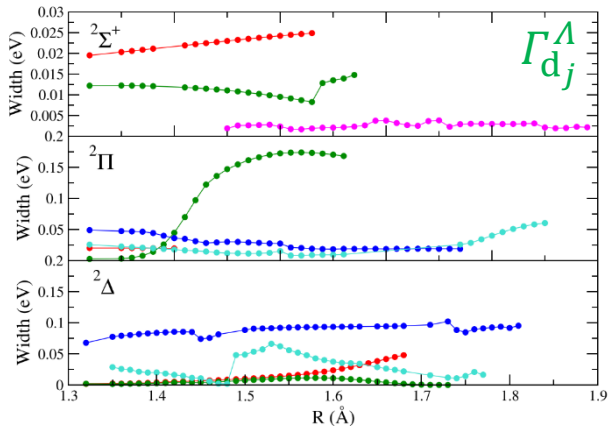
- Energy (real part) and autoionization width: $E = E^r - i \frac{\Gamma}{2}$

Energy of Feshbach resonances
Width

- Electronic coupling with ionization continuum: $V = \sqrt{\frac{\Gamma}{2\pi}}$



Results - Production of molecular structure data: autoionization widths



Global autoionization widths $\Gamma_{d_j}^A$ for the main symmetries and relevant dissociative states of NS

Figure 3: Resonance widths as a function of internuclear distance for $^2\Sigma^+$, $^2\Pi$ and $^2\Delta$ symmetries of NS (Iacob *et al*, 2022).

Published paper: Dissociative recombination of NS^+ :

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. **57** (2024) 165201 (7pp)

<https://doi.org/10.1088/1361-6455/ad5e20>

Dissociative recombination of NS^+ in collision with slow electrons

Published in 2024

R Hassaine^{1,*}, **F Gauchet**¹, **F Iacob**², **J Zs Mezei**^{1,3,*}, **E Roueff**⁴, **J Tennyson**^{3,5}
and **I F Schneider**^{1,6}

¹ LOMC CNRS-UMR6294, Université le Havre Normandie, F-76058 Le Havre, France

² Physics Faculty, West University of Timisoara, 300223 Timisoara, Romania

³ HUN-REN Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary

⁴ LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Universités, F-92190 Meudon, France

⁵ Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom

⁶ LAC CNRS-UMR9188, Université Paris-Saclay, F-91405 Orsay, France

E-mail: riyad.hassaine@etu.univ-lehavre.fr and mezei.zsolt@atomki.hu

Theory - Fragmentation dynamics : ionisation et dissociation

Step-wise MQDT

1) Construction of the interaction matrix:

$$\mathcal{V}_{d_j,lv^+}^\Lambda(E, E) = \langle \chi_{d_j}^\Lambda | V_{d_j,l}^{(e)\Lambda} | \chi_{v^+} \rangle$$

Vibrational wavefunction of the DISSOCIATING NEUTRAL

2) Construction of the reaction matrix:

$$\mathcal{K} = \mathcal{V} + \mathcal{V} \frac{1}{E - H_0} \mathcal{K}$$

Vibrational wavefunction of the ION

3) Diagonalization of the reaction matrix:

$$\mathcal{K} \mathbf{U} = -\frac{1}{\pi} \tan(\eta) \mathbf{U}$$

Eigenvectors

Eigenvalues

4) Frame transformation to the external region:

$$\begin{cases} \mathcal{C}_{lv^+, \Lambda\alpha} = \sum_v U_{lv,\alpha}^\Lambda \langle \chi_{v^+}(R) | \cos(\tau \mu_l^\Lambda(R) + \eta_\alpha^\Lambda) | \chi_v(R) \rangle \\ \mathcal{C}_{d_j, \Lambda\alpha} = U_{d_j\alpha}^\Lambda \cos \eta_\alpha^\Lambda \end{cases}$$

Quantum defect

Theory - Fragmentation dynamics : ionization et dissociation

5) **Construction of the generalized scattering matrix:** $X = \frac{c + iS}{c - iS} \quad X = \begin{pmatrix} X_{oo} & X_{oc} \\ X_{co} & X_{cc} \end{pmatrix}$

