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Dissociative recombination of NS^+ in collision with slow electrons

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Abstract

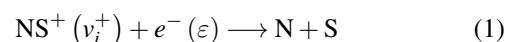
Cross sections and rate coefficients for the dissociative recombination (DR) of the NS^+ ion induced by collisions with low-energy electrons are reported for temperatures between 10 and 1000 K, relevant to a large range of interstellar cloud temperatures. Uncertainties are discussed for these rates. Comparisons are made with DR rates for the isovalent NO^+ molecular ion which are found to be much faster. The present findings lead to a moderate dissociative reaction rate coefficient, smaller by a factor of 2 than the current estimates reported in the different kinetic databases for a temperature of 10 K. We consider that our rate coefficients obtained through multichannel quantum defect theory for NS^+ are likely to be better than those displayed in the different kinetic databases.

Keywords: dissociative recombination, multichannel quantum defect theory, nitrogen sulfide cation, interstellar medium, low temperature electrons, super excited states

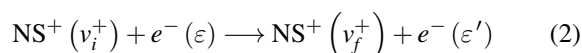
1. Introduction

Nitrogen sulfide (NS) was first detected in the early years of radio astronomy toward ‘SgrB2 interstellar cloud [1] and its presence has later been found in giant molecular clouds [2], dense cores [3] as well as in comets [4]. Recently, new observations have led to the discovery of the NS^+ cation thanks to laboratory spectroscopy [5]; the ion is found to be ubiquitous, from cold molecular cores, prestellar cores, and shocks

[5] to photon dominated regions [6]. Dissociative recombination (DR):



where v_i^+ is the initial vibrational number of the target and ε is the energy of the incident electron - is likely the major removal mechanism for the ion. It competes with autoionization, resulting in vibrational transitions:



i.e. vibrational excitation—when v_f^+ is larger than v_i^+ and ε exceeds the threshold of reaching this excited level—or vibrational de-excitation—when v_f^+ is smaller than v_i^+ , while ε' is the energy of the scattered electron.

We focus on calculating DR (equation (1)) cross sections and rate coefficients for collision energies/temperatures up to

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1 eV/1000 K, using the step-wise multichannel quantum defect theory (MQDT) explained in [7, 8] and references therein. The first attempt to provide uncertainties for our MQDT method is presented. Due to the lack of other theoretical or experimental results we will compare our results with those obtained for NO^+ , another closed shell molecular cation relevant for the upper atmosphere of Earth, that has similar electron structure and chemical properties to NS^+ .

The organisation of the paper is as follows: In section 2, a succinct presentation of our theoretical approach is given. Section 3 contains the major results—cross sections and rate coefficients—and section 4 summarizes the concluding remarks.

2. Theoretical method

The effectiveness of our theoretical approach based on the step-wise MQDT [7, 8] for modeling electron/diatomic cation collisions has been demonstrated through numerous previous studies involving various species. Examples of these include H_2^+ and its isotopologues, where we account for rotational and isotope effects across low to medium-high collision energies [9–14]. Additionally, we have explored core-excited effects for CH^+ [8] and for SH^+ [15, 16]. As the main elements of our approach have been extensively presented in previous works, such as [8], we will focus here on only outlining its main steps.

Reactions (1) and (2) encompass *ionization* channels, characterizing the interaction of an electron with the target cation, as well as *dissociation* channels, relating to atom-atom scattering. The interaction of these channels gives rise to quantum interference between the *direct* mechanism relying on open channels—where capture occurs into a doubly excited dissociative state of the neutral system (labeled as NS^{**})—and the *indirect* one—where capture takes place through a Rydberg bound state of the molecule (NS^*) pertaining to *closed* channels. These Rydberg states are predissociated by the dissociative channels. In both mechanisms, autoionization, which relies on the presence of *open* ionization channels, results in the vibrational excitation or de-excitation—reaction (2) of the cation. Each individual ionization channel is constructed by adding an electron to the NS^+ ion within its fundamental electronic state $X^1\Sigma^+$ at a specific (v_i^+) vibrational level. These ionization channels interact with all available dissociation exit channels, via Rydberg-valence interaction, for all relevant molecular symmetries— $^2\Sigma^+$, $^2\Pi$, and $^2\Delta$, labeled ‘sym’ within this article.

