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Accurate Einstein coefficients for electric dipole transitions in the first negative band of N_2^+

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ABSTRACT

Context. The N_2^+ fluorescence spectrum of comet C/2016 R2 is modelled in a companion paper. That work relies on accurate Einstein coefficients for electric dipole transitions between the $B^2\Sigma_u^+$ and $X^2\Sigma_g^+$ electronic states of N_2^+ .

Aims. These coefficients are provided in the present paper.

Methods. The potential energy curves and transition dipole moments were computed at a high level of ab initio theory and include relativistic corrections. Rovibrational wavefunctions were then obtained without assuming separability of vibrational and rotational motions.

Results. Vibrationally and rotationally resolved Einstein coefficients are presented in a convenient three-parameter functional form for three isotopologues. A possible explanation is given for the large variation in the experimental radiative lifetimes.

Key words. radiative transfer – comets: general – molecular data – planets and satellites: atmospheres

1. Introduction

The emission spectra of the first negative, $B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$, and Meinel, $A^2\Pi_u \rightarrow X^2\Sigma_g^+$, bands of N_2^+ are well studied due to their importance for airglow and planetary entry physics (Qin et al. 2017). N_2^+ has also been detected recently in a few comets, especially in comet C/2016 R2, which presented unusual bright emission lines due to N_2^+ (Biver et al. 2018; Cochran & McKay 2018b,a; Opatom et al. 2019; Venkataramani et al. 2020). The focus of many experimental and theoretical works has been the accurate determination of vibrational energy levels and rotational constants from which rovibrational energy levels and hence transition frequencies can easily be computed. The electronic dipole moment functions and Einstein coefficients are less well investigated. There are two compilations of Einstein coefficients, one by Lofthus & Krupenie (1977) and a more recent one by Gilmore et al. (1992). Lofthus and Krupenie reported data that were originally obtained by Jain & Sahni (1967), who employed the experimental RKR potential determined by Singh & Rai (1966). The integral over the transition dipole moment was approximated by the R -centroid method, that is, it was replaced by a single value of the dipole moment, at $R = R_{\text{centroid}}$. Ten years later, Langhoff, Bauschlicher, and Partridge (Langhoff et al. 1987; Langhoff & Bauschlicher 1988) published the results of their thorough ab initio investigations of the potential energy curves of the four lowest electronic states and transition dipole moments. For the $B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$ transitions, which are the subject of the present investigation, they found that the computed transition dipole moment is

significantly different from the dipole moments used before. Gilmore et al. (1992) then re-evaluated the Einstein coefficients. Just as before (Lofthus & Krupenie 1977), experimental RKR potential energy curves were applied, but the integrals over the transition dipole moments were evaluated numerically using a second-order fit in R of the ab initio transition dipole moments in Langhoff & Bauschlicher (1988). The fit was made with the intention to provide A coefficients for a wide range of transitions. Unfortunately, it washes out some features of the ab initio curve.

In the present work, we have recomputed the potential energy curves and transition dipole moment function at a very high level of ab initio theory: explicitly correlated multi-reference configuration interaction (MRCI-F12b) with the large aug-cc-pCVQZ-F12 basis. Moreover, all electrons were correlated, and relativistic corrections were applied. Rovibrational transition dipole moments were computed without assuming separation of vibrational and rotational motions. The rotational dependence of these matrix elements is represented in a functional form. For the complete determination of the Einstein A coefficients, our functions need still to be multiplied by the rotational line intensity factors, or Hönl-London factors. These must satisfy certain sum rules, and we note in passing that Hansson and Watson corrected some errors in the expressions for perpendicular singlet (Hansson & Watson 2005) and perpendicular multiplet dipole transitions (Watson 2008). The Hönl-London factors for the $B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$ system of N_2^+ , which are parallel transitions, were first derived by Mulliken (1931). To summarise, we provide in the present work Einstein A coefficients for the first negative

Table 1. Experimentally derived vs. computed energies of the $v = 0$ vibrational states of $^{14}\text{N}_2^+$, and relative energies.

State	Experiment (1)		Calculation A		Calculation B	
$X^2\Sigma_g^+$	1099.6	0	-109.017724	0	-109.014939	0
$A^2\Pi_u$	10116.1	9016.5	-108.976659	9012.88	-108.973968	8992.10
$B^2\Sigma_u^+$	26665.6	25566.0	-108.901214	25571.26	-108.898416	25573.90

Notes. Experimental energy values are with respect to the minimum of the electronic ground-state potential. Computed energy values are given in Hartree units (E_h), and the experimental and relative energy values are given in cm^{-1} . All calculations are MRCI-F12b with core correlation and relativistic correction (DKHO=8, DKHP=2), A: basis=aug-cc-pCVQZ-F12, B: basis=cc-pVQZ-F12.

References. (1) Singh & Rai (1966).

Table 2. $X^2\Sigma_g^+$: computed vibrational energies, rotational constants, and their comparison with experiment.

v	E_v	$E_v^{(1)}$	Diff.	B_v	$D_v \times 10^6$	$B_v^{(1)}$	$D_v^{(2)} \times 10^6$
0	0.00	0.00	0.00	1.9229	5.91	1.92229	5.9099
1	2175.62	2186.30	-10.68	1.9039	5.96	1.90350	5.9223
2	4318.73	4318.10	0.63	1.8848	6.02	1.88422	5.9350
3	6429.17	6436.90	-7.73	1.8656	6.07	1.8651	5.9354
4	8506.64	8490.90	15.74	1.8462	6.14	1.8459	5.8864
5	10551.06	10548.60	2.46	1.8266	6.21	1.8265	5.7508
6	12562.02	12552.20	9.82	1.8068	6.30	1.8060	5.352
7	14539.71	14530.10	9.61	1.7869	6.40	1.7855	5.763
8	16484.00	16470.80	13.20	1.7668	6.49	1.766	6.560

Notes. Energy values are relative to the vibrational zero-point energy reported in Table 1. All data are given in cm^{-1} .

References. (1) Lofthus & Krupenie (1977), (2) Gottscho et al. (1979).

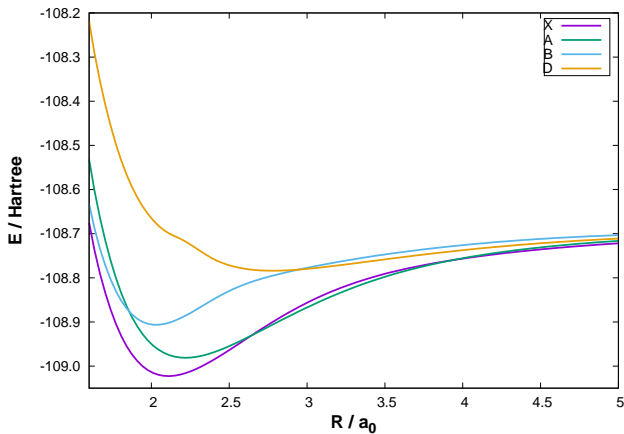


Fig. 1. Potential energy curves of the four lowest electronic doublet states, $X^2\Sigma_g^+$, $A^2\Pi_u$, $B^2\Sigma_u^+$, and $D^2\Pi_g$. Atomic units are used: 1 Hartree (E_h) = 27.211... eV, 1 Bohr (a_0) = 5.29177... 10^{-11} m.

band of N_2^+ with much higher precision than reported before. These data were used in the companion publication to analyse the fluorescence spectrum of comet C/2016 R2 (Rousselot et al. 2022).

2. Computational and theoretical approach

2.1. Lowest electronic states of N_2^+ and transition dipole moments

Electronic structure calculations for N_2^+ are not trivial due to many curve crossings, as shown in Fig. 1 for the four lowest doublet states or in Fig. 1 of Cartwright & Dunning (1975) for full appreciation. Multi-reference approaches are therefore

necessary. The potential energy and transition dipole moment curves for the three lowest doublet states of N_2^+ were computed from first principles with the Molpro package (Werner et al. 2021) using the explicitly correlated MRCI-F12b method with Davidson correction and the large aug-cc-pCVQZ-F12 basis. Moreover, all electrons were correlated, including atomic 1s electrons, and scalar relativistic corrections were applied using the eighth-order Douglas-Kroll-Hess Hamiltonian. Our approach goes beyond the level of theory reported before (see e.g. Cartwright & Dunning 1975; Langhoff & Bauschlicher 1988; Spelsberg & Meyer 2001; Polák & Fišer 2003; Bruna & Grein 2004; Shi et al. 2011; Liu et al. 2014; Ayari et al. 2020 and references therein). The accuracy obtained here is demonstrated in Table 1, where the energy values corresponding to the minima of the potential curves including the vibrational zero-point energy are presented and compared with data derived from experiments. The error is about 5 cm^{-1} . The rovibrational calculations of the lowest vibrational states on the X and B potential energy curves, which are of interest to the present work, are also more accurate than reported before, as can be inferred from Tables 2 and 3.

The potential energy curves $V(R)$ were computed in D_{2h} symmetry between $1.3 a_0 \leq R \leq 10 a_0$ on a very fine grid with spacing $\Delta R = 0.01 a_0$. MRCI transition dipole matrix elements were computed in C_s symmetry with a somewhat larger spacing $\Delta R = 0.05 a_0$.

The rovibrational energies and wavefunctions were computed with our own Numerov code by numerical integration of the rovibrational Schrödinger equation

$$\left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + V(R) + \frac{\hbar^2 N(N+1)}{2\mu R^2} - E_{vN} \right) \Psi_{vN}(R) = 0, \quad (1)$$

Table 3. $B^2\Sigma_u^+$: computed vibrational energies, rotational constants, and their comparison with experiment.

v	E_v	$E_v^{(1)}$	Diff.	B_v	$D_v \times 10^6$	$B_v^{(1)}$	$D_v^{(1)} \times 10^6$
0	0.00	0.00	0.00	2.0750	6.24	2.07461	6.33
1	2373.63	2371.62	2.01	2.0520	6.46	2.05171	6.53
2	4695.10	4690.59	4.51	2.0276	6.67	2.02750	6.89
3	6958.96	6951.54	7.42	2.0013	7.03	2.00083	7.12
4	9159.11	9148.14	10.97	1.9728	7.46	1.97220	7.79
5	11287.52	11272.04	15.48	1.9411	8.11	1.9394	7.8
6	13334.82	13313.43	21.39	1.9055	8.96	1.90398	9.4
7	15289.05	15260.69	28.36	1.8649	10.09	1.86191	9.2
8	17137.77	17101.39	36.38	1.8189	11.37	1.81558	10.8

Notes. Energy values are relative to the vibrational zero-point energy reported in Table 1. All data are given in cm^{-1} .

References. (1) Klynning & Pagès (1982).

Table 4. Hönl-London factors for ${}^2\Sigma - {}^2\Sigma$ transitions expressed in terms of $N = N''$ (third column) or $J = J''$ (fourth column).

Branch	J	$S(0, N', 0, N'')$	$S(0, J', 0, J'')$
P_1	$N + 1/2$	$\frac{2N(N+1)}{2N+1}$	$\frac{J^2-1/4}{J}$
R_1	$N + 1/2$	$\frac{2(N+1)(N+2)}{2N+3}$	$\frac{(J+1)^2-1/4}{J+1}$
${}^R Q_{21}$	$N + 1/2$	$\frac{2(N+1)}{(2N+1)(2N+3)}$	$\frac{2J+1}{4J(J+1)}$
${}^P Q_{12}$	$N - 1/2$	$\frac{2N}{(2N-1)(2N+1)}$	$\frac{2J+1}{4J(J+1)}$
P_2	$N - 1/2$	$\frac{2N(N-1)}{2N-1}$	$\frac{J^2-1/4}{J}$
R_2	$N - 1/2$	$\frac{2N(N+1)}{2N+1}$	$\frac{(J+1)^2-1/4}{J+1}$
$I_1 = I(P_1 + {}^R Q + R_1)$		$2(N + 1)$	$2J + 1$
$I_2 = I(P_2 + {}^P Q + R_2)$		$2N$	$2J + 1$
$I_1 + I_2$		$2(2N + 1)$	$2(2J + 1)$

where $N = J - S$ is the total angular momentum minus the spin, a good quantum number for Hund's case b molecules. Each rovibrational level E_{vN} is weakly split into two components denoted as F_1 and F_2 , which correspond to $J = N + 1/2$ and $J = N - 1/2$, respectively. The energy splitting is $\Delta E = E(F_1) - E(F_2) = \gamma(N + 1/2)$, where γ is the spin-rotation constant. Gottscho et al. (1979) reported numerical values for the spin-rotation constant of the order of 10^{-2} cm^{-1} . Although corrections could have been applied to the potential $V(R)$, this has not been done as the splitting is too small to be resolved within the present theoretical approach. It can be accounted for by substituting experimental transition frequencies in the expressions for the Einstein coefficients. Rotational constants were obtained as

$$B_{vN} = \left\langle vN \left| \frac{1}{2\mu R^2} \right| vN \right\rangle \quad (2)$$

and then expanded in powers of $N(N + 1)$ as

$$B_{vN}N(N + 1) = B_vN(N + 1) - D_v[N(N + 1)]^2 + \dots \quad (3)$$

2.2. Electric dipole transitions

Electric dipole transitions (E1 transitions) between two ${}^2\Sigma$ electronic states ($\Lambda = 0$) must satisfy the selection rules $\Delta N = \pm 1$ and $\Delta J = 0, \pm 1$. Transitions with $\Delta J = \Delta N$ occur between F_1 or F_2 spin components, while transitions with $\Delta N = \pm 1$ and $\Delta J = 0$

require a spin flip. The Einstein coefficients read

$$A_{\Lambda'=0v'J' \rightarrow \Lambda''=0v''J''} = \left(\frac{16\pi^3 \nu^3}{3\epsilon_0 h c^3} \right) \frac{S(0, J', 0, J'')}{2J' + 1} \left| \langle v'N' | \mu_{\Lambda'\Lambda''} | v''N'' \rangle_R \right|^2 \quad (4)$$

$$A_{\Lambda'=0v'N' \rightarrow \Lambda''=0v''N''} = \left(\frac{16\pi^3 \nu^3}{3\epsilon_0 h c^3} \right) \frac{S(0, N', 0, N'')}{2J' + 1} \left| \langle v'N' | \mu_{\Lambda'\Lambda''} | v''N'' \rangle_R \right|^2. \quad (5)$$

In the above equations, ν is the transition frequency, ϵ_0 is the vacuum permittivity, h is the Planck constant, and c is the vacuum speed of light. $S(\Lambda', J', \Lambda'', J'')$ or $S(\Lambda', N', \Lambda'', N'')$ are the Hönl-London factors, first derived by Mulliken (1931). They are presented in Table 4 in terms of N and of J . As demonstrated in the table, they are normalised as

$$\sum_{J''} S(0, J', 0, J'') = (2 - \delta_{0,\Lambda'} \delta_{0,\Lambda''}) (2S' + 1)(2J' + 1) \quad (6)$$

$$\sum_{N''} S(0, N', 0, N'') = (2 - \delta_{0,\Lambda'} \delta_{0,\Lambda''}) (2S' + 1)(2N' + 1) \quad (7)$$

according to the standard convention (Whiting et al. 1980). The sum rule is satisfied for both $J = J'$ and $J = J''$, and the same is true for N . Schadee (1964) reported these factors using a normalisation that does not include the electronic spin term. His factors must be multiplied by two to normalise them according

Table 5. Allowed combinations of Ψ_{vib} , Ψ_{el} , Ψ_{rot} , and Ψ_{ns} as well as the statistical weights, g_{ns} , of the corresponding states.