6) **Elimination of closed channels: (physical matrix)** $\left\{ \begin{array}{l} S = X_{oo} - \boxed{X_{oc} \frac{1}{X_{cc} - \exp(-i2\pi\nu)} X_{co}} \\ \nu_{v^+} = [2(E_{v^+} - E)]^{-1/2} \end{array} \right.$ Indirect process

7) **Cross sections evaluation:** $\sigma_{diss \leftarrow v_i^+}^{sym, \Lambda} = \frac{\pi}{\boxed{4\varepsilon}} \rho^{sym, \Lambda} \sum_{l, j} |S_{d_j, l v_i^+}^{\Lambda}|^2$ Incident electron energy

8) **Rate coefficients evaluation:** $k(T) = \frac{2}{k_B T} \sqrt{\frac{2}{\pi m k_B T}} \int_0^{+\infty} \boxed{\sigma(\varepsilon)} \varepsilon \exp(-\varepsilon/k_B T) d\varepsilon$ Cross section

Results - Dissociative recombination of NS^+ : Cross sections

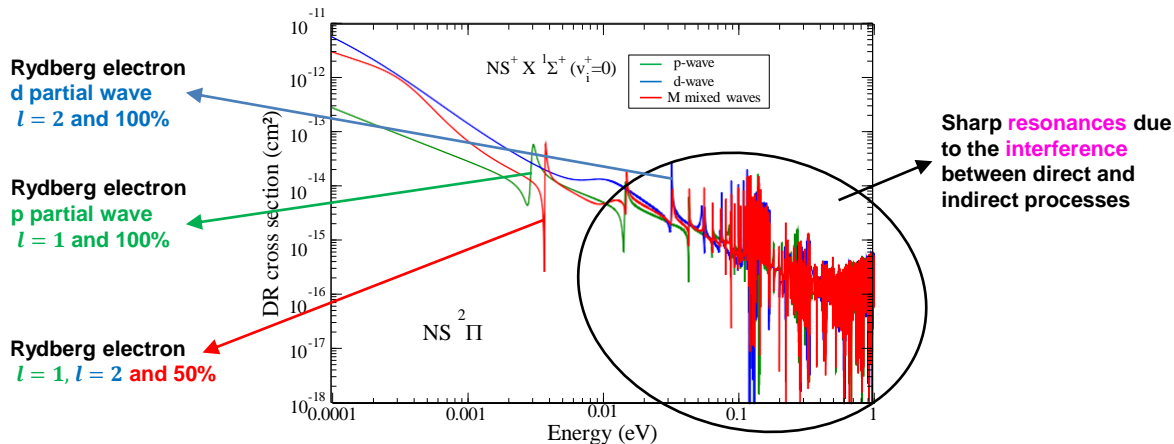


Figure. 4: Dissociative recombination cross section of $\text{NS}^+(v_i^+ = 0)$, for the 2Π molecular symmetry of NS (Hassaine *et al*, 2024).