The MQDT approach for studying DR relies on prior knowledge of the potential energy curves (PECs) corresponding to the ion’s ground state as well as that of the dissociative states of the neutral molecule and of its mono-excited Rydberg states. These latter states, which we can organize in Rydberg series, each of them characterized by geometry-dependent quantum defects. Additionally, the electronic couplings between the dissociation and ionization continua (referred as Rydberg-valence couplings) are needed.

A summary of the relevant PECs, taken from Iacob *et al* [17], can be seen in figure 1. The black curve stands for the

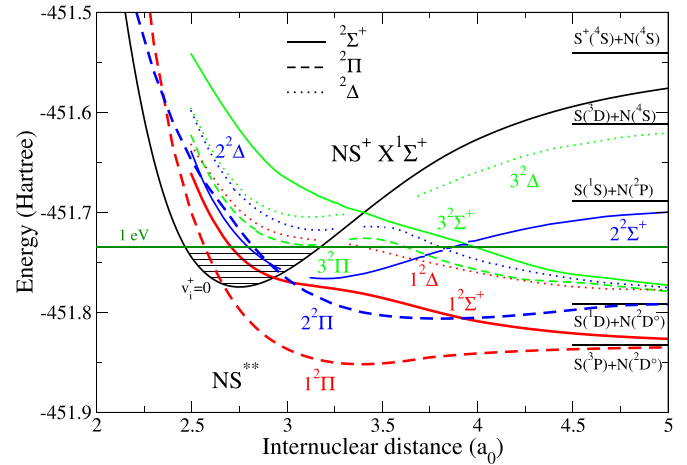


Figure 1. Energy diagram of the NS^+/NS molecular system, relevant for dissociative recombination, compiled from [17]. Given are the potential energy curves (PECs) and the atomic states of their corresponding asymptotic limits are given as short horizontal lines at large internuclear separation. The thick black solid curve represents the PEC of the ground electronic state of the NS^+ ion, while the colored solid, dashed and dotted curves represent NS^{**} dissociative states computed by the R-matrix method. The thin black horizontal lines denote the lowest vibrational levels of the ion. Reproduced from [17]. © The Author(s). Published by IOP Publishing Ltd. CC BY 4.0.

ground electronic state of the cation, while the colored solid, dashed and dotted lines represent the dissociative states of NS belonging to the $^2\Sigma^+$, $^2\Pi$ and $^2\Delta$ symmetries.

The current MQDT calculations neglect rotational effects. Within each of the symmetries involved, focus is directed towards the few lowest dissociative states accessible at low energy of the incident electron—below 1 eV—relevant for the interstellar media. For a given total symmetry, here we consider $^2\Sigma^+$, $^2\Pi$ and $^2\Delta$, the initial step of our methodology involves constructing the *interaction matrix* \mathcal{V} , which serves as the driving force during the collision process. Its elements quantify the interconnections between the ionization and the dissociation channels.

The next step consists of construction of the short-range reaction matrix \mathcal{K} . This is achieved using a second-order perturbative solution of the Lippmann-Schwinger equation. The \mathcal{K} -matrix is then diagonalized, its eigenvalues being related to the long-range phase-shifts of the eigenfunctions. Applying a Cayley transformation on these matrices [18] allows the generalized scattering matrix \mathcal{X} to be constructed. Elimination of the closed channels [19] is then performed, yielding the physical scattering matrix \mathcal{S} :

$$\mathcal{S} = \mathcal{X}_{oo} - \mathcal{X}_{oc} \frac{1}{\mathcal{X}_{cc} - \exp(-i2\pi\nu)} \mathcal{X}_{co}, \quad (3)$$

which relies on the block-matrices built not only for the open channels, \mathcal{X}_{oo} , but also for the closed ones, \mathcal{X}_{oc} , \mathcal{X}_{co} and \mathcal{X}_{cc} . The diagonal matrix ν appearing in the denominator of equation (3) incorporates the effective quantum numbers corresponding to the vibrational thresholds of the closed ionization channels at the given total energy of the system.