Molecule	Electr. state	$\Psi_{\text{vib}} \times \Psi_{\text{el}}$	$\Psi_{\text{rot}} \times \Psi_{\text{ns}}$	N	I	g_{ns}
$^{14}\text{N}_2^+$	X	s	s	Even	0, 2	6
				Odd	1	3
	B	a	a	Even	1	3
				Odd	0, 2	6
$^{15}\text{N}_2^+$	X	s	a	Even	0	1
				Odd	1	3
	B	a	s	Even	1	3
				Odd	0	1

Notes. The product of the four terms must be symmetric, s , with respect to nuclear permutation for the $^{14}\text{N}_2^+$ molecule and anti-symmetric, a , for $^{15}\text{N}_2^+$.

to Eq. (6). The expression for the Einstein coefficients can be written explicitly as

$$A_{\Lambda'=0v'N' \rightarrow \Lambda''=0v''N''} = \frac{2 - \delta_{0,\Lambda'}}{2 - \delta_{0,\Lambda'+\Lambda''}} \left(\frac{16\pi^3 \nu^3}{3\epsilon_0 h c^3} \right) \frac{S(0, N', 0, N'')}{2J' + 1} \frac{|\langle v'N' | \mu_{\Lambda'\Lambda''} | v''N'' \rangle_R|^2}{(8)} \quad (8)$$

to indicate the normalisation, with an analogous expression using J instead of N . In the remainder of the text, we mostly suppress the labels for Λ in the expressions for the Einstein coefficients and the Hönl-London factors.

The radiative lifetime τ of a rovibrational state (v', J') is given by

$$1/\tau = \sum_{v'', J''} A_{v'J' \rightarrow v''J''}. \quad (9)$$

To obtain the intensity of the emission from a rovibrational state (v', J') , the Einstein coefficients must be multiplied with $N_{v', J'}$, the number of molecules in that state,

$$I = N_{v', J'} \sum_{v'', J''} A_{v'J' \rightarrow v''J''} \quad (10)$$

with

$$N_{v', J'} = \frac{g'_{\text{ns}}(2J' + 1)e^{-E(v', J')/kT}}{Q}, \quad (11)$$

where Q denotes the partition function. $N_{v', J'}$ is proportional to the statistical weight g' of the state. $g' = g'_{\text{ns}} \times (2N' + 1)$, if the levels with $\Sigma = \pm 1/2$ are counted separately. If this is not the case, as intensities are additive, there is an additional factor of two. g'_{ns} is the degeneracy of the nuclear spin state.

2.3. Symmetry considerations

To make this paper self-contained, we briefly state the well-known symmetry properties. The total wavefunction can be written as a product of vibrational, rotational, electronic, and nuclear spin functions,

$$\Psi = \Psi_{\text{vib}} \Psi_{\text{rot}} \Psi_{\text{el}} \Psi_{\text{ns}}. \quad (12)$$

Physically allowed functions for homonuclear N_2^+ must be either symmetric or anti-symmetric with respect to nuclear permutation, depending on the nitrogen isotope. The principal isotope of

nitrogen is ^{14}N , which is a boson with nuclear spin $i = 1$. The second stable isotope, far less abundant, is ^{15}N , a fermion with $i = 1/2$. The nuclear spin states of $^{14}\text{N}_2^+$ are $I = 2, 1, 0$. States with $I = 2$ and $I = 0$ are symmetric with respect to a permutation of the two nuclei, while $I = 1$ is anti-symmetric. The nuclear spin states of $^{15}\text{N}_2^+$ are $I = 1, 0$. States with $I = 1$ are symmetric, and the state with $I = 0$ is anti-symmetric. The behaviour of the electronic wavefunctions with respect to nuclear permutation is indicated by the g/u label. Hence $\Psi_{X^2\Sigma_g^+}$ is symmetric and $\Psi_{B^2\Sigma_u^+}$ is anti-symmetric. The vibrational function is symmetric. The rotational functions are symmetric for even N and anti-symmetric for odd N . The allowed combinations and degeneracy factors are presented in Table 5. For a $^2\Sigma$ electronic state, there is no electronic spin degeneracy because the two components have different energy. The statistical weights g_{ns} of the rovibrational functions in the electronic $B^2\Sigma_u^+$ state enter into Eq. (11) as g'_{ns} . For the mixed isotopologue, $^{14}\text{N}^{15}\text{N}^+$, no restrictions occur. The statistical weight is $g_{\text{ns}} = 6$ for all rovibronic states.

3. Results

Rousselot et al. (2022) compiled a list of accurate rovibronic frequencies for transitions between the three lowest vibrational levels of the B state and the eight lowest vibrational levels of the X state from the references cited in that paper. These bands were investigated in the present work. The Einstein coefficients were obtained numerically for angular momenta $N = 0, \dots, 50$ and are represented in terms of two sets of analytical expressions: In the first set, the square of the rovibrational transition dipole moment was fitted to a polynomial in N ,

$$|\langle v'N' | \mu_{\Lambda'\Lambda''} | v''N'' \rangle_R|^2 = \tilde{\mu}^2 (1 + \alpha N + \beta N^2), \quad (13)$$

where N is the smaller of N' and N'' . The Einstein coefficient then becomes

$$A_{v'N' \rightarrow v''N''} = \left(\frac{16\pi^3 \nu^{*3}}{3\epsilon_0 h c^3} \right) \frac{S(N', N'')}{2J' + 1} \tilde{\mu}^2 (1 + \alpha N + \beta N^2) \quad (14)$$

$$= 2.026 \times 10^{-6} \nu^{*3} \frac{S(N', N'')}{2J' + 1} \tilde{\mu}^2 (1 + \alpha N + \beta N^2).$$

In the above equations, the transition dipole moment is expressed in atomic units. ν^* is the (experimental) transition frequency measured in cm^{-1} . A is obtained in s^{-1} . The coefficients of the two fits, for $\Delta N = \pm 1$, are collected in Tables B.3 and B.4.

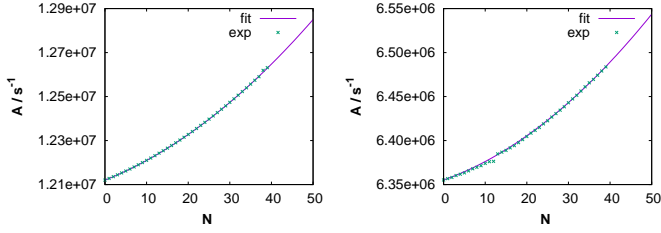


Fig. 2. $F_{v'=0N' \rightarrow v''=0N''}^{(1)}$ (left) and $F_{v'=0N' \rightarrow v''=1N''}^{(1)}$ (right) functions.

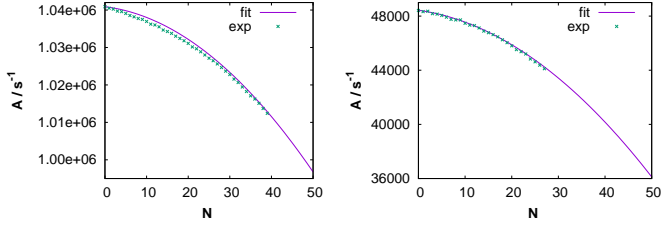


Fig. 3. $F_{v'=0N' \rightarrow v''=2N''}^{(1)}$ (left) and $F_{v'=0N' \rightarrow v''=3N''}^{(1)}$ (right) functions.

In the second set of fits, Tables B.1 and B.2, the complete radial part in Eq. (5) including the v^3 factor was represented by a polynomial in N ,

$$F_{v'N' \rightarrow v''N''} = \left(\frac{16\pi^3 v^3}{3\epsilon_0 h c^3} \right) |\langle v'N' | \mu_{\Lambda'\Lambda''} | v''N'' \rangle_R|^2 \quad (15)$$

$$= \tilde{A} (1 + aN + bN^2), \quad (16)$$

so that the Einstein coefficients can conveniently be evaluated through

$$A_{v'N' \rightarrow v''N''} \approx \frac{S(N', N'')}{2J' + 1} F_{v'N' \rightarrow v''N''}. \quad (17)$$

We have verified explicitly through sample calculations at $N = 100$ that the expansions are stable, allowing extrapolation. The fits may be used to compute Einstein coefficients for transitions without spin-flip, $\Delta N = \Delta J = \pm 1$, that is, the F_1 or F_2 branches, and for those with spin-flip, $\Delta N = \pm 1$ with $\Delta J = 0$, since electronic spin effects are not resolved in the present theoretical approach. The form of the expansion in Eq. (16) was chosen such that the parameter \tilde{A} , if desired, can be replaced by an experimental value. Figures 2 and 3 present examples of the fits for $v' = 0$ and $v'' = 0, 1, 2, 3$. Transitions from $v' = 0$ to higher vibrational levels of the X electronic state, $v'' > 4$, have very small Franck-Condon factors and the N -expansions are not meaningful. To the best of our knowledge, these angular momentum-dependent transition dipole moments have never before been reported in the literature.

The Einstein coefficients presented by Lofthus & Krupenie (1977) and by Gilmore et al. (1992) are somewhat different, as mentioned in the introduction. Lofthus and Krupenie reported the original data from Jain & Sahni (1967), who used RKR potentials and applied the R centroid method to estimate the transition dipole moments. The Einstein coefficients reported by Gilmore et al. (1992) are equally based on the experimental RKR potential energy curves, but the integrals over the transition dipole moments were evaluated numerically using RKR wavefunctions and a second-order fit in R of the ab initio transition dipole moments in Langhoff & Bauschlicher (1988). These dipole moments are more accurate than those used by previous works. The fit, however, does not reproduce some features of the

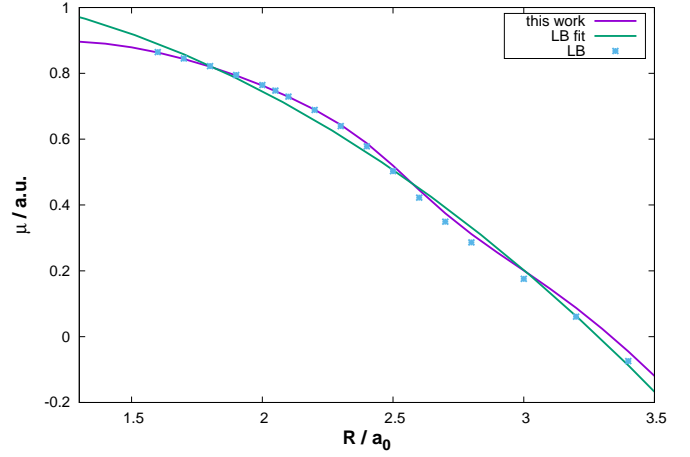


Fig. 4. Comparison of transition dipole moment functions. LB refers to Langhoff & Bauschlicher (1988), and LB-fit to a fit of their data by Gilmore et al. (1992). See main text for details. The dipole moment is expressed in atomic units: 1 a.u. = $ea_0 = 8.478353 \dots 10^{-30}$ Cm = 2.54175 Debye.

ab initio curve faithfully, such as the curvature near $R = 2.7 a_0$, which, as Langhoff & Bauschlicher (1988) wrote, is probably caused by the interaction between the B and C states. The two potential curves cross there, as shown in Fig. 1. Figure 4 demonstrates the limitations of the fit. It also shows that the present transition dipole moments and those computed by Langhoff and Bauschlicher are similar.

A comparison of purely vibrational A coefficients is provided in Table A.1. A (LB) and A (LB fit) were obtained using our ab initio potential energy curve and the transition moment based on the original data of Langhoff and Bauschlicher or based on Gilmore's fit, respectively. In A (exp) the experimental transition frequencies provided by Rousselot et al. (2022) were used together with the present ab initio data. A (Gilmore) and A (Jain) are taken from the respective publications. It can be seen that A (Gilmore) and A (LB fit) are very similar, but different from A (Jain). A (LB) and A (this work) are comparable. They are close to the RKR data reported in Table VII of Langhoff & Bauschlicher (1988), which are for $v' \leq 3$. The present A values are thus more accurate than those presented in the compilations by Lofthus & Krupenie (1977) or by Gilmore et al. (1992), and they are more complete than the data by Langhoff and Bauschlicher.