Results - Dissociative recombination of NS^+ : Rate coefficients

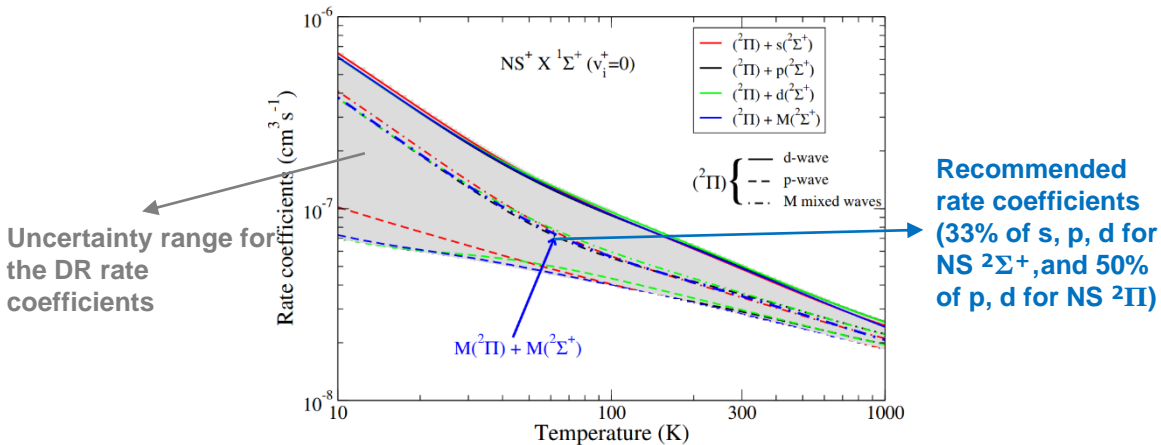


Figure. 5: Rate coefficients for dissociative recombination of $\text{NS}^+(v_1^+ = 0)$ (Hassaine *et al*, 2024).

Results - Dissociative recombination of NS^+ : Fitting

Fit formula

$$\alpha(T) = a_0 \left(\frac{T}{300} \right)^{a_1}$$

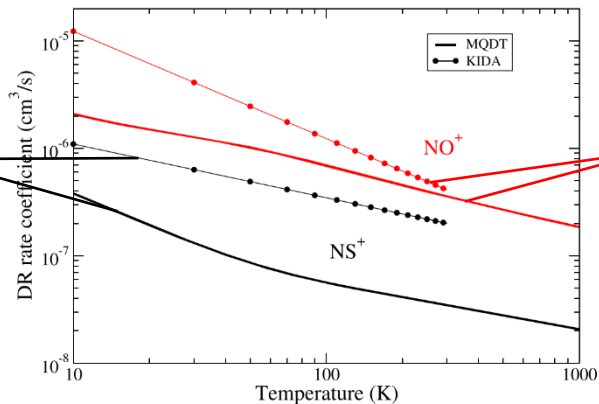
Very good RMS with a two-parameter fit

Model	Temperature (K)	v_i^+	a_0 ($\text{cm}^3 \text{s}^{-1}$)	a_1	RMS
$\text{M}(^2\Pi) + \text{M}(^2\Sigma^+)$	$10 \leq T \leq 33$	0	1.426×10^{-8}	-0.963 555	0.0058
	$33 < T \leq 78$		2.3193×10^{-8}	-0.741 244	0.0127
	$78 < T \leq 1000$		$3.48\,726 \times 10^{-8}$	-0.43 795	0.0075
$\text{M}(^2\Pi) + \text{M}(^2\Sigma^+)$	$10 \leq T \leq 31$	1	$1.00\,126 \times 10^{-7}$	-0.509 637	0.0089
	$31 < T \leq 160$		$1.22\,272 \times 10^{-7}$	-0.420 919	0.0025
	$160 < T \leq 1000$		$1.32\,716 \times 10^{-7}$	-0.280 971	0.0057

Tab. 1: Fitting parameters corresponding to rate coefficients for DR on NS^+ (Hassaine *et al*, 2024).

Results - Dissociative recombination of NS^+ : Rate coefficients

Comparison of MQDT rate coefficients with KIDA for the DR of NS^+



Comparison of MQDT rate coefficients with KIDA for the DR of NO^+ (isovalent to NS^+)

Figure. 6: DR rate coefficients of $NS^+(v_i^+ = 0)$ (in black) and $NO^+(v_i^+ = 0)$ (in red) compared with those existing in KIDA database (Hassaine *et al*, 2024), (Schneider *et al*, 2000), (Motapon *et al*, 2006), (Wakelam, Faure, Talbi, Tennyson *et al*, 2012).

1) Introduction

2) Theory & Results

3) Conclusions

4) Perspectives

Conclusions

- First estimation of rate coefficients for the dissociative recombination of NS^+ with low-energy electrons (Hassaine *et al*, 2024).

Conclusions

- First estimation of rate coefficients for the dissociative recombination of NS^+ with low-energy electrons (Hassaine *et al*, 2024).
- DR: effective process

Conclusions

- First estimation of rate coefficients for the dissociative recombination of NS^+ with low-energy electrons (Hassaine *et al*, 2024).
- DR: effective process
- Important role of the Rydberg resonances in the XS and RC.