Finally, the global cross section for the DR is:

$$\sigma_{\text{diss} \leftarrow v_i^+} = \frac{\pi}{4\varepsilon} \sum_{\text{sym}} \rho^{(\text{sym})} \sum_{l,j} |S_{d_j, v_i^+ l}^{(\text{sym})}|^2, \quad (4)$$

where ρ represents the ratio of multiplicities between the neutral system and the ion for a specific neutral symmetry. The thermal rate coefficients are determined by convoluting the cross section with the Maxwell energy distribution function of the free electrons:

$$\alpha(T) = \frac{2}{kT} \sqrt{\frac{2}{\pi mkT}} \int_0^{+\infty} \sigma(\varepsilon) \varepsilon \exp(-\varepsilon/kT) d\varepsilon, \quad (5)$$

where m is the electron's mass, T the temperature, and k the Boltzmann constant.

3. Results and discussions

Applying the step-wise MQDT method outlined in the previous section, we have calculated the DR (equation (4)) cross sections of NS^+ for the lowest two vibrational levels of the ground electronic state of the cation. Since NS^+ molecular cation has been observed in the diffuse interstellar medium (ISM) for temperatures between 10 and 300 K [5], corresponding to electron energies in the range between 0.01 meV and 1 eV, here we focus on producing cross sections for the lowest relevant open dissociative states of the neutral.

The present nuclear dynamics study relies on the molecular data sets recently calculated in the framework of the R-matrix theory [17]. We have found five molecular states of the cation, and for the ionization channels, the partial waves we took into account for the incident electron are s , p , and d for the $^2\Sigma^+$ states and p and d for the $^2\Pi$ ones [17]. In order to calculate the energy positions and resonance widths of the resonant dissociative states, in some of our previous studies, the Time-delay matrix method [20] was successfully tested and applied for molecular systems like $e^- + \text{CO}^+$ [21] relying on one single ionic core and three partial waves, or $e^- + \text{N}_2^+$ [22] relying on three ionic cores and one partial wave. The $e^- + \text{NS}^+$ molecular system relying on five ionic cores and three partial waves is a more complex system, and we had technical difficulties in using the same method. Thus, we have used the module RESON [23] that automatically detects resonances and fit them to a Breit–Wigner profile to determine their positions and widths. Consequently, we produced global electronic couplings, which are not resolved neither on partial waves nor on ionic cores.

Starting from figure 1 containing the PECs of the ground electronic state of NS^+ and doubly excited dissociative states of NS, and considering the temperature ranges relevant for the ISM we reduced the input molecular data to those curves presented in figure 2. We also limited our calculations to collision energies up to 1 eV shown with dark green line in figures 1 and 2. This restricts the open dissociation channels to those whose asymptotic limits are given in the first column of table 1. In addition, the unfavorable crossing points—far from the Franck-Condon region—between the PEC's of the

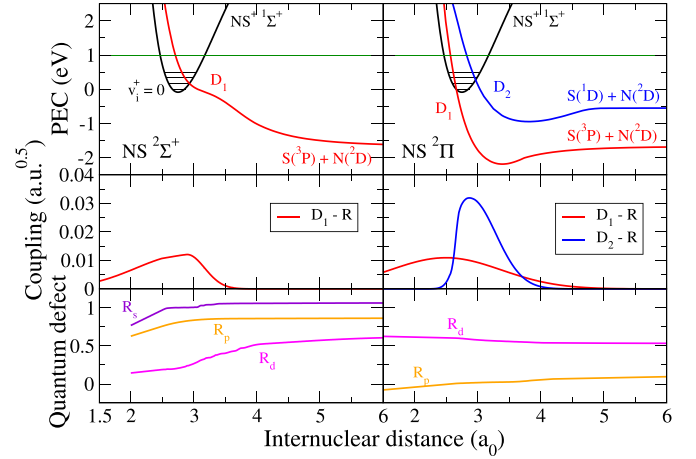


Figure 2. Relevant molecular data sets used in the nuclear dynamics calculations. In the top row, the thick red solid curves (D_1) stand for the PEC of $\text{NS}^{**} 1^2\Sigma^+$ (left panel) and $1^2\Pi$ (right panel), while the thick blue solid curve (D_2) represents $\text{NS}^{**} 2^2\Pi$ state. 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.