Tables B.1 and B.2 list the fit parameters from which very accurate rovibrational Einstein A coefficients can be computed according to Eqs. (16) and (17). No separation of vibrational and rotational motions was made. For transitions with very weak vibrational Franck-Condon factors, (<0.002), a fit is not meaningful, and a constant value of A should be used for all N .

Radiative lifetimes were computed according to Eq. (9). The vibrational lifetimes are collected in Table 6 for three isotopologues. As expected, they do not vary much upon isotopic substitution. A number of experiments were conducted quite some time ago to measure the lifetime of the $v' = 0$ vibrational state. The most recent data seem to be those by Scholl et al. (1995) and by Schmoranzler et al. (1989), who reported $\tau = 61.8 \pm 0.5$ ns and $\tau = 61.35 \pm 0.29$ ns, respectively. They are slightly higher than our ab initio value. Johnson & Fowler (1970) reported $\tau = 59.1 \pm 1.4$ ns for $v' = 0$ and $\tau = 58.5 \pm 1.4$ ns for $v' = 1$, which are close to the present values. However, as shown in the literature review by Johnson and Fowler or

Table 6. Radiative $B \rightarrow X$ lifetimes, in ns, of the lowest vibrational states of the three isotopologues $^{14}\text{N}_2^+$, $^{15}\text{N}_2^+$, and $^{14}\text{N}^{15}\text{N}^+$.

v'	τ		
	$^{14}\text{N}_2^+$	$^{14}\text{N}^{15}\text{N}^+$	$^{15}\text{N}_2^+$
0	58.820	58.829	58.837
1	57.988	58.003	58.025
2	57.500	57.514	57.526
3	57.400	57.399	57.388
4	57.755	57.710	57.667
5	58.677	58.563	58.454
6	60.326	60.102	59.885
7	62.971	62.574	62.189
8	66.950	66.282	66.643

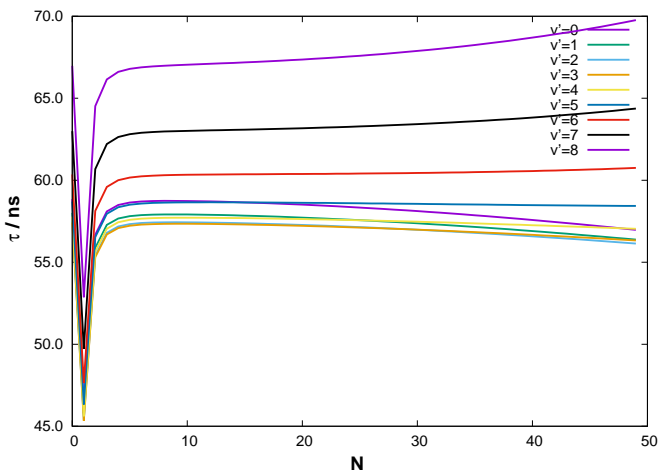


Fig. 5. Radiative rovibrational lifetimes, in ns, for B rovibrational states with $\Sigma = 1/2$ (F_1).

Schmoranzner et al., the experimental lifetimes vary considerable, between $\tau = 40 \pm 20$ ns and $\tau = 80 \pm 20$ ns.

It is instructive to analyse the radiative lifetimes with rotational resolution. These lifetimes were computed according to Eq. (9) for the F_1 and F_2 upper levels, and the three possible routes denoted I_1 and I_2 in Table 4 were accounted for each of them. They are presented graphically in Figs. 5 and 6. Considerable deviations from the vibrational lifetimes presented in Table 6 can be found for low values of N . The F_1 rovibrational lifetimes approach the vibrational lifetimes from below as N increases, while the F_2 rovibrational lifetimes approach them from above. This behaviour is real and follows from the numerical values of the Hönl-London factors. If the spin-splitting is neglected, that is, if the two spin-components are treated as a single rovibrational state, the lifetimes, computed as $1/\tau = 1/\tau(F_1) + 1/\tau(F_2)$, yield average values that vary very little with the rotational quantum number N . This is demonstrated in Fig. 7 for the vibrational ground state $v' = 0$. In these calculations, the degree of degeneracy in Eqs. (4) and (5) must be set to $2(2J' + 1)$. This large variation of τ for low values of N might perhaps explain the spread in the experimental lifetimes.

4. Conclusions

Very accurate rovibronic Einstein A coefficients for transitions between the $B^2\Sigma_u^+$ and $X^2\Sigma_g^+$ electronic states of N_2^+ were computed for N up to 50 and represented in a compact form.

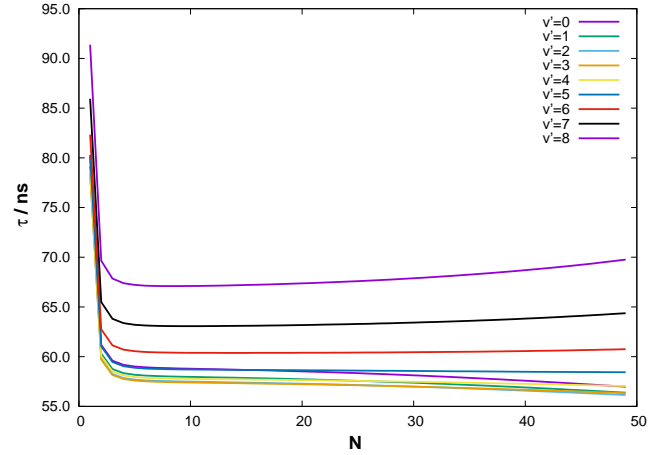


Fig. 6. Radiative rovibrational lifetimes, in ns, for B rovibrational states with $\Sigma = -1/2$ (F_2).

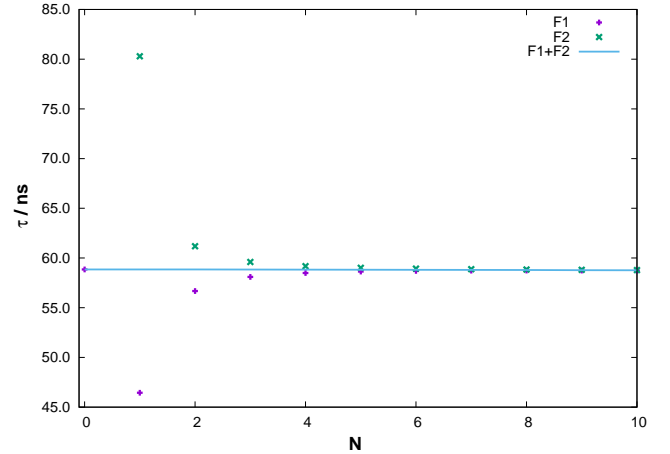


Fig. 7. Radiative lifetimes, in ns, for B rovibrational levels belonging to $v' = 0$ and the F_1 and F_2 spin components. The average value is also shown.

Rovibrational wavefunctions were used for the two electronic states, that is, no separation of vibration and rotation was assumed. Data for the principal isotopologue $^{14}\text{N}_2^+$ as well as those for $^{14}\text{N}^{15}\text{N}^+$ and the rare $^{15}\text{N}_2^+$ are collected in the appendix. These coefficients were used in the companion paper on comet spectra, Rousselot et al. (2022). That work is based on unique observational data obtained for comet C/2016 R2 in February 2018 with the 8 m Very large Telescope (VLT) of the European Southern Observatory equipped with a high-resolution spectrograph (spectral resolution of about 0.06 \AA). These spectra clearly show tens of emission lines with a good signal-to-noise ratio belonging to the (0,0) and (1,1) band of the $B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$ transition. These spectra reveal differences between the near-nucleus region, corresponding to ‘‘young’’ N_2^+ ions that are freshly created by photoionisation of N_2 , and spectra at the extremities of the slit, corresponding to a projected distance of about 6000 km from the nucleus, that is, at least a few thousand seconds of travel time from it. This difference is interpreted in terms of time necessary to reach a fluorescence equilibrium (because pure rotational transitions are forbidden), and the spectra obtained at the end of the slit can be satisfactorily explained by a Monte Carlo simulation based on the transition probabilities computed in this work. Some fluorescence efficiencies (the number of photons $\text{s}^{-1} \text{ ion}^{-1}$, which depends on the

solar radiation density received by the comet) were also computed, allowing a quantitative study of the N_2 production rate in this comet and in future comets with a significant amount of this species. These fluorescence efficiencies diverge by about 30% from the previous estimates (Lutz et al. 1993) and predict a correct ratio of the (1,1) and (0,0) bands (in contrast to the previous estimate of these factors). Given the importance of N_2 in comets, these improved transition probabilities will be very useful for tracing the physical properties during their formation process.

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Appendix A: Vibrational Einstein coefficients for the $^{14}\text{N}_2^+$ isotopologue

Table A.1. Vibrational transition dipole moments (μ , in atomic units), Franck-Condon factors (FC), R -centroids (in Angstrom) and a comparison of vibrational Einstein A coefficients (in s^{-1}) for electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. v' and v'' denote the vibrational quantum numbers of the B and X electronic states, using standard spectroscopic notation.

v'	v''	μ^2	FC	R -centroid	A (this work)	A (LB)	A (LB fit)	A (Gilmore)	A (Jain)	A (exp)
0	0	0.35778	0.66043	1.09936	0.12120E+08	0.12141E+08	0.11358E+08	0.11400E+08	0.96400E+07	0.12113E+08
1	0	0.14381	0.29338	1.15234	0.63585E+07	0.63509E+07	0.58055E+07	0.57600E+07	0.48700E+07	0.63533E+07
2	0	0.01855	0.04395	1.21807	0.10422E+07	0.10338E+07	0.92433E+06	0.90200E+06	0.75700E+06	0.10412E+07
3	0	0.00070	0.00223	1.31924	0.48538E+05	0.47044E+05	0.41779E+05	0.39800E+05	0.28100E+05	0.48473E+05
4	0	0.00000	0.00001	1.78097	0.21028E+01	0.16024E-01	0.33176E+01	0.22100E+00		0.20996E+01
5	0	0.00000	0.00000	1.16099	0.15460E+03	0.16415E+03	0.11483E+03	0.10200E+03		0.15422E+03
6	0	0.00000	0.00000	1.48536	0.28261E+01	0.27201E+01	0.18746E+01	0.84300E+00		
7	0	0.00000	0.00000	1.01526	0.59942E+00	0.66884E+00	0.39725E+00	0.44100E+00		
0	1	0.15065	0.25483	1.05085	0.39087E+07	0.39248E+07	0.37421E+07	0.37100E+07	0.34800E+07	0.39064E+07
1	1	0.12291	0.23395	1.11124	0.42613E+07	0.42601E+07	0.39862E+07	0.40300E+07	0.30800E+07	0.42580E+07
2	1	0.19247	0.40165	1.16065	0.86439E+07	0.86190E+07	0.78847E+07	0.78800E+07	0.63600E+07	0.86353E+07
3	1	0.04222	0.10307	1.22733	0.23924E+07	0.23662E+07	0.21232E+07	0.20800E+07	0.16400E+07	0.23892E+07
4	1	0.00187	0.00648	1.33835	0.13051E+06	0.12523E+06	0.11307E+06	0.10800E+06	0.62300E+05	0.13031E+06
5	1	0.00001	0.00000	2.73467	0.45079E+03	0.60978E+03	0.31441E+03	0.16500E+04		0.44963E+03
6	1	0.00001	0.00002	1.23182	0.10006E+04	0.10436E+04	0.74676E+03	0.63500E+03		
7	1	0.00000	0.00000	1.68778	0.17132E+01	0.11743E+01	0.10411E+01	0.28400E-02		
0	2	0.04176	0.06654	1.01127	0.81220E+06	0.81593E+06	0.79329E+06	0.78400E+06	0.77500E+06	0.81179E+06
1	2	0.16867	0.28836	1.05663	0.45068E+07	0.45245E+07	0.43028E+07	0.42800E+07	0.38700E+07	0.45035E+07
2	2	0.02756	0.05622	1.13492	0.97552E+06	0.96981E+06	0.91309E+06	0.92700E+06	0.57400E+06	0.97457E+06
3	2	0.19393	0.41593	1.17003	0.88220E+07	0.87762E+07	0.80480E+07	0.80900E+07	0.62400E+07	0.88099E+07
4	2	0.06399	0.16179	1.23751	0.36465E+07	0.35934E+07	0.32429E+07	0.31900E+07	0.23500E+07	0.36408E+07
5	2	0.00285	0.01107	1.36348	0.19894E+06	0.18799E+06	0.17430E+06	0.16400E+06	0.72600E+05	0.19841E+06
6	2	0.00007	0.00002	0.10585	0.60591E+04	0.69619E+04	0.45578E+04	0.11800E+04		
7	2	0.00003	0.00008	1.29543	0.31318E+04	0.31894E+04	0.23609E+04	0.19900E+04		
0	3	0.00960	0.01458	0.97580	0.13644E+06	0.13708E+06	0.13563E+06	0.13500E+06	0.13600E+06	0.13639E+06
1	3	0.08082	0.12989	1.01663	0.16310E+07	0.16383E+07	0.15890E+07	0.15700E+07	0.15300E+07	0.16300E+07
2	3	0.13443	0.23235	1.06237	0.36891E+07	0.37029E+07	0.35120E+07	0.34700E+07	0.30300E+07	0.36857E+07
3	3	0.00115	0.00361	1.25765	0.41362E+05	0.39322E+05	0.39724E+05	0.37700E+05	0.36200E+04	0.41306E+05
4	3	0.17689	0.39254	1.18093	0.81238E+07	0.80551E+07	0.74228E+07	0.74600E+07	0.55500E+07	0.81111E+07
5	3	0.08073	0.21283	1.24891	0.46087E+07	0.45202E+07	0.41147E+07	0.40700E+07	0.27800E+07	0.45962E+07
6	3	0.00294	0.01362	1.39991	0.20398E+06	0.18781E+06	0.18239E+06	0.18200E+06		
7	3	0.00038	0.00036	0.94040	0.31040E+05	0.33627E+05	0.24067E+05	0.16800E+05		
0	4	0.00200	0.00292	0.94355	0.20169E+05	0.20260E+05	0.20366E+05	0.20700E+05	0.20600E+05	0.20165E+05
1	4	0.02654	0.04060	0.98100	0.39498E+06	0.39682E+06	0.39165E+06	0.39200E+06	0.39200E+07	0.39478E+06
2	4	0.10183	0.16507	1.02187	0.21255E+07	0.21349E+07	0.20658E+07	0.20400E+07	0.19400E+07	0.21238E+07
3	4	0.08959	0.15652	1.06789	0.25166E+07	0.25258E+07	0.23886E+07	0.23200E+07	0.19800E+07	0.25133E+07
4	4	0.00307	0.00347	0.92487	0.11221E+06	0.11709E+06	0.10102E+06	0.11900E+06	0.15400E+06	0.11204E+06
5	4	0.15727	0.36434	1.19380	0.72618E+07	0.71681E+07	0.66593E+07	0.66800E+07	0.48300E+07	0.72417E+07