1) Introduction

2) Theory & Results

3) Conclusions

4) Perspectives

Perspectives

- **Improvements** needed for NS^+ DR:
 - resolution of autoionization width
 - considering the rotational effects
 - considering the role of core-excited states of the ion (multiply-excited Rydberg states).

Perspectives

- **Improvements** needed for NS^+ DR:
 - resolution of autoionization width
 - considering the rotational effects
 - considering the role of the excited states of the ion (core-excited Rydberg states).
- Studies on **other systems** of astrophysical interest...

Perspectives - other systems

Theoretical study of the excited states of NeH and of their non-adiabatic couplings

R. Hassaine,¹ D. Talbi,² R. P. Brady,³ J. Zs. Mezei,^{1,4} J. Tennyson,^{1,3} and I. F. Schneider^{1,5}

¹LOMC CNRS-UMR6294, Université le Havre Normandie, F-76058 Le Havre, France

²LUPM CNRS-UMR5299, Université de Montpellier, F-34095 Montpellier, France

³Department of Physics and Astronomy, University College London, WC1E 6BT London, UK

⁴HUN-REN Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary

⁵LAC CNRS-UMR9188, Université Paris-Saclay, F-91405 Orsay, France

(*Electronic mail: ioan.schneider@univ-lehavre.fr)

(*Electronic mail: mezei.zsolt@atomki.hu)

(*Electronic mail: dahbia.talbi@umontpellier.fr)

Article in preparation

? NeH^+ in ISM ?
Future discovery ?

- NeH^+ (XS and RC production for dissociative recombination at low energy)
- H_2^+ and HD^+ (XS and RC production for DR, Rovibrational Excitation & DE)
- He_2^+ (XS and RC production for DR)
- N_2H^+ (and, soon, NH^+ , NH_2^+ , HCO^+ ...)

Support

Research supported by the Normandy region, LabEx EMC³, Graduate School Materials & Energy Sciences (GS-MES), IEPE, CNRS-CEA-CNES/PCMI, ANR-MONA, NKFIH-OTKA.

I would like to thank my coauthors for their assistance with this research, and our funding agencies for their support.

Special thanks to Dr. Evelyne Roueff for having pointed to us the discovery and the importance of NS^+ in ISM.

Thank you for your attention!



References

- 1 C.A. Gotlieb *et al*, Detection of interstellar nitrogen sulfide. *ApJL*, 1975.
- 2 D. McGonagle *et al*, Nitrogen Sulfide in Giant Molecular Clouds. *ApJ*, 1997.
- 3 P. Hily-Blant, G. Pineau Des Forêts, A. Faure, F. Lique, Sulfur gas-phase abundance in dense cores. *AA*, 2022.
- 4 W. M. Irvine *et al*, NOTE: Detection of Nitrogen Sulfide in Comet Hale-Bopp. *Icarus*, 2000.
- 5 J. Cernicharo, E. Roueff *et al*, Discovery of the Ubiquitous Cation NS^+ in Space Confirmed by Laboratory Spectroscopy. *ApJL*, 2018.
- 6 P. Rivière-Marichalar, Pety, Gratier, Roueff, Loison, Wakelam, Gérin *et al*, Abundances of sulphur molecules in the Horsehead nebula. First NS^+ detection in a photodissociation region. *AA*, 2019.
- 7 DA. Little, Electron- N_2^+ scattering and dynamics, 2015.
- 8 F. Iacob, Study of bound and resonant states of NS molecule in the R-matrix approach, *J. Phys. B*, 2022.
- 9 R. Hassaine *et al*, Dissociative recombination of NS^+ in collisions with slow electrons. *J. Phys. B*, 2024.
- 10 I. F. Schneider *et al*, Dissociative recombination of NO^+ : calculations and comparison with experiment. *J. Phys. B*, 2000.
- 11 O. Motapon *et al*, Reactive collisions between electrons and NO^+ ions: rate coefficient computations and relevance for the air plasma kinetics. *Plasma Sources Sci. Technol.*, 2006.
- 12 V. Wakelam, A. Faure, D. Talbi, J. Tennyson *et al*, A kinetic database for astrochemistry (KIDA). *ApJS*, 2012.