Table 1. Asymptotic states of NS^{**} relevant for low-energy impact collisions. The corresponding energies are given with respect to NS^{**} lowest limit: $\text{S}(^3\text{P}) + \text{N}(^4\text{S})$.

State	Energy (eV)	Symmetry
$\text{S}(^3\text{P}) + \text{N}(^2\text{D}^o)$	2.381	$1^2\Sigma^+, 1^2\Pi$
$\text{S}(^1\text{D}) + \text{N}(^2\text{D}^o)$	3.524	$2^2\Pi$

remaining open dissociative channels $1^2\Delta$, $2^2\Delta$, $3^2\Sigma$, $3^2\Pi$ and that of the target ion—make them irrelevant for DR at low energy. Consequently, $1^2\Sigma^+$, $1^2\Pi$, $2^2\Pi$ are the only relevant dissociative paths to be considered in this study. Figure 2 contains the molecular data characterizing these dissociative states. The middle panels represent their electronic couplings with the ionization continuum. The quantum defects generating the complete Rydberg series corresponding to the partial waves s , p , d for $^2\Sigma^+$ symmetry and p , d for $^2\Pi$ symmetry are displayed in the bottom panels.

Figure 3 shows the DR cross sections obtained for the two dissociative states of the $^2\Pi$ symmetry corresponding to the case when we chose for the incoming electron 100% d partial wave. We give here the *direct*—smooth cross section due to the direct capture of the electron into doubly excited dissociative states, responsible for the bulk part of the cross section—and *total*, i.e. *direct* and *indirect*, cross sections—infinite number of resonances, due to the temporary capture into highly excited Rydberg states. The D_1 dissociative state (black curve) has a more favorable crossing with the cation compared to D_2 (blue curve) leading thus to larger DR cross sections, although the vibronic coupling of D_1 is a factor of two smaller than the coupling of D_2 . Figure 4 shows the total DR cross sections associated to the $^2\Pi$ molecular states considering three scenarios for the partial waves of the incoming electron. Dark green stands for p wave, blue for the d and

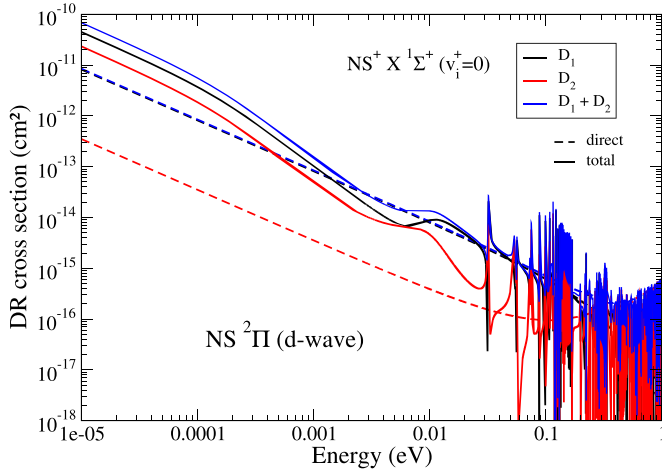


Figure 3. Dissociative recombination of NS⁺ in its ground state with an electron into NS states—D₁ or/and D₂ of ²Π symmetry—restricted to the contribution of the *d* partial wave: Total vs direct mechanism.