Continued on next page

Table A.1. continued.

v'	v''	μ^2	FC	R -centroid	A (this work)	A (LB)	A (LB fit)	A (Gilmore)	A (Jain)	A (exp)
6	4	0.09123	0.25301	1.26194	0.51923E+07	0.50616E+07	0.46647E+07	0.46900E+07		
7	4	0.00181	0.01188	1.46349	0.12390E+06	0.10755E+06	0.11586E+06	0.13900E+06		
0	5	0.00040	0.00056	0.91381	0.27243E+04	0.27359E+04	0.27908E+04	0.29700E+04	0.28300E+04	0.27245E+04
1	5	0.00722	0.01061	0.94878	0.76996E+05	0.77352E+05	0.77558E+05	0.79400E+05	0.78500E+05	0.76974E+05
2	5	0.04502	0.06935	0.98600	0.69896E+06	0.70223E+06	0.69143E+06	0.69000E+06	0.68000E+06	0.69850E+06
3	5	0.10448	0.17087	1.02696	0.22475E+07	0.22571E+07	0.21794E+07	0.21300E+07	0.20000E+07	0.22448E+07
4	5	0.05202	0.09170	1.07257	0.14899E+07	0.14956E+07	0.14090E+07	0.13100E+07	0.11400E+07	0.14877E+07
5	5	0.01210	0.01679	1.00694	0.44648E+06	0.45950E+06	0.40424E+06	0.45900E+06	0.43100E+06	0.44522E+06
6	5	0.14310	0.34981	1.20893	0.66095E+07	0.64854E+07	0.60984E+07	0.59700E+07		
7	5	0.09439	0.27873	1.27720	0.53246E+07	0.51501E+07	0.48274E+07	0.50200E+07		
0	6	0.00008	0.00011	0.88611	0.34168E+03	0.34310E+03	0.35475E+03	0.41500E+03		0.34186E+03
1	6	0.00177	0.00251	0.91911	0.13048E+05	0.13107E+05	0.13333E+05	0.14500E+05		0.13048E+05
2	6	0.01536	0.02270	0.95384	0.17265E+06	0.17347E+06	0.17350E+06	0.17900E+06		0.17258E+06
3	6	0.05998	0.09303	0.99067	0.96756E+06	0.97207E+06	0.95503E+06	0.94900E+06		0.96652E+06
4	6	0.09456	0.15610	1.03197	0.20871E+07	0.20956E+07	0.20198E+07	0.19300E+07		0.20842E+07
5	6	0.02654	0.04682	1.07432	0.77139E+06	0.77513E+06	0.72570E+06	0.61200E+06		0.76921E+06
6	6	0.01865	0.02530	0.99940	0.69071E+06	0.71257E+06	0.62131E+06	0.76400E+06		
7	6	0.13799	0.35967	1.22604	0.63355E+07	0.61709E+07	0.58971E+07	0.55000E+07		
0	7	0.00001	0.00002	0.85999	0.39812E+02	0.40000E+02	0.41859E+02	0.57400E+02		0.39861E+02
1	7	0.00041	0.00056	0.89156	0.19917E+04	0.20008E+04	0.20624E+04	0.24800E+04		0.19927E+04
2	7	0.00452	0.00646	0.92426	0.35648E+05	0.35814E+05	0.36340E+05	0.40000E+05		0.35646E+05
3	7	0.02495	0.03711	0.95861	0.29428E+06	0.29568E+06	0.29508E+06	0.30600E+06		0.29405E+06
4	7	0.06875	0.10731	0.99487	0.11466E+07	0.11519E+07	0.11294E+07	0.11100E+07		0.11452E+07
5	7	0.07879	0.13146	1.03712	0.17749E+07	0.17816E+07	0.17150E+07	0.15700E+07		0.17700E+07
6	7	0.01179	0.02018	1.06524	0.34566E+06	0.34866E+06	0.32186E+06	0.20300E+06		
7	7	0.01947	0.02287	0.94287	0.71913E+06	0.74994E+06	0.63727E+06	0.89000E+06		

Appendix B: Expansion parameters for the $^{14}\text{N}_2^+$ isotopologue

Table B.1. Isotopologue $^{14}\text{N}^{14}\text{N}^+$: Franck-Condon factors (FC) and parameters for the evaluation of rovibrational Einstein A coefficients for $\Delta N = N' - N'' = 1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$

v'	v''	FC	\tilde{A} (this work)	\tilde{A} (exp)	a	b
0	0	0.66051	0.12128E+08	0.12120E+08	0.62136E-03	0.11646E-04
1	0	0.29334	0.63603E+07	0.63553E+07	0.26433E-03	0.65655E-05
2	0	0.04392	0.10419E+07	0.10409E+07	-0.13235E-03	-0.14309E-04
3	0	0.00223	0.48480E+05	0.48415E+05	-0.99177E-03	-0.81785E-04
4	0	0.00001	0.19279E+01	0.19250E+01		
5	0	0.00000	0.15450E+03	0.15427E+03		
6	0	0.00000	0.28189E+01			
7	0	0.00000	0.60040E+00			
0	1	0.25479	0.39102E+07	0.39079E+07	0.40561E-03	0.15030E-04
1	1	0.23407	0.42656E+07	0.42623E+07	0.10012E-02	0.14570E-04
2	1	0.40163	0.86469E+07	0.86384E+07	0.38945E-03	0.69807E-05
3	1	0.10301	0.23918E+07	0.23886E+07	-0.78061E-04	-0.20763E-04
4	1	0.00647	0.13027E+06	0.13007E+06	-0.13617E-02	-0.10938E-03
5	1	0.00000	0.45313E+03	0.45245E+03		
6	1	0.00002	0.10003E+04			
7	1	0.00000	0.16891E+01			
0	2	0.06652	0.81234E+06	0.81194E+06	0.21646E-03	0.25051E-04
1	2	0.28835	0.45091E+07	0.45059E+07	0.57283E-03	0.10828E-04
2	2	0.05631	0.97764E+06	0.97670E+06	0.17884E-02	0.38892E-04
3	2	0.41597	0.88265E+07	0.88146E+07	0.51512E-03	0.10714E-04
4	2	0.16169	0.36453E+07	0.36396E+07	-0.50338E-05	-0.29091E-04
5	2	0.01105	0.19865E+06	0.19835E+06	-0.20907E-02	-0.14863E-03
6	2	0.00002	0.60786E+04			
7	2	0.00008	0.31285E+04			
0	3	0.01457	0.13644E+06	0.13639E+06	0.45295E-04	0.38705E-04
1	3	0.12985	0.16315E+07	0.16305E+07	0.33015E-03	0.19193E-04
2	3	0.23240	0.36918E+07	0.36885E+07	0.77551E-03	0.81510E-05
3	3	0.00364	0.41758E+05	0.41702E+05	0.39115E-02	0.40886E-03
4	3	0.39267	0.81295E+07	0.81169E+07	0.64018E-03	0.19142E-04
5	3	0.21273	0.46079E+07	0.46010E+07	0.81420E-04	-0.40811E-04
6	3	0.01359	0.20348E+06		-0.41868E-02	-0.19520E-03
7	3	0.00036	0.31083E+05			
0	4	0.00292	0.20162E+05	0.20158E+05	-0.12039E-03	0.56073E-04
1	4	0.04058	0.39506E+06	0.39487E+06	0.13631E-03	0.31659E-04
2	4	0.16504	0.21263E+07	0.21246E+07	0.45557E-03	0.13547E-04
3	4	0.15660	0.25192E+07	0.25160E+07	0.10407E-02	0.85220E-05
4	4	0.00345	0.11156E+06	0.11139E+06	-0.58304E-02	-0.14324E-03
5	4	0.36450	0.72678E+07	0.72571E+07	0.75732E-03	0.33453E-04
6	4	0.25287	0.51908E+07		0.19561E-03	-0.59765E-04
7	4	0.01185	0.12343E+06		0.10504E+59	
0	5	0.00056	0.27227E+04	0.27230E+04		
1	5	0.01060	0.77003E+05	0.76983E+05	-0.36681E-04	0.47878E-04
2	5	0.06931	0.69904E+06	0.69859E+06	0.24375E-03	0.23950E-04
3	5	0.17086	0.22486E+07	0.22460E+07	0.59278E-03	0.86457E-05
4	5	0.09180	0.14923E+07	0.14901E+07	0.14001E-02	0.15352E-04
5	5	0.01673	0.44546E+06	0.44483E+06	-0.22108E-02	-0.13963E-03
6	5	0.35003	0.66164E+07		0.86548E-03	0.52922E-04
7	5	0.27857	0.53227E+07			
0	6	0.00010	0.34151E+03	0.34169E+03		
1	6	0.00251	0.13046E+05	0.13046E+05	-0.20609E-03	0.68280E-04
2	6	0.02268	0.17264E+06	0.17257E+06	0.65381E-04	0.38573E-04
3	6	0.09300	0.96778E+06	0.96677E+06	0.35068E-03	0.16047E-04
4	6	0.15611	0.20884E+07	0.20856E+07	0.74363E-03	0.53613E-05

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Table B.1. Einstein coefficients $\Delta J = 0, 1, \Delta N = 1$, continued.

v'	v''	FC	\tilde{A} (this work)	\tilde{A} (exp)	a	b
5	6	0.04689	0.77291E+06	0.77190E+06	0.19241E-02	0.35275E-04
6	6	0.02522	0.68939E+06		-0.16861E-02	-0.16213E-03
7	6	0.35993	0.63426E+07			
0	7	0.00002	0.39822E+02	0.39872E+02		
1	7	0.00056	0.19909E+04	0.19920E+04		
2	7	0.00645	0.35643E+05	0.35641E+05	-0.10719E-03	0.57277E-04
3	7	0.03709	0.29429E+06	0.29407E+06	0.16177E-03	0.28539E-04
4	7	0.10727	0.11468E+07	0.11455E+07	0.46505E-03	0.78710E-05
5	7	0.13150	0.17764E+07	0.17744E+07	0.90697E-03	0.50515E-05
6	7	0.02023	0.34678E+06		0.27224E-02	0.82949E-04
7	7	0.02280	0.71782E+06			

Table B.2. Isotopologue ¹⁴N¹⁴N⁺: Franck-Condon factors (FC) and parameters for the evaluation of rovibrational Einstein A coefficients for $\Delta N = N' - N'' = -1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$

v'	v''	FC	\tilde{A} (this work)	\tilde{A} (exp)	a	b
0	0	0.66034	0.12113E+08	0.12106E+08	-0.57785E-03	0.11380E-04
1	0	0.29345	0.63574E+07	0.63522E+07	-0.17837E-03	0.73219E-05
2	0	0.04398	0.10425E+07	0.10414E+07	0.38219E-03	-0.12457E-04
3	0	0.00223	0.48562E+05	0.48496E+05	0.13776E-02	-0.86916E-04
4	0	0.00001	0.21511E+01	0.21478E+01		
5	0	0.00000	0.15386E+03	0.15348E+03		
6	0	0.00000	0.28528E+01			
7	0	0.00000	0.56872E+00			
0	1	0.25486	0.39071E+07	0.39049E+07	-0.29465E-03	0.15440E-04
1	1	0.23384	0.42574E+07	0.42542E+07	-0.10559E-02	0.12950E-04
2	1	0.40167	0.86408E+07	0.86324E+07	-0.31828E-03	0.76521E-05
3	1	0.10312	0.23927E+07	0.23895E+07	0.34641E-03	-0.18510E-04
4	1	0.00649	0.13067E+06	0.13047E+06	0.13703E-02	-0.11859E-03
5	1	0.00000	0.44544E+03	0.44431E+03		
6	1	0.00002	0.10002E+04			
7	1	0.00000	0.18550E+01			
0	2	0.06657	0.81207E+06	0.81166E+06	-0.83555E-04	0.25936E-04
1	2	0.28835	0.45044E+07	0.45012E+07	-0.46570E-03	0.11080E-04
2	2	0.05614	0.97369E+06	0.97276E+06	-0.22301E-02	0.30728E-04
3	2	0.41590	0.88178E+07	0.88058E+07	-0.48673E-03	0.11223E-04
4	2	0.16186	0.36469E+07	0.36412E+07	0.33649E-03	-0.25933E-04
5	2	0.01108	0.19918E+06	0.19865E+06	0.13637E-02	-0.16765E-03
6	2	0.00002	0.60421E+04			
7	2	0.00008	0.31312E+04			
0	3	0.01459	0.13645E+06	0.13640E+06	0.69442E-04	0.40586E-04
1	3	0.12993	0.16306E+07	0.16296E+07	-0.17427E-03	0.19835E-04
2	3	0.23229	0.36864E+07	0.36830E+07	-0.69805E-03	0.83174E-05
3	3	0.00359	0.41002E+05	0.40947E+05	-0.10366E-01	0.22491E-03
4	3	0.39245	0.81187E+07	0.81061E+07	-0.67753E-03	0.19314E-04
5	3	0.21293	0.46093E+07	0.45969E+07	0.37028E-03	-0.36288E-04
6	3	0.01364	0.20432E+06		0.87469E-03	-0.24204E-03
7	3	0.00036	0.31010E+05			
0	4	0.00293	0.20173E+05	0.20170E+05	0.15533E-03	0.59577E-04
1	4	0.04062	0.39498E+06	0.39478E+06	0.24763E-04	0.33101E-04
2	4	0.16510	0.21248E+07	0.21231E+07	-0.28683E-03	0.14120E-04
3	4	0.15644	0.25140E+07	0.25108E+07	-0.10172E-02	0.86218E-05
4	4	0.00350	0.11277E+06	0.11259E+06	0.58939E-02	-0.21008E-03