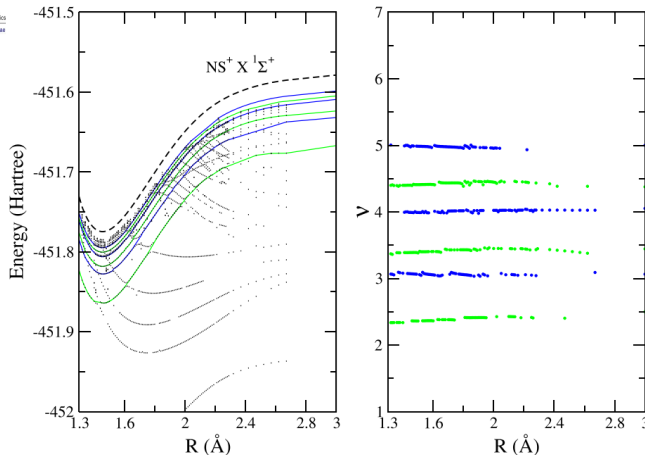
Additional material

OPEN ACCESS

IOP Publishing

J. Phys. B: At. Mol. Opt. Phys. 55 (2022) 235202 (9pp)

Journal of Physics B: Atomic, Molecular and Optical Physics

<https://doi.org/10.1088/1361-6455/ac2a9a>Study of bound and resonant states of NS molecule in the R -matrix approachFelix Iacob¹, Thomas Meltzer², János Zsolt Mezei^{3,4},
Ioan F Schneider^{4,5} and Jonathan Tennyson^{2,3,4,6,*}¹ West University of Timişoara, 300223 Timişoara, Romania² Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom³ Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary⁴ LOMC, CNRS, Université Le Havre Normandie, 76056 Le Havre, France⁵ LAC, CNRS, Université Paris-Saclay, 91195 Orsay, FranceE-mail: j.tennyson@ucl.ac.uk

π
symmetry
of the
neutral:
Rydberg
states and
effective
principal
quantum
numbers

Figure 3. $\text{NS } ^2\Pi$, bound states: left panel PECs. Right panel effective principal quantum numbers. Bound states belong to series that converge to $X^1\Sigma^+$ symmetry of ion. The partial wave characterizing the Rydberg π -wave electron is indicated using colours: green p -wave, blue d -wave.

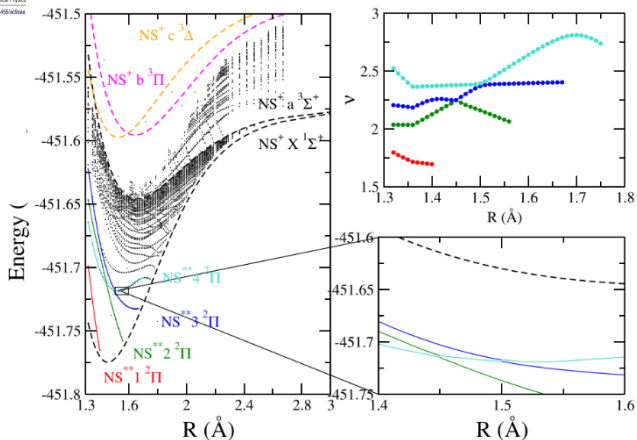
Additional material

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 55 (2022) 23502 (9pp)

<https://doi.org/10.1088/1361-6455/ac9a2a>Study of bound and resonant states of NS molecule in the R -matrix approachFelix Iacob¹, Thomas Meltzer², János Zsolt Mezei^{3,4},
Ioan F Schneider^{4,5} and Jonathan Tennyson^{2,3,4,6,*}¹ West University of Timișoara, 300223 Timișoara, Romania² Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom³ Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary⁴ LOMC, CNRS, Université Le Havre Normandie, 76056 Le Havre, France⁵ LMC, CNRS, Université Paris-Saclay, 91190 Orsay, FranceE-mail: j.tennyson@ucl.ac.uk

Π
symmetry
of the
neutral:
resonances
- PECs of
 NS^+ ground
and lower
excited
states

Figure 6. $\text{NS}^+ 2\Pi$ symmetry resonances curves (left panel) and effective principal quantum numbers (right panel) for some specific curves of special interest for DR.