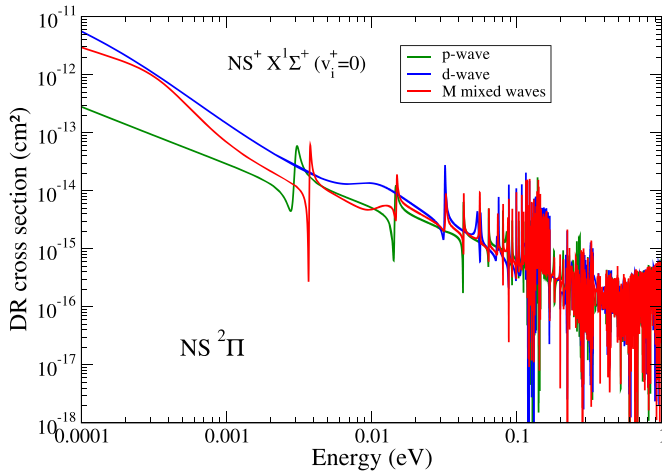


Figure 4. Dissociative recombination cross section of NS⁺ for the ²Π molecular symmetry for *p*, *d* and mixed “M” = (1/2) × *p* + (1/2) × *d* partial waves for the incident electron.

red for the 0.5 × *p* + 0.5 × *d* mixture. The overall behavior of the three cross sections seems the same, at least starting from 100 meV collision energies. For very low collision energies we obtained smaller cross sections for the *p* incident electrons.

The molecular data sets produced in our electron structure and electron scattering calculation using the R-matrix theory [17] relevant for the present study contains one ion core (NS⁺ X¹Σ⁺), three molecular symmetries (NS ²Σ⁺, ²Π, and ²Δ) and two or three partial waves for the incident electron for the three symmetries relevant for low-energy DR. RESON provides global autoionization widths for the doubly excited dissociative resonant states, meaning that the electronic couplings are not resolved for the angular momentum of the incident electron. As a consequence, neither our cross sections nor rate coefficients are resolved. In order to overcome this we assume certain partial wave distributions for the vibronic couplings. This is the case for example in figure 4, where we

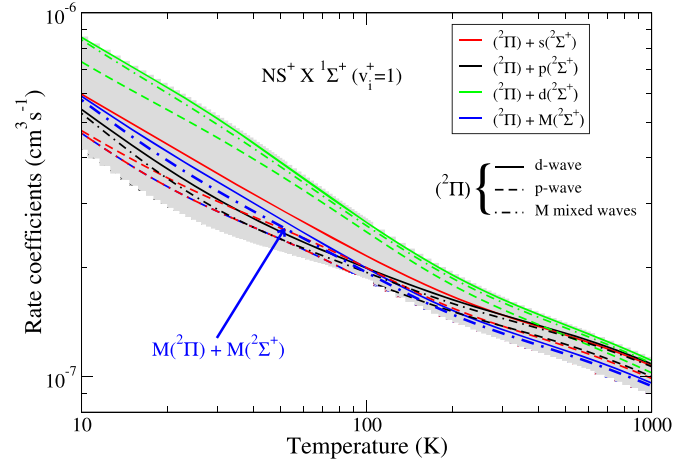
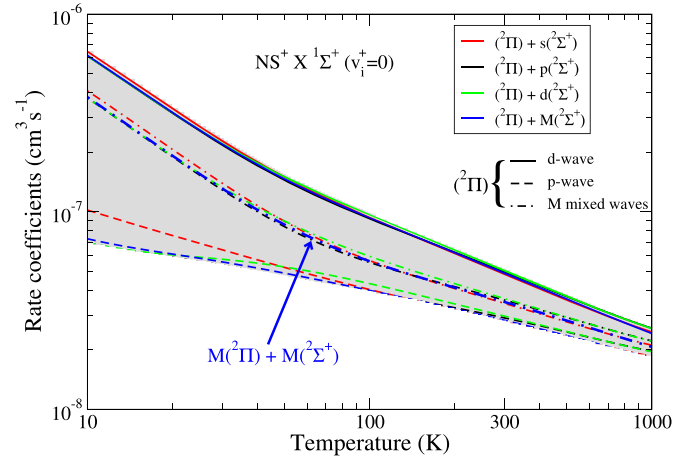


Figure 5. Rate coefficients for dissociative recombination of NS⁺ cation from its lowest two vibrational levels and uncertainties due to the use of different partial waves for the incident electrons. Curves give the partial wave contributions for the incident electron. ‘M’ denotes mixed partial waves ((1/2) × *p* + (1/2) × *d* for ²Π states and (1/3) × *s* + (1/3) × *p* + (1/3) × *d* for ²Σ⁺ 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.

have assumed either 100% *p* or *d* waves or 0.5 × *p* + 0.5 × *d* mixture.