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Table B.2. Einstein coefficients $\Delta J = 0, -1$, $\Delta N = -1$, continued.

v'	v''	FC	\tilde{A} (this work)	\tilde{A} (exp)	a	b
5	4	0.36420	0.72561E+07	0.72360E+07	-0.87863E-03	0.33084E-04
6	4	0.25313	0.51932E+07		0.48351E-03	-0.53195E-04
7	4	0.01191	0.12425E+06			
0	5	0.00056	0.27253E+04	0.27256E+04		
1	5	0.01062	0.77012E+05	0.76989E+05	0.14700E-03	0.50767E-04
2	5	0.06938	0.69891E+06	0.69845E+06	-0.25743E-04	0.25211E-04
3	5	0.17088	0.22464E+07	0.22437E+07	-0.42726E-03	0.93396E-05
4	5	0.09161	0.14877E+07	0.14855E+07	-0.14675E-02	0.14837E-04
5	5	0.01685	0.44751E+06	0.44625E+06	0.27014E-02	-0.15345E-03
6	5	0.34961	0.66033E+07		-0.10561E-02	0.52113E-04
7	5	0.27888	0.53259E+07			
0	6	0.00011	0.34179E+03	0.34197E+03		
1	6	0.00251	0.13050E+05	0.13051E+05	0.18822E-03	0.73334E-04
2	6	0.02272	0.17265E+06	0.17258E+06	0.14388E-03	0.41013E-04
3	6	0.09306	0.96731E+06	0.96629E+06	-0.89993E-04	0.17256E-04
4	6	0.15608	0.20857E+07	0.20829E+07	-0.59986E-03	0.63773E-05
5	6	0.04676	0.76991E+06	0.76775E+06	-0.21341E-02	0.32511E-04
6	6	0.02535	0.69147E+06		0.19601E-02	-0.17103E-03
7	6	0.35951	0.63299E+07			
0	7	0.00002	0.39828E+02	0.39878E+02		
1	7	0.00056	0.19923E+04	0.19934E+04		
2	7	0.00647	0.35655E+05	0.35653E+05	0.22013E-03	0.61651E-04
3	7	0.03713	0.29427E+06	0.29404E+06	0.12506E-03	0.30691E-04
4	7	0.10734	0.11462E+07	0.11449E+07	-0.17213E-03	0.94555E-05
5	7	0.13142	0.17734E+07	0.17685E+07	-0.80753E-03	0.64982E-05
6	7	0.02013	0.34468E+06		-0.31603E-02	0.72185E-04
7	7	0.02292	0.71994E+06			

Table B.3. Isotopologue $^{14}\text{N}^{14}\text{N}^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = N' - N'' = 1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. For transitions with very weak Franck-Condon factors, a constant value, μ_0^2 , should be used.

v'	v''	FC	μ_0^2	α	β
0	0	0.66051	0.33531E+00	0.11077E-03	-0.78211E-05
1	0	0.29334	0.13128E+00	-0.21542E-03	-0.79646E-05
2	0	0.04392	0.16443E-01	-0.61813E-03	-0.23099E-04
3	0	0.00223	0.59808E-03	-0.15377E-02	-0.81733E-04
4	0	0.00001	0.36667E-07		
5	0	0.00000	0.11306E-05		
6	0	0.00000	0.15668E-07		
7	0	0.00000	0.28784E-08		
0	1	0.25479	0.14421E+00	-0.15657E-03	-0.82019E-05
1	1	0.23407	0.11504E+00	0.51575E-03	-0.50839E-05
2	1	0.40163	0.17555E+00	-0.81529E-04	-0.68571E-05
3	1	0.10301	0.37445E-01	-0.56760E-03	-0.28044E-04
4	1	0.00647	0.16139E-02	-0.19172E-02	-0.10603E-03
5	1	0.00000	0.37393E-05		
6	1	0.00002	0.74334E-05		
7	1	0.00000	0.87365E-08		
0	2	0.06652	0.40774E-01	-0.38482E-03	-0.35052E-05
1	2	0.28835	0.16103E+00	0.14130E-04	-0.11508E-04
2	2	0.05631	0.25841E-01	0.13883E-02	0.16671E-04

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Table B.3. Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = 1$, continued.

v'	v''	FC	μ_0^2	α	β
3	2	0.41597	0.17693E+00	0.59267E-04	-0.24170E-05
4	2	0.16169	0.56866E-01	-0.49881E-03	-0.34463E-04
5	2	0.01105	0.24923E-02	-0.26225E-02	-0.14136E-03
6	2	0.00002	0.54536E-04		
7	2	0.00008	0.23849E-04		
0	3	0.01457	0.95373E-02	-0.58880E-03	0.29998E-05
1	3	0.12985	0.78721E-01	-0.27414E-03	-0.79137E-05
2	3	0.23240	0.12801E+00	0.22509E-03	-0.13400E-04
3	3	0.00364	0.11125E-02		
4	3	0.39267	0.16167E+00	0.20459E-03	0.68266E-05
5	3	0.21273	0.72037E-01	-0.41775E-03	-0.43719E-04
6	3	0.01359	0.26207E-02		
7	3	0.00036	0.29135E-03		
0	4	0.00292	0.20207E-02	-0.77699E-03	0.10785E-04
1	4	0.04058	0.26308E-01	-0.50595E-03	-0.20402E-05
2	4	0.16504	0.98949E-01	-0.15116E-03	-0.12011E-04
3	4	0.15660	0.85078E-01	0.50938E-03	-0.12566E-04
4	4	0.00345	0.27474E-02	-0.70000E-02	-0.13580E-03
5	4	0.36450	0.14428E+00	0.34437E-03	0.22249E-04
6	4	0.25287	0.81902E-01	-0.31017E-03	-0.59460E-04
7	4	0.01185	0.16818E-02		
0	5	0.00056	0.40594E-03		
1	5	0.01060	0.72698E-02	-0.70829E-03	0.53403E-05
2	5	0.06931	0.44512E-01	-0.41024E-03	-0.75167E-05
3	5	0.17086	0.10131E+00	-0.13325E-04	-0.15292E-04
4	5	0.09180	0.49253E-01	0.90715E-03	-0.59529E-05
5	5	0.01673	0.10928E-01	-0.31418E-02	-0.13902E-03
6	5	0.35003	0.13212E+00	0.46756E-03	0.43554E-04
7	5	0.27857	0.85513E-01	-0.19161E-03	-0.88076E-04
0	6	0.00010	0.79414E-04		
1	6	0.00251	0.18061E-02	-0.89255E-03	0.13778E-04
2	6	0.02268	0.15421E-01	-0.62667E-03	-0.94269E-06
3	6	0.09300	0.59182E-01	-0.31440E-03	-0.13011E-04
4	6	0.15611	0.91522E-01	0.14294E-03	-0.16877E-04
5	6	0.04689	0.25010E-01	0.15068E-02	0.12282E-04
6	6	0.02522	0.16733E-01	-0.26256E-02	-0.16079E-03
7	6	0.35993	0.12853E+00	0.63638E-03	0.64299E-04
0	7	0.00002	0.15376E-04		
1	7	0.00056	0.42203E-03		
2	7	0.00645	0.46071E-02	-0.82387E-03	0.68822E-05
3	7	0.03709	0.24997E-01	-0.55145E-03	-0.76870E-05
4	7	0.10727	0.67704E-01	-0.21061E-03	-0.18518E-04
5	7	0.13150	0.76160E-01	0.32041E-03	-0.15401E-04
6	7	0.02023	0.11012E-01	0.24621E-02	0.55074E-04
7	7	0.02280	0.17210E-01	-0.33516E-02	-0.19653E-03

Table B.4. Isotopologue $^{14}\text{N}^{14}\text{N}^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = N' - N'' = -1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. For transitions with very weak Franck-Condon factors, a constant value, μ_0^2 , should be used.

v'	v''	FC	μ_0^2	α	β
0	0	0.66034	0.35773E+00	-0.15224E-03	-0.62452E-05
1	0	0.29345	0.14385E+00	0.22024E-03	-0.65501E-05
2	0	0.04398	0.18565E-01	0.75467E-03	-0.22855E-04
3	0	0.00223	0.69653E-03	0.17317E-02	-0.94394E-04
4	0	0.00001	0.25311E-07		
5	0	0.00000	0.15170E-05		
6	0	0.00000	0.23888E-07		
7	0	0.00000	0.41099E-08		
0	1	0.25486	0.15067E+00	0.17515E-03	-0.66633E-05
1	1	0.23384	0.12285E+00	-0.65136E-03	-0.36158E-05
2	1	0.40167	0.19249E+00	0.69118E-04	-0.53826E-05
3	1	0.10312	0.42242E-01	0.70846E-03	-0.27967E-04
4	1	0.00649	0.18700E-02	0.17115E-02	-0.12506E-03
5	1	0.00000	0.52710E-05		
6	1	0.00002	0.99673E-05		
7	1	0.00000	0.15832E-07		
0	2	0.06657	0.41778E-01	0.45080E-03	-0.19984E-05
1	2	0.28835	0.16866E+00	-0.18419E-04	-0.98355E-05
2	2	0.05614	0.27522E-01	-0.18499E-02	0.15452E-04
3	2	0.41590	0.19392E+00	-0.10898E-03	-0.83697E-06
4	2	0.16186	0.64022E-01	0.69311E-03	-0.34350E-04
5	2	0.01108	0.28543E-02	0.16938E-02	-0.17306E-03
6	2	0.00002	0.72097E-04		
7	2	0.00008	0.31686E-04		
0	3	0.01459	0.96075E-02	0.69389E-03	0.50694E-05
1	3	0.12993	0.80846E-01	0.33183E-03	-0.66315E-05
2	3	0.23229	0.13440E+00	-0.27265E-03	-0.11286E-04
3	3	0.00359	0.11386E-02		
4	3	0.39245	0.17685E+00	-0.30884E-03	0.84513E-05
5	3	0.21293	0.80773E-01	0.72373E-03	-0.43445E-04
6	3	0.01364	0.29450E-02	0.11677E-02	-0.24587E-03
7	3	0.00036	0.37509E-03		
0	4	0.00293	0.20050E-02	0.90608E-03	0.14062E-04
1	4	0.04062	0.26558E-01	0.61222E-03	-0.52560E-06
2	4	0.16510	0.10184E+00	0.19145E-03	-0.10739E-04
3	4	0.15644	0.89538E-01	-0.61075E-03	-0.95735E-05
4	4	0.00350	0.30877E-02		
5	4	0.36420	0.15721E+00	-0.51995E-03	0.23785E-04
6	4	0.25313	0.91275E-01	0.84183E-03	-0.58960E-04
7	4	0.01191	0.18115E-02		
0	5	0.00056	0.39724E-03		
1	5	0.01062	0.72275E-02	0.84859E-03	0.77502E-05
2	5	0.06938	0.45040E-01	0.52454E-03	-0.63503E-05
3	5	0.17088	0.10448E+00	0.25281E-04	-0.13768E-04
4	5	0.09161	0.51968E-01	-0.10767E-02	-0.18112E-05
5	5	0.01685	0.12136E-01	0.30398E-02	-0.16435E-03
6	5	0.34961	0.14302E+00	-0.71372E-03	0.45040E-04
7	5	0.27888	0.94445E-01	0.10887E-02	-0.87706E-04
0	6	0.00011	0.76686E-04		
1	6	0.00251	0.17708E-02	0.10512E-02	0.17780E-04
2	6	0.02272	0.15366E-01	0.79395E-03	0.73009E-06
3	6	0.09306	0.59999E-01	0.42318E-03	-0.12033E-04

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Table B.4. Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = -1$, continued.

v'	v''	FC	μ_0^2	α	β
4	6	0.15608	0.94541E-01	-0.16991E-03	-0.14820E-04
5	6	0.04676	0.26506E-01	-0.17506E-02	0.17486E-04
6	6	0.02535	0.18675E-01	0.22804E-02	-0.17980E-03
7	6	0.35951	0.13792E+00	-0.79213E-03	0.66839E-04
0	7	0.00002	0.14657E-04		
1	7	0.00056	0.40855E-03		
2	7	0.00647	0.45275E-02	0.10169E-02	0.97056E-05
3	7	0.03713	0.24960E-01	0.72783E-03	-0.67007E-05
4	7	0.10734	0.68769E-01	0.30983E-03	-0.17412E-04
5	7	0.13142	0.78767E-01	-0.39535E-03	-0.12574E-04
6	7	0.02013	0.11765E-01	-0.27873E-02	0.59272E-04
7	7	0.02292	0.19496E-01	0.17689E-02	-0.22325E-03