Additional material

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 57 (2024) 165201 (7pp)

<https://doi.org/10.1088/1361-6455/ad5a20>Dissociative recombination of NS^+ in collision with slow electronsR Hassaine^{1,*}, F Gauchet², F Iacob³, J Zs Mezei^{1,3,*}, E Roueff⁴, J Tennyson^{1,3,5} and I F Schneider^{1,6}¹ LOMC CNRS-UMR6294, Université de Havre Normandie, F-76058 Le Havre, France² Physics Faculty, West University of Timisoara, 300223 Timisoara, Romania³ HUN-REN Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary⁴ LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Université, F-92190

Meudon, France

⁵ Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom⁶ LAC CNRS-UMR9188, Université Paris-Saclay, F-91405 Orsay, France

E-mail: riyad.hassaine@eta.univ-lehavre.fr and mezei.zsolt@atomki.hu

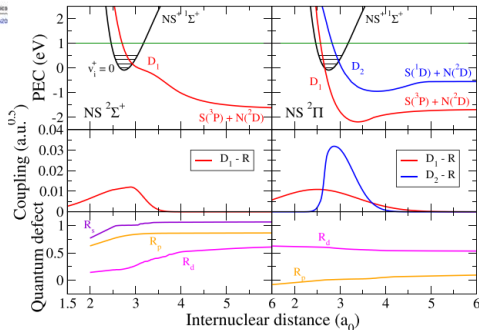


Figure 2. Relevant molecular data sets used in the nuclear dynamics calculations. In the top row, the thick red solid curves (D_1) stand for the PEC of $NS^{**} 1^2\Sigma^+$ (left panel) and $1^2\Pi$ (right panel), while the thick blue solid curve (D_2) represents $NS^{**} 2^2\Pi$ state. The middle row displays the electronic couplings between these dissociative states and the ionization continuum. The quantum defects μ characterizing the Rydberg series of dominant partial waves s , p , and d are shown in the bottom row.

Molecular data of NS^+ and NS

Additional material

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 57 (2024) 165201 (7pp)

<https://doi.org/10.1088/1361-6455/ad5a20>Dissociative recombination of NS^+
in collision with slow electronsR Hassaine^{1,*}, F Gauchet¹, F Iacob², J Zs Mezei^{3,4}, E Roueff⁵, J Tennyson^{1,3,5}
and I F Schneider^{1,6}¹LOMIC CNRS-UMR6294, Université le Havre Normandie, F-76058 Le Havre, France²Physics Faculty, West University of Timisoara, 300223 Timisoara, Romania³HUN-REN Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary⁴LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Université, F-92190

Meudon, France

⁵Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom⁶LAC CNRS-UMR9188, Université Paris-Saclay, F-91405 Orsay, France

*Corresponding author

E-mail: riyad.hassaine@eta.univ-lehavre.fr and mezei.zsolt@atomki.hu

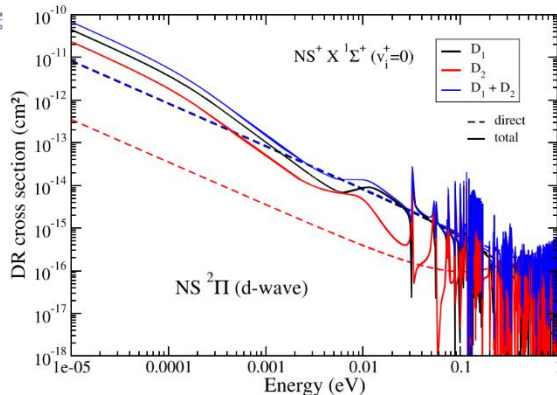


Figure 3. Dissociative recombination of NS^+ in its ground state with an electron into NS states— D_1 or/and D_2 of $^2\Pi$ symmetry—restricted to the contribution of the d partial wave: Total vs direct mechanism.