Following this idea, we made a detailed study considering ²Σ⁺ and ²Π symmetries of NS and *s*, *p*, *d* or *p* and *d* partial waves for the two symmetries. The calculated rate coefficients are presented in figure 5 for different partial wave distribution scenarios. The recommended rate coefficients for the DR of NS⁺ X¹Σ⁺ (v_i⁺ = 0, 1) are given in blue dashed-dotted lines labeled as M(²Π)+M(²Σ⁺). The grey area enclosed by the different scenarios can be regarded as uncertainties of MQDT calculations caused by the unresolved electronic couplings.

Due to the lack of any theoretical or experimental studies regarding the electron induced reactive processes of NS⁺, we have instead compared our present NS⁺ results with those previously obtained for NO⁺ [24, 25], which due to its chemical similarity could be a proxy for NS⁺. In figure 6 we have compared the molecular states most relevant for DR of the NS⁺/NS and NO⁺/NO molecular systems. In black we represent the

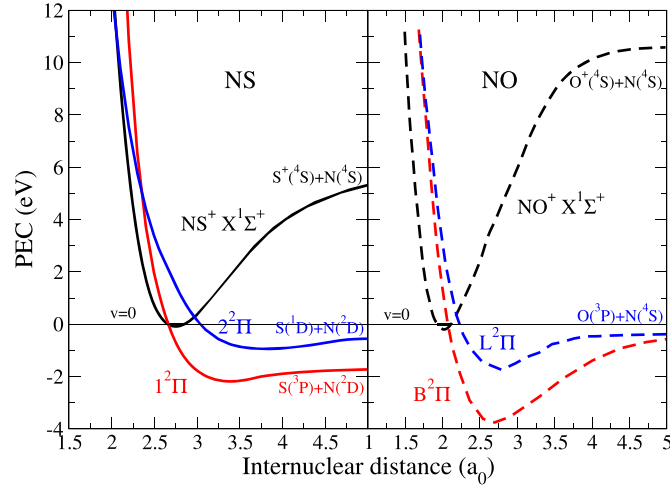


Figure 6. Potential energy curves of the NS⁺/NS (left figure) and NO⁺/NO molecular (right figure) systems relevant for low energy dissociative recombination compiled from [17] and [24] respectively. The solid curves stand for NS while the dashed ones for NO. The black curves show the ground electronic state of the target, while in red and blue we present the most important dissociative molecular states with ²Π 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.

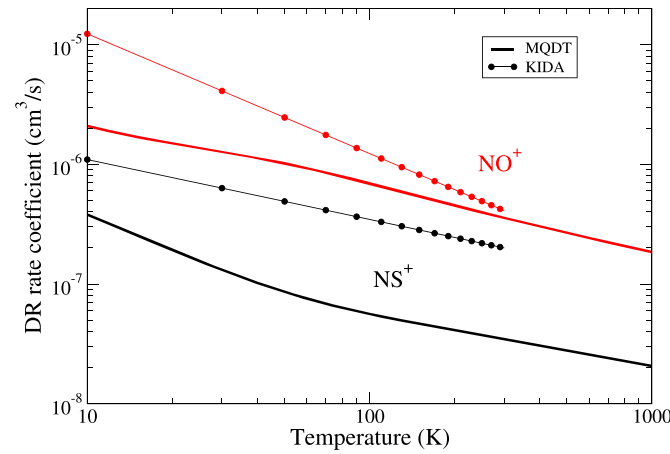


Figure 7. Dissociative recombination rate coefficients of NS⁺ (in black) and NO⁺ [24, 25] (in red) molecular targets for $v_i^+ = 0$ compared with the rates available in the KIDA database [26]. Reproduced from [24]. © IOP Publishing Ltd. All rights reserved.

Table 2. Fitting parameters for the equation (6), corresponding to the rate coefficients for DR on NS⁺, with $v_i^+ = 0$ and $v_i^+ = 1$. Electron temperature range was divided in three regions and they vary between 10 and 1000 K.