Appendix C: Expansion parameters for the $^{14}\text{N}^{15}\text{N}^+$ isotopologue**Table C.1.** Isotopologue $^{14}\text{N}^{15}\text{N}^+$: Franck-Condon factors (FC) and parameters for the evaluation of rovibrational Einstein A coefficients for $\Delta N = N' - N'' = 1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$

v'	v''	FC	\tilde{A} (this work)	a	b
0	0	0.65575	0.12040E+08	0.60285E-03	0.11254E-04
1	0	0.29629	0.64088E+07	0.26231E-03	0.64356E-05
2	0	0.04551	0.10774E+07	-0.13649E-03	-0.12720E-04
3	0	0.00242	0.53204E+05	-0.99681E-03	-0.73407E-04
4	0	0.00001	0.20456E+02		
5	0	0.00000	0.15125E+03		
6	0	0.00000	0.37207E+01		
7	0	0.00000	0.49705E+00		
0	1	0.25740	0.39622E+07	0.39893E-03	0.14351E-04
1	1	0.22675	0.41317E+07	0.97474E-03	0.14218E-04
2	1	0.40231	0.86441E+07	0.38186E-03	0.70079E-05
3	1	0.10642	0.24693E+07	-0.66766E-04	-0.18852E-04
4	1	0.00710	0.14534E+06	-0.12229E-02	-0.10014E-03
5	1	0.00001	0.21572E+03		
6	1	0.00002	0.10136E+04		
7	1	0.00000	0.46358E+01		
0	2	0.06803	0.83734E+06	0.20974E-03	0.23981E-04
1	2	0.28878	0.45272E+07	0.55753E-03	0.10512E-04
2	2	0.05144	0.89150E+06	0.18096E-02	0.38034E-04
3	2	0.41265	0.87434E+07	0.50664E-03	0.10780E-04
4	2	0.16671	0.37622E+07	-0.85479E-06	-0.26063E-04
5	2	0.01232	0.22781E+06	-0.17716E-02	-0.13645E-03
6	2	0.00001	0.45510E+04		
7	2	0.00008	0.33231E+04		
0	3	0.01504	0.14281E+06	0.40599E-04	0.37009E-04
1	3	0.13211	0.16716E+07	0.32039E-03	0.18441E-04
2	3	0.23021	0.36643E+07	0.75979E-03	0.80125E-05
3	3	0.00232	0.23546E+05		
4	3	0.38508	0.79680E+07	0.63192E-03	0.19221E-04
5	3	0.21913	0.47619E+07	0.83600E-04	-0.36212E-04
6	3	0.01562	0.24664E+06	-0.32732E-02	-0.18326E-03
7	3	0.00026	0.26396E+05		
0	4	0.00304	0.21412E+05	-0.12519E-03	0.53541E-04
1	4	0.04174	0.41148E+06	0.13213E-03	0.30240E-04
2	4	0.16696	0.21649E+07	0.44216E-03	0.13129E-04
3	4	0.15286	0.24624E+07	0.10246E-02	0.85764E-05
4	4	0.00517	0.15084E+06	-0.43498E-02	-0.12979E-03
5	4	0.35284	0.70389E+07	0.74749E-03	0.33768E-04
6	4	0.26089	0.53902E+07	0.19364E-03	-0.52474E-04
7	4	0.01454	0.17151E+06		
0	5	0.00058	0.29338E+04		
1	5	0.01099	0.81401E+05	-0.34739E-04	0.45549E-04
2	5	0.07104	0.72481E+06	0.23271E-03	0.23045E-04
3	5	0.17176	0.22739E+07	0.57793E-03	0.85494E-05
4	5	0.08771	0.14264E+07	0.13889E-02	0.15763E-04
5	5	0.02061	0.52481E+06	-0.17516E-02	-0.12384E-03
6	5	0.33416	0.63279E+07	0.84497E-03	0.54224E-04
7	5	0.28928	0.55890E+07	0.32155E-03	-0.80580E-04
0	6	0.00011	0.37379E+03		
1	6	0.00262	0.13991E+05	-0.20119E-03	0.64800E-04
2	6	0.02346	0.18178E+06	0.55856E-04	0.36934E-04
3	6	0.09498	0.99909E+06	0.33564E-03	0.15673E-04
4	6	0.15578	0.20959E+07	0.72728E-03	0.55942E-05

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Table C.1. Isotopologue ¹⁴N¹⁵N⁺: Einstein coefficients $\Delta J = 0, 1, \Delta N = 1$, continued.

v'	v''	FC	\tilde{A} (this work)	a	b
5	6	0.04336	0.71338E+06	0.19284E-02	0.37053E-04
6	6	0.03049	0.79488E+06	-0.12690E-02	-0.14453E-03
7	6	0.33937	0.60000E+07	0.98728E-03	0.74655E-04
0	7	0.00002	0.44389E+02		
1	7	0.00059	0.21671E+04		
2	7	0.00672	0.38062E+05	-0.10622E-03	0.54485E-04
3	7	0.03826	0.30875E+06	0.15192E-03	0.27496E-04
4	7	0.10919	0.11792E+07	0.44850E-03	0.80727E-05
5	7	0.13005	0.17671E+07	0.89139E-03	0.55927E-05
6	7	0.01767	0.30108E+06	0.27498E-02	0.91321E-04
7	7	0.02872	0.83869E+06	-0.15609E-02	-0.18248E-03

Table C.2. Isotopologue ¹⁴N¹⁵N⁺: Franck-Condon factors (FC) and parameters for the evaluation of rovibrational Einstein A coefficients for $\Delta N = N' - N'' = -1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$

v'	v''	FC	\tilde{A} (this work)	a	b
0	0	0.65559	0.12026E+08	-0.56130E-03	0.11005E-04
1	0	0.29641	0.64063E+07	-0.17147E-03	0.71265E-05
2	0	0.04557	0.10781E+07	0.34938E-03	-0.11017E-04
3	0	0.00243	0.53338E+05	0.11964E-02	-0.77202E-04
4	0	0.00001	0.21120E+02		
5	0	0.00000	0.15189E+03		
6	0	0.00000	0.37397E+01		
7	0	0.00000	0.51582E+00		
0	1	0.25748	0.39594E+07	-0.28047E-03	0.14721E-04
1	1	0.22648	0.41232E+07	-0.10441E-02	0.12658E-04
2	1	0.40235	0.86383E+07	-0.31483E-03	0.75996E-05
3	1	0.10654	0.24704E+07	0.32376E-03	-0.16744E-04
4	1	0.00711	0.14567E+06	0.12873E-02	-0.10746E-03
5	1	0.00001	0.21216E+03		
6	1	0.00002	0.10149E+04		
7	1	0.00000	0.47317E+01		
0	2	0.06809	0.83712E+06	-0.78782E-04	0.24796E-04
1	2	0.28877	0.45226E+07	-0.45647E-03	0.10718E-04
2	2	0.05126	0.88761E+06	-0.22450E-02	0.30046E-04
3	2	0.41256	0.87348E+07	-0.48387E-03	0.11187E-04
4	2	0.16688	0.37636E+07	0.30273E-03	-0.23140E-04
5	2	0.01235	0.22840E+06	0.13233E-02	-0.15109E-03
6	2	0.00001	0.45327E+04		
7	2	0.00008	0.33302E+04		
0	3	0.01506	0.14284E+06	0.69819E-04	0.38771E-04
1	3	0.13220	0.16709E+07	-0.17072E-03	0.19022E-04
2	3	0.23010	0.36590E+07	-0.68794E-03	0.81262E-05
3	3	0.00228	0.22962E+05		
4	3	0.38487	0.79574E+07	-0.67666E-03	0.19240E-04
5	3	0.21933	0.47634E+07	0.32530E-03	-0.32021E-04
6	3	0.01567	0.24746E+06	0.10727E-02	-0.21775E-03
7	3	0.00026	0.26335E+05		
0	4	0.00304	0.21424E+05	0.15050E-03	0.56891E-04
1	4	0.04179	0.41145E+06	0.25607E-04	0.31585E-04
2	4	0.16701	0.21633E+07	-0.28481E-03	0.13627E-04
3	4	0.15270	0.24575E+07	-0.10091E-02	0.85527E-05

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Table C.2. Isotopologue $^{14}\text{N}^{15}\text{N}^+$: Einstein coefficients $\Delta J = 0, -1, \Delta N = -1$, continued.

v'	v''	FC	\tilde{A} (this work)	a	b
4	4	0.00522	0.15194E+06	0.48492E-02	-0.16860E-03
5	4	0.35258	0.70282E+07	-0.88381E-03	0.33100E-04
6	4	0.26110	0.53912E+07	0.41749E-03	-0.46352E-04
7	4	0.01460	0.17234E+06		
0	5	0.00059	0.29366E+04		
1	5	0.01101	0.81424E+05	0.15059E-03	0.48249E-04
2	5	0.07111	0.72463E+06	-0.28928E-04	0.24174E-04
3	5	0.17177	0.22716E+07	-0.42560E-03	0.91521E-05
4	5	0.08755	0.14224E+07	-0.14715E-02	0.15009E-04
5	5	0.02072	0.52663E+06	0.23630E-02	-0.13124E-03
6	5	0.33382	0.63165E+07	-0.10788E-02	0.52777E-04
7	5	0.28955	0.55912E+07	0.61601E-03	-0.71930E-04
0	6	0.00011	0.37415E+03		
1	6	0.00262	0.13998E+05	0.19742E-03	0.69502E-04
2	6	0.02349	0.18180E+06	0.13775E-03	0.39166E-04
3	6	0.09505	0.99866E+06	-0.97841E-04	0.16769E-04
4	6	0.15573	0.20932E+07	-0.59906E-03	0.64653E-05
5	6	0.04323	0.71053E+06	-0.21758E-02	0.33535E-04
6	6	0.03062	0.79692E+06	0.17391E-02	-0.14780E-03
7	6	0.33893	0.59874E+07	-0.11724E-02	0.73613E-04
0	7	0.00002	0.44401E+02		
1	7	0.00059	0.21687E+04		
2	7	0.00673	0.38083E+05	0.22296E-03	0.58550E-04
3	7	0.03832	0.30879E+06	0.11607E-03	0.29489E-04
4	7	0.10925	0.11785E+07	-0.18053E-03	0.94925E-05
5	7	0.12996	0.17641E+07	-0.80795E-03	0.68167E-05
6	7	0.01758	0.29919E+06	-0.33416E-02	0.77474E-04
7	7	0.02888	0.84136E+06	0.13922E-02	-0.18866E-03

Table C.3. Isotopologue $^{14}\text{N}^{15}\text{N}^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = N' - N'' = 1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. For transitions with very weak Franck-Condon factors, a constant value, μ_0^2 , should be used.

v'	v''	FC	μ_0^2	α	β
0	0	0.65575	0.35531E+00	0.11220E-03	-0.60594E-05
1	0	0.29629	0.14552E+00	-0.19333E-03	-0.63416E-05
2	0	0.04551	0.19321E-01	-0.58567E-03	-0.20555E-04
3	0	0.00242	0.77054E-03	-0.14862E-02	-0.74569E-04
4	0	0.00001	0.24398E-06		
5	0	0.00000	0.15117E-05		
6	0	0.00000	0.31661E-07		
7	0	0.00000	0.36545E-08		
0	1	0.25740	0.15197E+00	-0.14356E-03	-0.64827E-05
1	1	0.22675	0.11918E+00	0.50779E-03	-0.33931E-05
2	1	0.40231	0.19326E+00	-0.64420E-04	-0.53081E-05
3	1	0.10642	0.43893E-01	-0.51833E-03	-0.25648E-04
4	1	0.00710	0.20996E-02	-0.17315E-02	-0.99208E-04
5	1	0.00001	0.25820E-05		
6	1	0.00002	0.10229E-04		
7	1	0.00000	0.40088E-07		
0	2	0.06803	0.42614E-01	-0.37247E-03	-0.19201E-05
1	2	0.28878	0.16870E+00	0.19602E-04	-0.95064E-05
2	2	0.05144	0.25196E-01	0.14259E-02	0.17518E-04
3	2	0.41265	0.19298E+00	0.75784E-04	-0.11637E-05

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Table C.3. Isotopologue ¹⁴N¹⁵N⁺: Squares of transition dipole moments, continued.

v'	v''	FC	μ_0^2	α	β
4	2	0.16671	0.66482E-01	-0.45468E-03	-0.31603E-04
5	2	0.01232	0.32937E-02	-0.22986E-02	-0.13295E-03
6	2	0.00001	0.54885E-04		
7	2	0.00008	0.34025E-04		
0	3	0.01504	0.98834E-02	-0.57602E-03	0.44208E-05
1	3	0.13211	0.82056E-01	-0.26384E-03	-0.61399E-05
2	3	0.23021	0.13302E+00	0.23021E-03	-0.11278E-04
3	3	0.00232	0.65388E-03		
4	3	0.38508	0.17417E+00	0.22181E-03	0.76119E-05
5	3	0.21913	0.83961E-01	-0.37503E-03	-0.40130E-04
6	3	0.01562	0.35841E-02		
7	3	0.00026	0.32236E-03		
0	4	0.00304	0.20755E-02	-0.76702E-03	0.12076E-04
1	4	0.04174	0.27228E-01	-0.49149E-03	-0.50507E-06
2	4	0.16696	0.10281E+00	-0.14285E-03	-0.10070E-04
3	4	0.15286	0.87350E-01	0.51257E-03	-0.10242E-04
4	4	0.00517	0.41305E-02	-0.51858E-02	-0.12407E-03
5	4	0.35284	0.15298E+00	0.36314E-03	0.22553E-04
6	4	0.26089	0.95260E-01	-0.27338E-03	-0.54247E-04
7	4	0.01454	0.25185E-02		
0	5	0.00058	0.41305E-03		
1	5	0.01099	0.74635E-02	-0.69021E-03	0.66073E-05
2	5	0.07104	0.46016E-01	-0.39963E-03	-0.56999E-05
3	5	0.17176	0.10485E+00	-0.56252E-05	-0.13224E-04
4	5	0.08771	0.49635E-01	0.91060E-03	-0.31153E-05
5	5	0.02061	0.14230E-01	-0.25053E-02	-0.12185E-03
6	5	0.33416	0.13741E+00	0.48399E-03	0.43815E-04
7	5	0.28928	0.99561E-01	-0.15618E-03	-0.79571E-04
0	6	0.00011	0.80021E-04		
1	6	0.00262	0.18383E-02	-0.87516E-03	0.14840E-04
2	6	0.02346	0.15830E-01	-0.61507E-03	0.69149E-06
3	6	0.09498	0.61103E-01	-0.30509E-03	-0.10925E-04
4	6	0.15578	0.94218E-01	0.15047E-03	-0.14750E-04
5	6	0.04336	0.24463E-01	0.15150E-02	0.17014E-04
6	6	0.03049	0.21453E-01	-0.20147E-02	-0.14100E-03
7	6	0.33937	0.13095E+00	0.63360E-03	0.66120E-04
0	7	0.00002	0.15338E-04		
1	7	0.00059	0.42551E-03		
2	7	0.00672	0.46903E-02	-0.80599E-03	0.82239E-05
3	7	0.03826	0.25657E-01	-0.53746E-03	-0.57941E-05
4	7	0.10919	0.69802E-01	-0.20081E-03	-0.16155E-04
5	7	0.13005	0.77843E-01	0.32865E-03	-0.13325E-04
6	7	0.01767	0.10232E-01	0.24595E-02	0.67923E-04
7	7	0.02872	0.22676E-01	-0.23114E-02	-0.17566E-03