**XS for the DR
of NS^+ for
each of the
dissociative
channels**

Additional material

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 57 (2024) 165201 (7pp)

<https://doi.org/10.1088/1361-6455/ad5a00>Dissociative recombination of NS^+
in collision with slow electronsR Hassaine^{1,*}, F Gauchet², F Jacob², J Zs Mezei^{3,4,*}, E Roueff⁵, J Tennyson^{1,3,5}
and I F Schneider^{1,6}¹LOMIC CNRS-UMR6294, Université le Havre Normandie, F-76058 Le Havre, France²Physics Faculty, West University of Timisoara, 300223 Timisoara, Romania³HUN-REN Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary⁴LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Université, F-92190

Meudon, France

⁵Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom⁶LAC CNRS-UMR9188, Université Paris-Saclay, F-91405 Orsay, France

E-mail: riyad.hassaine@eta.univ-lehavre.fr and mezei.zsolt@atomki.hu

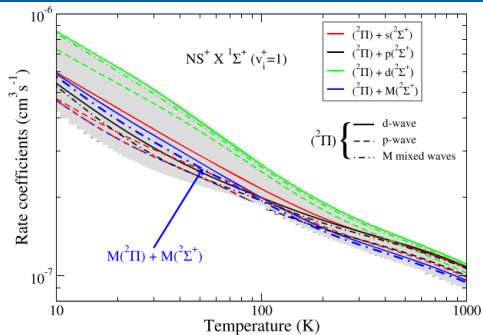


Figure 5. Rate coefficients for dissociative recombination of NS^+ cation from its lowest two vibrational levels and uncertainties due to the use of different partial waves for the incident electrons. Curves give the partial wave contributions for the incident electron. ‘M’ denotes mixed partial waves ($(1/2) \times p + (1/2) \times d$ for $^2\Pi$ states and $(1/3) \times s + (1/3) \times p + (1/3) \times d$ for $^2\Sigma^+$ states). The lower limit of the grey band stands for the minimum rate coefficient as a function of temperature while its upper limit stands for the maximum rate coefficient as a function of temperature.

RC for the
DR of NS^+
for $V_i=1$

Additional material

OPEN ACCESS

IOP Publishing

Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 57 (2024) 165201 (7pp)

<https://doi.org/10.1088/1361-4105/ad5a20>Dissociative recombination of NS^+
in collision with slow electronsR Hassaine^{1,*}, F Gauchet¹, F Jacob², J Zs Mezei^{1,3,*}, E Roueff⁴, J Tennyson^{1,3,5}
and I F Schneider^{1,6}¹ LOMC CNRS-UMR6294, Université de Havre Normandie, F-76058 Le Havre, France² Physics Faculty, West University of Timisoara, 300223 Timisoara, Romania³ HUN-REN Institute for Nuclear Research (ATOMKI), H-4001 Debrecen, Hungary⁴ LERMA, Observatoire de Paris, PSL Research University, CNRS, Sorbonne Université, F-92190

Meudon, France

⁵ Department of Physics and Astronomy, University College London, WC1E 6BT London, United Kingdom⁶ LAC CNRS-UMR9188, Université Paris-Saclay, F-91405 Orsay, France