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

molecular state of the target cations, in red and blue the first two dissociative states of the neutral belonging to the ²Π symmetry. The solid line stands for NS, while the dashed line for NO. The two target states are different, the NS⁺ has a shallower but wider PEC, leading to less vibrational levels, thus

fewer ionization channels. While the second pair of dissociative states (2 and L²Π) presented in blue show similarities: they have unfavorable crossing points with the target states, similar shapes and asymptotic limits, we can see more important differences for the first two states (1 and B²Π) given in red. These

have different shapes and asymptotic limits, but most importantly the NO dissociative state has more favorable crossing with the cation. This latter is mostly responsible for the larger rate coefficients obtained for the DR of NO⁺.

The comparison between the NO⁺ DR rate coefficient and the NS⁺ one for $v_i^+ = 0$ is performed in figure 7. We also compare here our MQDT-based rate coefficients with those displayed in the kinetic database for astrochemistry (KIDA) [26, 27]. Our thermal rates are lower than the latter ones by a factor up to 7 for NO⁺, and with a factor between 3 and 9 for NS⁺. In [26, 27] it is stated that these KIDA results are just estimates, assuming a recombination coefficient $\alpha \approx (1 - 2) \times 10^{-7} (300/T)^{1/2} \text{ cm}^3 \text{ s}^{-1}$ for diatomic cations, and $\alpha \approx (3 - 6) \times 10^{-7} (300/T)^{1/2} \text{ cm}^3 \text{ s}^{-1}$ for complex cations. Without giving details, the KIDA database displays $\alpha = 2 \times 10^{-7} (300/T)^{1/2} \text{ cm}^3 \text{ s}^{-1}$ for the DR of NS⁺ and $\alpha = 4.1 \times 10^{-7} (300/T) \text{ cm}^3 \text{ s}^{-1}$ for the DR of NO⁺. As a conclusion, we consider that our rate coefficients obtained through MQDT for NS⁺ are likely to be more reliable than those given by KIDA. As for NO⁺, we note that our MQDT cross sections and rate coefficients [24, 25] show excellent agreement with the experimental values and should also be more reliable than those given by KIDA.

Finally, in order to simplify the use of our recombination rate coefficients for kinetic modeling, we have fitted their temperature dependence by using a simple power formula:

$$\alpha(T) = a_0 \left(\frac{T}{300} \right)^{a_1} \quad (6)$$

where T is in Kelvin and α in $\text{cm}^3 \text{ s}^{-1}$. The fitting coefficients from the exponent are very small numbers, so the commonly used Arrhenius formula is reducing to equation (6). The fitting parameters for the DR of the lowest 2 vibrational levels of the target, mainly populated in the ISM for temperatures up to 300 K, are summarized in table 2. The RMS values given in the table show that the fitted parameters reproduce our MQDT rate coefficients within 1.3% over the whole temperature range $10 < T < 1000$ K.

4. Conclusions

Using the step-wise MQDT, we calculate cross sections and thermal rate coefficients for the DR of electrons with NS⁺ ($X^1\Sigma^+$) ions. The cross sections are computed within the energy range of 0.01 meV to 1 eV, and the corresponding thermal rate coefficients were evaluated for temperatures ranging from 10 to 1000 K, focusing on the two lowest vibrational levels of the ions.

Our model considers all pertinent electronic states and symmetries of the cation target, along with the relevant vibronic electronic couplings, by taking into account the quantum interference among the direct and indirect mechanisms. We estimate the uncertainty of our MQDT calculations caused by the global electronic couplings unresolved in the angular

momentum of the incident electron. Comparing our results with those obtained for the similar molecular cation NO⁺ and with values given in the KIDA database, suggests that the database values are too high. We suggest that rate coefficients obtained through MQDT for NS⁺ and NO⁺ are likely to be more reliable than those currently recommended in the KIDA database. The relatively moderate DR rate we evaluate explains—at least partially—the ubiquitous presence of NS⁺ in interstellar space.

The numerical data, ready to be used in the kinetic modeling in astrochemistry and plasma physics is available upon request to the authors.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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