Table C.4. Isotopologue $^{14}\text{N}^{15}\text{N}^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = N' - N'' = -1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. For transitions with very weak Franck-Condon factors, a constant value, μ_0^2 , should be used.

v'	v''	FC	μ_0^2	α	β
0	0	0.65559	0.35522E+00	-0.15025E-03	-0.60336E-05
1	0	0.29641	0.14559E+00	0.21238E-03	-0.63026E-05
2	0	0.04557	0.19348E-01	0.70238E-03	-0.20987E-04
3	0	0.00243	0.77303E-03	0.15179E-02	-0.84014E-04
4	0	0.00001	0.25207E-06		
5	0	0.00000	0.15190E-05		
6	0	0.00000	0.31842E-07		
7	0	0.00000	0.37945E-08		
0	1	0.25748	0.15201E+00	0.17106E-03	-0.65244E-05
1	1	0.22648	0.11904E+00	-0.65051E-03	-0.34354E-05
2	1	0.40235	0.19329E+00	0.59522E-04	-0.50633E-05
3	1	0.10654	0.43945E-01	0.66761E-03	-0.25841E-04
4	1	0.00711	0.21058E-02	0.16039E-02	-0.11348E-03
5	1	0.00001	0.25410E-05		
6	1	0.00002	0.10249E-04		
7	1	0.00000	0.40941E-07		
0	2	0.06809	0.42648E-01	0.43330E-03	-0.19451E-05
1	2	0.28877	0.16869E+00	-0.25357E-04	-0.94284E-05
2	2	0.05126	0.25108E-01	-0.18653E-02	0.14951E-04
3	2	0.41256	0.19294E+00	-0.11646E-03	-0.61827E-06
4	2	0.16688	0.66555E-01	0.63887E-03	-0.31200E-04
5	2	0.01235	0.33045E-02	0.16429E-02	-0.15643E-03
6	2	0.00001	0.54700E-04		
7	2	0.00008	0.34118E-04		
0	3	0.01506	0.98970E-02	0.66590E-03	0.49183E-05
1	3	0.13220	0.82106E-01	0.31429E-03	-0.63317E-05
2	3	0.23010	0.13295E+00	-0.27620E-03	-0.10820E-04
3	3	0.00228	0.63822E-03		
4	3	0.38487	0.17408E+00	-0.31492E-03	0.84762E-05
5	3	0.21933	0.84050E-01	0.65432E-03	-0.38801E-04
6	3	0.01567	0.35986E-02	0.14127E-02	-0.22294E-03
7	3	0.00026	0.32182E-03		
0	4	0.00304	0.20794E-02	0.86500E-03	0.13689E-04
1	4	0.04179	0.27257E-01	0.58607E-03	-0.47507E-06
2	4	0.16701	0.10284E+00	0.17468E-03	-0.10231E-04
3	4	0.15270	0.87256E-01	-0.61355E-03	-0.91132E-05
4	4	0.00522	0.41641E-02	0.51655E-02	-0.18033E-03
5	4	0.35258	0.15287E+00	-0.52749E-03	0.23687E-04
6	4	0.26110	0.95348E-01	0.74192E-03	-0.51593E-04
7	4	0.01460	0.25324E-02		
0	5	0.00059	0.41407E-03		
1	5	0.01101	0.74753E-02	0.81681E-03	0.74282E-05
2	5	0.07111	0.46057E-01	0.49646E-03	-0.59520E-05
3	5	0.17177	0.10485E+00	0.10443E-04	-0.13091E-04
4	5	0.08755	0.49542E-01	-0.10871E-02	-0.13020E-05
5	5	0.02072	0.14291E-01	0.26730E-02	-0.14152E-03
6	5	0.33382	0.13727E+00	-0.73248E-03	0.45283E-04
7	5	0.28955	0.99672E-01	0.94435E-03	-0.75499E-04
0	6	0.00011	0.80236E-04		
1	6	0.00262	0.18418E-02	0.10140E-02	0.17021E-04
2	6	0.02349	0.15852E-01	0.75643E-03	0.87529E-06
3	6	0.09505	0.61144E-01	0.39398E-03	-0.11270E-04

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Table C.4. Isotopologue ¹⁴N¹⁵N⁺: Squares of transition dipole moments, continued.

v'	v''	FC	μ_0^2	α	β
4	6	0.15573	0.94188E-01	-0.18268E-03	-0.14034E-04
5	6	0.04323	0.24387E-01	-0.17951E-02	0.18650E-04
6	6	0.03062	0.21526E-01	0.20404E-02	-0.15628E-03
7	6	0.33893	0.13077E+00	-0.84634E-03	0.68936E-04
0	7	0.00002	0.15372E-04		
1	7	0.00059	0.42651E-03		
2	7	0.00673	0.46993E-02	0.97415E-03	0.94819E-05
3	7	0.03832	0.25690E-01	0.68807E-03	-0.60705E-05
4	7	0.10925	0.69839E-01	0.28034E-03	-0.16260E-04
5	7	0.12996	0.77786E-01	-0.40610E-03	-0.11765E-04
6	7	0.01758	0.10177E-01	-0.29560E-02	0.64168E-04
7	7	0.02888	0.22766E-01	0.16990E-02	-0.19545E-03

Appendix D: Expansion parameters for the $^{15}\text{N}^{15}\text{N}^+$ isotopologue**Table D.1.** Isotopologue $^{15}\text{N}^{15}\text{N}^+$: Franck-Condon factors (FC) and parameters for the evaluation of rovibrational Einstein A coefficients for $\Delta N = N' - N'' = 1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$

v'	v''	FC	\tilde{A} (this work)	a	b
0	0	0.65080	0.11948E+08	0.58456E-03	0.10852E-04
1	0	0.29933	0.64583E+07	0.25359E-03	0.64479E-05
2	0	0.04720	0.11152E+07	-0.12479E-03	-0.11527E-04
3	0	0.00264	0.58538E+05	-0.91660E-03	-0.67583E-04
4	0	0.00002	0.63099E+02		
5	0	0.00000	0.14974E+03		
6	0	0.00000	0.47295E+01		
7	0	0.00000	0.51744E+00		
0	1	0.26012	0.40163E+07	0.38128E-03	0.13931E-04
1	1	0.21916	0.39932E+07	0.96404E-03	0.13507E-04
2	1	0.40288	0.86386E+07	0.37375E-03	0.70333E-05
3	1	0.11002	0.25507E+07	-0.66024E-04	-0.16807E-04
4	1	0.00779	0.16191E+06	-0.10990E-02	-0.91479E-04
5	1	0.00002	0.58015E+02		
6	1	0.00002	0.10194E+04		
7	1	0.00000	0.87884E+01		
0	2	0.06963	0.86376E+06	0.19877E-03	0.23007E-04
1	2	0.28911	0.45439E+07	0.54092E-03	0.10214E-04
2	2	0.04661	0.80624E+06	0.18422E-02	0.37110E-04
3	2	0.40898	0.86526E+07	0.49922E-03	0.10794E-04
4	2	0.17189	0.38818E+07	-0.11600E-05	-0.23142E-04
5	2	0.01371	0.26033E+06	-0.15228E-02	-0.12428E-03
6	2	0.00000	0.31326E+04		
7	2	0.00008	0.34847E+04		
0	3	0.01555	0.14968E+06	0.35803E-04	0.35279E-04
1	3	0.13447	0.17135E+07	0.30730E-03	0.17740E-04
2	3	0.22778	0.36331E+07	0.74043E-03	0.79233E-05
3	3	0.00127	0.10193E+05		
4	3	0.37703	0.77959E+07	0.62675E-03	0.19211E-04
5	3	0.22564	0.49177E+07	0.80998E-04	-0.31842E-04
6	3	0.01788	0.29567E+06	-0.26142E-02	-0.16874E-03
7	3	0.00017	0.21604E+05		
0	4	0.00316	0.22781E+05	-0.11716E-03	0.50708E-04
1	4	0.04298	0.42909E+06	0.12538E-03	0.28894E-04
2	4	0.16891	0.22045E+07	0.43062E-03	0.12672E-04
3	4	0.14887	0.24015E+07	0.10083E-02	0.86214E-05
4	4	0.00729	0.19700E+06	-0.33503E-02	-0.11411E-03
5	4	0.34060	0.67973E+07	0.74016E-03	0.33944E-04
6	4	0.26886	0.55882E+07	0.18848E-03	-0.45656E-04
7	4	0.01761	0.22953E+06		
0	5	0.00061	0.31679E+04		
1	5	0.01141	0.86195E+05	-0.42687E-04	0.43477E-04
2	5	0.07287	0.75216E+06	0.22295E-03	0.22137E-04
3	5	0.17258	0.22986E+07	0.56186E-03	0.84627E-05
4	5	0.08345	0.13577E+07	0.13843E-02	0.16036E-04
5	5	0.02493	0.61167E+06	-0.14284E-02	-0.10828E-03
6	5	0.31771	0.60261E+07	0.83833E-03	0.55071E-04
7	5	0.29972	0.58511E+07	0.31602E-03	-0.69545E-04
0	6	0.00012	0.41004E+03		
1	6	0.00273	0.15034E+05	-0.19795E-03	0.61447E-04
2	6	0.02429	0.19167E+06	0.52240E-04	0.35218E-04
3	6	0.09704	0.10320E+07	0.32220E-03	0.15252E-04
4	6	0.15528	0.21014E+07	0.71159E-03	0.57808E-05

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Table D.1. Isotopologue ¹⁵N¹⁵N⁺: Einstein coefficients $\Delta J = 0, 1, \Delta N = 1$, continued.

v'	v''	FC	\tilde{A} (this work)	a	b
5	6	0.03972	0.65242E+06	0.19450E-02	0.38668E-04
6	6	0.03623	0.90752E+06	-0.96456E-03	-0.12745E-03
7	6	0.31814	0.56413E+07	0.94422E-03	0.78239E-04
0	7	0.00002	0.49588E+02		
1	7	0.00062	0.23640E+04		
2	7	0.00700	0.40724E+05	-0.10375E-03	0.51729E-04
3	7	0.03952	0.32433E+06	0.14373E-03	0.26418E-04
4	7	0.11114	0.12126E+07	0.43289E-03	0.82051E-05
5	7	0.12837	0.17547E+07	0.87651E-03	0.60692E-05
6	7	0.01513	0.25598E+06	0.28145E-02	0.10040E-03
7	7	0.03524	0.96757E+06	-0.10467E-02	-0.16314E-03

Table D.2. Isotopologue ¹⁵N¹⁵N⁺: Franck-Condon factors (FC) and parameters for the evaluation of rovibrational Einstein A coefficients for $\Delta N = N' - N'' = -1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$

v'	v''	FC	\tilde{A} (this work)	a	b
0	0	0.65063	0.11935E+08	-0.54402E-03	0.10609E-04
1	0	0.29947	0.64567E+07	-0.17207E-03	0.70925E-05
2	0	0.04725	0.11157E+07	0.33030E-03	-0.99019E-05
3	0	0.00264	0.58565E+05	0.11491E-02	-0.70967E-04
4	0	0.00002	0.63290E+02		
5	0	0.00000	0.14740E+03		
6	0	0.00000	0.47692E+01		
7	0	0.00000	0.42145E+00		
0	1	0.26016	0.40131E+07	-0.27626E-03	0.14255E-04
1	1	0.21894	0.39856E+07	-0.10199E-02	0.12054E-04
2	1	0.40292	0.86327E+07	-0.31200E-03	0.75581E-05
3	1	0.11012	0.25513E+07	0.29371E-03	-0.14871E-04
4	1	0.00780	0.16225E+06	0.12094E-02	-0.97277E-04
5	1	0.00002	0.54553E+02		
6	1	0.00002	0.10175E+04		
7	1	0.00000	0.93173E+01		
0	2	0.06969	0.86359E+06	-0.79684E-04	0.23780E-04
1	2	0.28910	0.45395E+07	-0.44924E-03	0.10392E-04
2	2	0.04644	0.80248E+06	-0.22522E-02	0.29124E-04
3	2	0.40887	0.86441E+07	-0.47945E-03	0.11101E-04
4	2	0.17206	0.38834E+07	0.26547E-03	-0.20442E-04
5	2	0.01375	0.26098E+06	0.12508E-02	-0.13539E-03
6	2	0.00000	0.31140E+04		
7	2	0.00008	0.34954E+04		
0	3	0.01557	0.14973E+06	0.70534E-04	0.36894E-04
1	3	0.13456	0.17129E+07	-0.17127E-03	0.18273E-04
2	3	0.22766	0.36279E+07	-0.68024E-03	0.79628E-05
3	3	0.00124	0.98050E+04		
4	3	0.37679	0.77853E+07	-0.67221E-03	0.19084E-04
5	3	0.22584	0.49193E+07	0.27656E-03	-0.27962E-04
6	3	0.01794	0.29675E+06	0.11257E-02	-0.19379E-03
7	3	0.00017	0.21552E+05		
0	4	0.00317	0.22796E+05	0.16623E-03	0.53705E-04
1	4	0.04303	0.42909E+06	0.24547E-04	0.30123E-04
2	4	0.16896	0.22029E+07	-0.28213E-03	0.13122E-04