E-mail: riyad.hassaine@eta.univ-lehavre.fr and mezei.zsolt@atomki.hu

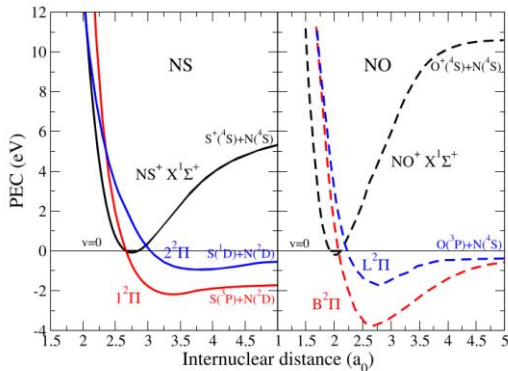
NS and
NO PECs

Figure 6. Potential energy curves of the NS^+/NS (left figure) and NO^+/NO molecular (right figure) systems relevant for low energy dissociative recombination compiled from [17] and [24] respectively. The solid curves stand for NS while the dashed ones for NO . The black curves show the ground electronic state of the target, while in red and blue we present the most important dissociative molecular states with $^2\Pi$ symmetry. Reproduced from [17]. © The Author(s). Published by IOP Publishing Ltd. **CC BY 4.0**. Reproduced from [24]. © IOP Publishing Ltd. All rights reserved.

Additional material

No interaction

$$H_0|\phi\rangle = E|\phi\rangle$$

Interacting
colliding systems

$$(H_0 + V)|\psi\rangle = E|\psi\rangle$$

Lippman-
Schwinger
formulation
and solutions

$$\Phi_E(r) = \psi_E(r) + \mathcal{P} \int dE' \frac{\mathcal{K}(E', E)}{E - E'} \psi_{E'}(r)$$

Lippman-Schwinger
equation

$$\mathcal{K}(E', E) = \langle \psi_{E'} | V | \psi_E \rangle + \mathcal{P} \int dE'' \frac{\langle \psi_{E''} | V | \psi_{E'} \rangle}{E - E''} \mathcal{K}(E'', E)$$

2nd order perturbative Solutions Hassaine-PCMI2024-Bordeaux

Possible questions:

- Slide 7: Products of the dissociation: $N+S^*$: why S in an excited state and Nitrogen in its ground state? Explain in a few words
- Slide 12: Physical meaning of autoionization widths: explain in a few words
- Slide 13: Why diabatic representation? explain in a few words
- Slide 16: Lippman-Schwinger equation: explain in a few words
- Slide 16: Eta (shift) in the 3rd point - 3): explain in a few words
- Slide 16: Physical meaning of the quantum defect: explain in a few words
- Slide 16: Frame transformation: explain in a few words
- Slide 17: Elimination of closed channels: explain in a few words
- Slide 21: why the comparison with NO^+ system? Explain in a few words

Answers:

- Slide 7: Sulfur has a lower excitation energy and ionization potential than Nitrogen (resp. 2.1 eV - 10.4 eV and 2.4 eV - 14.6 eV)
- Slide 12: rates at which an electron in a quasi-bound state transitions to an unbound, ionized state
- Slide 13: In the adiabatic representation, the natural coupling is the non-adiabatic coupling. In the case where PECs of neutral and ion exhibit avoided crossings, since the NACs are inversely proportional to the energy difference between the PECs, these couplings are infinite and non-physical. In the context of quasi-diabatic representation, avoided crossing rule is not required, and one can obtain physical couplings.
- Slide 16: Second-order perturbative solution of the Lippmann-Schwinger integral equation
- Slide 16: Shift of the total eigenfunction in the asymptotical region
- Slide 16: Basically it is a correction. This is the measure of how much energy levels of the Rydberg electron in an atom/molecule deviates from the expected values of a simple hydrogen-like model

Answers:

- Slide 16: In the external region, the incoming Rydberg electron is following the movement of nuclei, and has only a fraction of the kinetic energy it exhibits when accelerated by the coulomb potential in the short-range region. As a consequence, the Born-Oppenheimer approximation is not valid in the external region. The Frame transformation consists in projecting the molecular eigenstates of the short-range interactions region (where B.O approx. is ok) on the eigenstates in the external region, in order to ensure the continuity of the solutions in the region.
- Slide 17: In order to take into account reactive collision processes, it is necessary to eliminate closed channels in the diffusion matrix to calculate the probabilities of reaction corresponding to the process studied.
- Slide 21: NO^+ has a similar electronic configuration as NS^+ /same number of valence electrons. To remember in case of:
 - Atomic number of Nitrogen: 7
 - Atomic number of Sulfur: 16
 - Atomic number of Oxygen: 8