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Table D.2. Isotopologue $^{15}\text{N}^{15}\text{N}^+$: Einstein coefficients $\Delta J = 0, -1, \Delta N = -1$, continued.

v'	v''	FC	\tilde{A} (this work)	a	b
3	4	0.14871	0.23966E+07	-0.10023E-02	0.84922E-05
4	4	0.00735	0.19826E+06	0.40234E-02	-0.13657E-03
5	4	0.34033	0.67866E+07	-0.88670E-03	0.33003E-04
6	4	0.26908	0.55896E+07	0.35070E-03	-0.39968E-04
7	4	0.01767	0.23051E+06		
0	5	0.00061	0.31723E+04		
1	5	0.01143	0.86242E+05	0.14497E-03	0.45968E-04
2	5	0.07294	0.75212E+06	-0.34169E-04	0.23205E-04
3	5	0.17259	0.22965E+07	-0.42526E-03	0.89816E-05
4	5	0.08329	0.13537E+07	-0.14725E-02	0.15073E-04
5	5	0.02507	0.61405E+06	0.20277E-02	-0.11137E-03
6	5	0.31726	0.60130E+07	-0.10877E-02	0.53012E-04
7	5	0.30001	0.58538E+07	0.52026E-03	-0.61409E-04
0	6	0.00012	0.41051E+03		
1	6	0.00274	0.15043E+05	0.20422E-03	0.65797E-04
2	6	0.02433	0.19170E+06	0.13432E-03	0.37305E-04
3	6	0.09711	0.10316E+07	-0.10408E-03	0.16237E-04
4	6	0.15524	0.20987E+07	-0.59777E-03	0.65167E-05
5	6	0.03960	0.64973E+06	-0.22187E-02	0.34427E-04
6	6	0.03638	0.90978E+06	0.15149E-02	-0.12700E-03
7	6	0.31769	0.56290E+07	-0.12259E-02	0.75945E-04
0	7	0.00002	0.49586E+02		
1	7	0.00062	0.23653E+04		
2	7	0.00701	0.40742E+05	0.22833E-03	0.55463E-04
3	7	0.03957	0.32434E+06	0.11057E-03	0.28222E-04
4	7	0.11119	0.12119E+07	-0.18649E-03	0.94403E-05
5	7	0.12829	0.17518E+07	-0.80827E-03	0.70860E-05
6	7	0.01504	0.25422E+06	-0.35418E-02	0.83043E-04
7	7	0.03538	0.96979E+06	0.12888E-02	-0.16336E-03

Table D.3. Isotopologue $^{15}\text{N}^{15}\text{N}^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = N' - N'' = 1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. For transitions with very weak Franck-Condon factors, a constant value, μ_0^2 , should be used.

v'	v''	FC	μ_0^2	α	β
0	0	0.65080	0.35269E+00	0.11081E-03	-0.58745E-05
1	0	0.29933	0.14731E+00	-0.18611E-03	-0.60004E-05
2	0	0.04720	0.20157E-01	-0.55756E-03	-0.19320E-04
3	0	0.00264	0.85691E-03	-0.13842E-02	-0.69198E-04
4	0	0.00002	0.76237E-06		
5	0	0.00000	0.15187E-05		
6	0	0.00000	0.40892E-07		
7	0	0.00000	0.38690E-08		
0	1	0.26012	0.15336E+00	-0.14086E-03	-0.61479E-05
1	1	0.21916	0.11525E+00	0.51323E-03	-0.35163E-05
2	1	0.40288	0.19402E+00	-0.56883E-04	-0.49863E-05
3	1	0.11002	0.45693E-01	-0.49953E-03	-0.23663E-04
4	1	0.00779	0.23632E-02	-0.15829E-02	-0.91213E-04
5	1	0.00002	0.70302E-06		
6	1	0.00002	0.10432E-04		
7	1	0.00000	0.77137E-07		
0	2	0.06963	0.43528E-01	-0.36163E-03	-0.18298E-05

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Table D.3. Isotopologue ¹⁵N¹⁵N⁺: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = -1$, continued.

v'	v''	FC	μ_0^2	α	β
1	2	0.28911	0.16867E+00	0.23440E-04	-0.91099E-05
2	2	0.04661	0.22806E-01	0.14717E-02	0.17221E-04
3	2	0.40898	0.19185E+00	0.83632E-04	-0.89423E-06
4	2	0.17189	0.69115E-01	-0.43599E-03	-0.28852E-04
5	2	0.01371	0.38011E-02	-0.20239E-02	-0.12169E-03
6	2	0.00000	0.38220E-04		
7	2	0.00008	0.36140E-04		
0	3	0.01555	0.10192E-01	-0.55841E-03	0.42019E-05
1	3	0.13447	0.83360E-01	-0.25434E-03	-0.58788E-05
2	3	0.22778	0.13143E+00	0.23089E-03	-0.10727E-04
3	3	0.00127	0.28334E-03		
4	3	0.37703	0.17117E+00	0.23161E-03	0.77982E-05
5	3	0.22564	0.87327E-01	-0.35733E-03	-0.36085E-04
6	3	0.01788	0.43362E-02	-0.31272E-02	-0.16335E-03
7	3	0.00017	0.26664E-03		
0	4	0.00316	0.21559E-02	-0.73810E-03	0.11411E-04
1	4	0.04298	0.27969E-01	-0.47484E-03	-0.48959E-06
2	4	0.16891	0.10383E+00	-0.13230E-03	-0.96563E-05
3	4	0.14887	0.84927E-01	0.51562E-03	-0.96206E-05
4	4	0.00729	0.53997E-02	-0.41152E-02	-0.11131E-03
5	4	0.34060	0.14834E+00	0.37050E-03	0.22829E-04
6	4	0.26886	0.99400E-01	-0.25683E-03	-0.47960E-04
7	4	0.01761	0.33980E-02		
0	5	0.00061	0.43137E-03		
1	5	0.01141	0.77293E-02	-0.67296E-03	0.64359E-05
2	5	0.07287	0.47090E-01	-0.38408E-03	-0.54231E-05
3	5	0.17258	0.10517E+00	0.23325E-05	-0.12587E-04
4	5	0.08345	0.47105E-01	0.92613E-03	-0.23769E-05
5	5	0.02493	0.16597E-01	-0.21253E-02	-0.10812E-03
6	5	0.31771	0.13131E+00	0.49467E-03	0.44547E-04
7	5	0.29972	0.10480E+00	-0.13859E-03	-0.69320E-04
0	6	0.00012	0.83893E-04		
1	6	0.00273	0.19151E-02	-0.84915E-03	0.14249E-04
2	6	0.02429	0.16348E-01	-0.59287E-03	0.67782E-06
3	6	0.09704	0.62290E-01	-0.29169E-03	-0.10339E-04
4	6	0.15528	0.93769E-01	0.15886E-03	-0.13960E-04
5	6	0.03972	0.22305E-01	0.15536E-02	0.18891E-04
6	6	0.03623	0.24499E-01	-0.16572E-02	-0.12573E-03
7	6	0.31814	0.12344E+00	0.61229E-03	0.69244E-04
0	7	0.00002	0.16122E-04		
1	7	0.00062	0.44511E-03		
2	7	0.00700	0.48755E-02	-0.77875E-03	0.79187E-05
3	7	0.03952	0.26432E-01	-0.51727E-03	-0.54289E-05
4	7	0.11114	0.70889E-01	-0.18829E-03	-0.15217E-04
5	7	0.12837	0.76734E-01	0.33751E-03	-0.12389E-04
6	7	0.01513	0.86696E-02	0.25611E-02	0.76497E-04
7	7	0.03524	0.26144E-01	-0.17498E-02	-0.15830E-03

Table D.4. Isotopologue $^{15}\text{N}^{15}\text{N}^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = N' - N'' = -1$ electronic dipole transitions between the electronic states $X^2\Sigma_g^+$ and $B^2\Sigma_u^+$. For transitions with very weak Franck-Condon factors, a constant value, μ_0^2 , should be used.

v'	v''	FC	μ_0^2	α	β
0	0	0.65063	0.35260E+00	-0.14667E-03	-0.58583E-05
1	0	0.29947	0.14738E+00	0.19976E-03	-0.59556E-05
2	0	0.04725	0.20182E-01	0.67275E-03	-0.19662E-04
3	0	0.00264	0.85786E-03	0.14616E-02	-0.77708E-04
4	0	0.00002	0.76514E-06		
5	0	0.00000	0.14959E-05		
6	0	0.00000	0.41258E-07		
7	0	0.00000	0.31528E-08		
0	1	0.26016	0.15339E+00	0.15926E-03	-0.61912E-05
1	1	0.21894	0.11514E+00	-0.63908E-03	-0.35172E-05
2	1	0.40292	0.19404E+00	0.50541E-04	-0.47623E-05
3	1	0.11012	0.45738E-01	0.62759E-03	-0.23814E-04
4	1	0.00780	0.23698E-02	0.15165E-02	-0.10324E-03
5	1	0.00002	0.66149E-06		
6	1	0.00002	0.10418E-04		
7	1	0.00000	0.81826E-07		
0	2	0.06969	0.43563E-01	0.41257E-03	-0.18324E-05
1	2	0.28910	0.16866E+00	-0.32400E-04	-0.90303E-05
2	2	0.04644	0.22718E-01	-0.18860E-02	0.14539E-04
3	2	0.40887	0.19181E+00	-0.12322E-03	-0.41905E-06
4	2	0.17206	0.69191E-01	0.59218E-03	-0.28414E-04
5	2	0.01375	0.38131E-02	0.15592E-02	-0.14064E-03
6	2	0.00000	0.38017E-04		
7	2	0.00008	0.36272E-04		
0	3	0.01557	0.10206E-01	0.64046E-03	0.46434E-05
1	3	0.13456	0.83412E-01	0.29614E-03	-0.60523E-05
2	3	0.22766	0.13136E+00	-0.28194E-03	-0.10326E-04
3	3	0.00124	0.27279E-03		
4	3	0.37679	0.17106E+00	-0.32116E-03	0.85309E-05
5	3	0.22584	0.87417E-01	0.59649E-03	-0.34738E-04
6	3	0.01794	0.43548E-02	0.14490E-02	-0.19869E-03
7	3	0.00017	0.26616E-03		
0	4	0.00317	0.21601E-02	0.84398E-03	0.12792E-04
1	4	0.04303	0.28000E-01	0.56150E-03	-0.47380E-06
2	4	0.16896	0.10386E+00	0.16063E-03	-0.97968E-05
3	4	0.14871	0.84832E-01	-0.61978E-03	-0.85875E-05
4	4	0.00735	0.54386E-02	0.43425E-02	-0.14839E-03
5	4	0.34033	0.14822E+00	-0.54068E-03	0.23692E-04
6	4	0.26908	0.99495E-01	0.66544E-03	-0.45290E-04
7	4	0.01767	0.34148E-02		
0	5	0.00061	0.43256E-03		
1	5	0.01143	0.77428E-02	0.78079E-03	0.71907E-05
2	5	0.07294	0.47137E-01	0.47126E-03	-0.56225E-05
3	5	0.17259	0.10517E+00	-0.32182E-05	-0.12460E-04
4	5	0.08329	0.47007E-01	-0.10997E-02	-0.75859E-06
5	5	0.02507	0.16675E-01	0.23370E-02	-0.12172E-03
6	5	0.31726	0.13112E+00	-0.74904E-03	0.45420E-04
7	5	0.30001	0.10492E+00	0.83641E-03	-0.65104E-04
0	6	0.00012	0.84124E-04		
1	6	0.00274	0.19187E-02	0.97682E-03	0.16265E-04
2	6	0.02433	0.16371E-01	0.72556E-03	0.87480E-06
3	6	0.09711	0.62332E-01	0.37007E-03	-0.10654E-04

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Table D.4. Isotopologue $^{15}N^{15}N^+$: Parameters for the evaluation of the squares of transition dipole moments for $\Delta N = -1$, continued.

v'	v''	FC	μ_0^2	α	β
4	6	0.15524	0.93738E-01	-0.19451E-03	-0.13292E-04
5	6	0.03960	0.22232E-01	-0.18494E-02	0.19914E-04
6	6	0.03638	0.24579E-01	0.18139E-02	-0.13560E-03
7	6	0.31769	0.12326E+00	-0.90589E-03	0.70934E-04
0	7	0.00002	0.16151E-04		
1	7	0.00062	0.44605E-03		
2	7	0.00701	0.48841E-02	0.94008E-03	0.90684E-05
3	7	0.03957	0.26463E-01	0.65845E-03	-0.56911E-05
4	7	0.11119	0.70921E-01	0.25836E-03	-0.15327E-04
5	7	0.12829	0.76679E-01	-0.41917E-03	-0.10940E-04
6	7	0.01504	0.86174E-02	-0.31659E-02	0.69912E-04
7	7	0.03538	0.26224E-01	0.15878E-02	-0.17021E-03